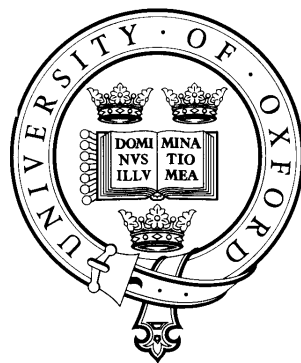


MODELLING RESIDUAL STRESSES AND DEFORMATION IN METAL AT DIFFERENT SCALES

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ABSTRACT

This thesis is devoted to the numerical and experimental investigation of residual stress and deformation in polycrystalline metallic alloys at different scales. The emphasis in the current study is placed on establishing the connection between the simulation of deformation by the Finite Element (FE) method and experimental characterisation by synchrotron X-Ray Diffraction (XRD). Of particular importance is the interpretation of modelling results and their validation by careful comparison with experimental data.

The concept of eigenstrain was used extensively throughout the report to study the residual elastic strain distributions and their sources. A pseudo-thermal strain FE procedure was used systematically to simulate the residual stress states in samples and engineering components of different shape and dimensionality. The case of 1-D strain variation was considered using the example of a plastically bent bar. The *direct* and *inverse* problems of eigenstrain analysis were solved, and validated experimentally by the use of XRD and EDM slitting methods. A novel 2-D discrete inverse eigenstrain algorithm was proposed and implemented to reconstruct the residual stress distribution in a worn rail head. The link between the residual stress and deformation history was studied via thermo-mechanical modelling of the Linear Friction Welding (LFW) process.

To advance the understanding of polycrystalline deformation behaviour across the scales, a crystal plasticity model was employed to simulate the elastic-plastic deformation behaviour of Ti-6Al-4V alloy. A post-processor was developed to extract the average elastic strains for orientation-specific grain groups and to compare them with XRD data. A “peak constructor” post-processor was developed that utilised the knowledge of both the elastic strain and dislocation density. In a further development step, a strain gradient crystal plasticity formulation was adopted to account for the local dislocation evolution. Intra-granular deformation analysis was carried out and micro-beam Laue experimental diffraction technique was used for validation. Thus, local lattice arrangement was studied at the microscopic, intragranular scale. Special attention was paid to the phenomenon of Laue spot “streaking”, indicative of the local lattice misorientation caused by dislocation activity during deformation.

The results presented in this thesis contributed to the fundamental understanding of the residual stress and deformation in polycrystalline metallic alloys and lead to more than 20 publications in peer-reviewed journals and conference proceedings, which are listed in the Appendix.

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Chapter 1 Introduction and Literature Review

1.1 Residual Stresses

Residual stresses are the stresses that remain after the original cause of deformation (external forces, heat gradient) has been removed [1]. Residual stresses are caused by mismatched permanent strains and may arise or become modified at every stage of the engineering component life cycle, from original material production to normal service operation. The significance of residual stresses is that they may greatly influence the material and component performance through various mechanisms. Modern engineering practice demands that they should be taken into consideration in design, performance prediction, and assessment [2].

Residual stresses may be deleterious or advantageous for material and component performance. However, when the cause, distribution and magnitude of residual stresses are not known, their presence introduces a level of uncertainty.

The cold working process of shot peening is a good example of a situation when residual stresses are introduced deliberately as a step of component preparation. Compressive residual stresses are introduced into the surface of a component in order to reduce the likelihood of crack initiation and to increase the fatigue life. The process involves repeated impact on the component surface by a stream of particles, or shots (metallic, glass or ceramic) with the force that is sufficient to induce plastic deformation (Figure 1.1 and 1.2). Close to the impacted surface the nature of this deformation is such that plastic compression occurs in the direction of the surface normal, and plastic stretching in the directions parallel to the surface plane.

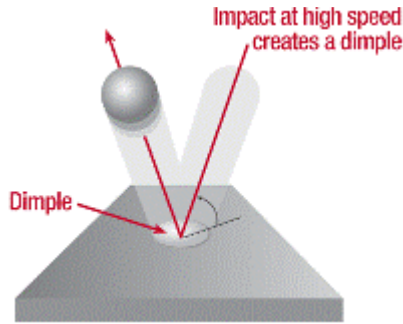


Figure 1.1: Illustration of shot peening process with single shot [3]



Figure 1.2: Illustration of the surface profile and the compression zone created by plastic deformation [3]

Plastic deformation induces a residual compressive stress in a peened surface, along with tensile stress deeper in the interior. It is the surface compressive stresses that prevent crack initiation and opening, impede crack propagation, and thus confer resistance to metal fatigue and to some forms of stress corrosion. Usually the presence of tensile stresses deep within the component does not cause any problems, since the cracks are most likely to start at component surface [4]. However, if the magnitude of near-surface compressive stresses increases, this causes attendant increase in the maximum tensile stresses, and may ultimately result in sub-surface crack initiation. This example demonstrates the important influence that can be exerted by the magnitude and distribution of residual stresses on the dominant mode of failure.

In brittle materials, the strength in response to static loading performance can be improved remarkably by the introduction of compressive residual stresses. Common examples include thermally toughened glass and pre-stressed concrete (although in the latter the strength improvement is also enhanced by the presence of tensile steel reinforcement) [5]. While in brittle materials residual stresses may be thought of as simply additional to the applied stresses, in ductile materials the combined effect is more intricate: it is necessary to consider the interaction and evolution of residual stresses in response of applied loading. Residual stresses may

promote or delay the onset of plastic deformation. Once plastic flow begins, however, additional permanent strains arise that cause the modification of residual stresses. For this reason, the effect of residual stresses on ductile failure under monotonic loading is often considered to be small, since the initial misfit strains are quickly “washed out” by subsequent comparatively large plasticity[5].

In contrast, residual stresses potentially produce a strong effect on material failure under repeated loading (fatigue). Fatigue is the progressive and localized structural damage that occurs when a material is subjected to cyclic loading. The maximum stress values are less than the ultimate tensile stress limit (Low Cycle Fatigue or LCF), and may be even below the nominal macroscopic yield stress limit of the material (High Cycle Fatigue or HCF) [6]. Reliable prediction of fatigue life of metallic components is a fundamental requirement in various branches of engineering applications. Material fatigue behaviour is a strong function of the load history. Residual stresses may affect the loading history in a variety of ways. If the residual stresses persist without change during cycling, then they do not vary with the applied load or cycle numbers. In this case they do not affect the loading amplitude, but they do influence the mean or the maximum value of the load in each cycle. It is well known that the variation of the mean (maximum) has a strong effect on fatigue lifetime under both LCF and HCF conditions [7]. It is conventionally believed that [7] the fatigue nucleation life (the number of cycles required to form a short fatigue crack) is a function of the alternating stress amplitude but not the mean stress, while the growth rates of fatigue cracks show a dependence on both the stress amplitude and mean stress. This view implies that residual stresses have relatively little influence on fatigue crack nucleation, but potentially a significant one on fatigue crack growth. The influence on fatigue crack growth may be especially pronounced when these cracks

are relatively short and the driving force for their growth lie close to the threshold. In this case, residual stress may make the critical difference between short fatigue crack growth or arrest. If the overall fatigue response (e.g. expressed in the form of the S-N curve) is dominated by crack nucleation, then the effects of residual stresses may be small. However, if the S-N curve is dominated by crack growth, including in the short crack regime, then the influence of residual stresses could be large. At any rate, in the context of fatigue performance it is important to be able to monitor and control the residual stresses.

Two classes of techniques are commonly used for measuring the residual stresses: destructive and non-destructive. The destructive method relies on monitoring the changes in component deformation, either in the process of residual stress introduction (e.g. coating deposition, welding), or subsequent relaxation e.g. due to mechanical or electro-chemical removal of material. Common destructive methods includes curvature measurement, hole drilling, crack compliance and etc. [5]. A typical curvature measurement experiment involves depositing a layer of coating onto the substrate, monitoring the resulting change in curvature, and calculating the corresponding variation of stress as a function of deposition thickness. The hole drilling method is based on the principle that different regions of a sample containing residual stresses will experience different amounts of strain relief when material is removed in their vicinity by hole drilling. The measurement of this strain relief provides the data for subsequent back-calculation (reconstruction) of residual stress. The strains around the progressively drilled hole can be measured e.g. using 45° triple strain gauge rosettes (Figure 1.3 and 1.4) [8]. Figure 1.4 is a schematic illustration of Figure 1.3, where a vertical welding line can be observed. Hence the vertical direction is nominated as the longitudinal and horizontal named as the transverse direction.



Figure 1.3: An illustration of a 45° strain gauge rosette on an Electron Beam (EB) weld sample [8]

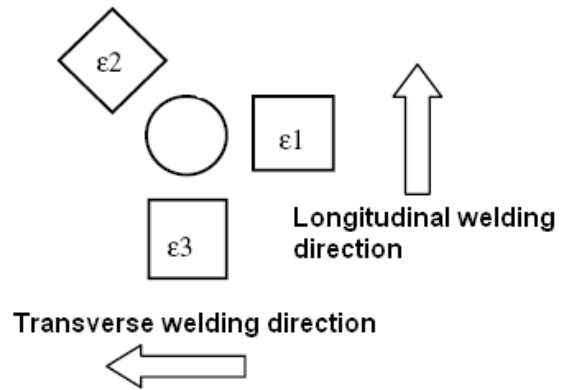


Figure 1.4: Schematic illustration of the 45° strain gauge rosette in Figure 1.5 [8]

The crack compliance method involves cutting a small slot and monitoring the relief of strain or displacement in the vicinity using strain gauge(s) or profilometry. By steadily increasing the depth of the slot it is possible to resolve the stress field normal to the cut as a function of depth for relatively simple stress distributions (Figure 1.5) [5, 9].

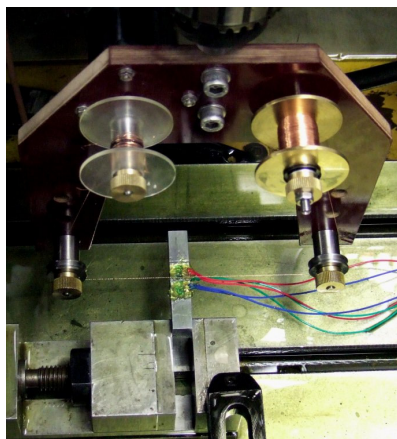
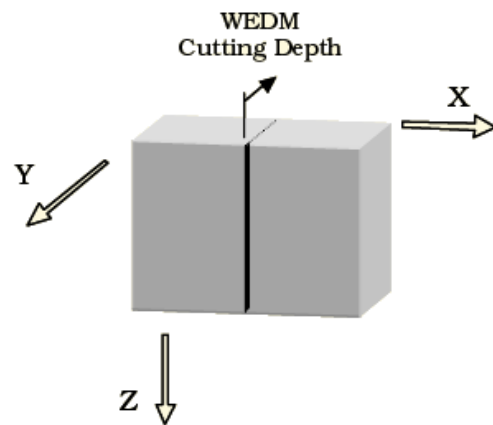


Figure 1.6: Illustration of the experimental setup for incremental slitting using Wire Electric Discharge Machining (WEDM). The strain gauges were mounted at the top sample surface [9]



Being portable and cheap to undertake, these methods are well suited to routine inspection procedures in the industrial setting. However, their limitations are (1) the comparative low accuracy of the residual stresses values measured [5], and (2)

the fact that drilling and slitting are irreversible processes leading to permanent damage of the sample under investigation.

In order to overcome this limitation, various non-destructive methods have been developed, including e.g. electromagnetic [10, 11] and ultrasonic [12] techniques. They possess the virtue of measuring residual stresses non-destructively and being easy to use, but suffer from high sensitivity to material microstructure, limited measurement accuracy, and lack of directional sensitivity [5]. Thermoelastic [13] and photoelastic [14] methods have also been also proposed for residual stresses measurement. However, the thermoelastic effect is relatively small compared to the sensitivity of the current infrared cameras [13]. The photoelastic method requires the sample to be birefringent and transparent, or to carry a coating of such material, which limits its application. It is also important to note that these methods measure “live” stresses, so that the determination of residual stresses remains problematic.

In the last decade, a significant increase has taken place in residual stress evaluation using diffraction methods, both in science and industry communities. It provides a powerful non-destructive method for determining the level of residual stress through careful characterisation of interplanar crystal lattice spacing in a localized region of the engineering component, requires no material removal, and gives very high precision. Hence, the diffraction method is widely considered as the most prominent non-destructive means of determining residual stress field within crystalline materials and engineering components [15]. Stress measurement by diffraction can be achieved via different sources: lab-based X-ray beams, synchrotron X-ray beams, neutrons, electrons, etc. The characteristics of these beams and their experimental implementation are quite different in various aspects. Their representative features are listed in Table 1.1, with typical values reflect the

technological advances at the beginning of the new millennium [5]. However different may appear, they share the common features of using the same principle for elastic strain measurement, the Bragg's Law.

Method	Laboratory X-Rays	Synchrotron X-Rays	Neutrons
Penetration	<50μm (Al)	50mm~150mm (Al)	~200mm (Al)
Resolution	1 mm (lateral)	20μm (lateral)	>500μm
Accuracy	±20MPa	±10 microstrain	±50 microstrain
Diffraction Mode	Reflection (surface)	Reflection or Transmission	Transmission
Table 1.1 Diffraction techniques and their attributes [5]			

X-rays interact with atoms primarily via the electromagnetic forces exerted on and from the electron clouds. For the purposes of the present discussion, the process of interaction can be thought of as re-emission of electromagnetic waves of the same frequency (elastic scattering). These re-emitted waves may interfere with each other constructively or destructively. The intensity of diffracted beam is only high when constructive interference occurs, i.e., when the path difference is equal to an integer number of wavelengths [16]. This condition is expressed in the form of Bragg's law as:

$$2d \sin \theta = n\lambda, \quad (1.1)$$

where λ is the wavelength; d is the inter-planar spacing; θ is the angle between the incident ray and the scattering planes; n is the order of reflection. By knowing the photon energy E (and hence the wavelength $\lambda = \frac{hc}{E}$, where h is Planck's constant and c is the speed of light) and the diffraction angle, the inter-planar spacing can be found.

The elastic strains (corresponding to the change of interplanar lattice spacing) can be readily calculated as follows:

$$\varepsilon = \frac{d - d_0}{d_0} = \frac{\Delta d}{d_0}. \quad (1.2)$$

Here d is the deformed lattice spacing; d_0 denotes the unstrained lattice spacing.

Although the principles of diffraction strain measurement are fairly straight-forward, the experimental setups and interpretation procedures can sometimes be quite complicated and intricate, since very high measurement accuracy is required. Details of the diffraction techniques employed in the current research are further described in Chapter 3.

1.2 Inelastic Deformation and the Length Scale Effects

Residual stresses arise due to various reasons: plastic deformations, thermal expansion mismatch, phase transformation, etc. The prediction of residual stresses that arise as a consequence of a particular processing operation is one of the purposes of *process modelling*. Reliable prediction of residual stresses as a function of processing conditions requires good understanding of the operative mechanisms, as well as the knowledge of (time-, temperature- and history-dependent) material properties. It is, however, also possible to take an alternative view that focuses on the characterisation and reconstruction (simulation) of the final residual stress state, without trying to reproduce the complex history that led to its creation. It will be shown in this thesis that sometimes this approach (closely linked with the concept of eigenstrain) offers certain advantages from the point of view of simplicity and validation.

The stresses are always related to the *elastic* strains via the generalised

Hooke's law. In the tensor form this relationship is expressed as follows:

$$\boldsymbol{\sigma}_{\text{res}} = \boldsymbol{C} : \boldsymbol{\varepsilon}_{\text{el}} . \quad (1.3)$$

Here $\boldsymbol{C}$ is fourth order tensor of material constants; $\boldsymbol{\varepsilon}_{\text{el}}$ is the second order elastic strain tensor. The latter may be, as a particular special case, *residual elastic strain*.

Throughout this thesis, the definitions of elasticity and elastic strain are as follows. *Elasticity* is the physical property of a material to return to its original shape after the removal of external forces or other modes of loading. *Elastic strain* can be obtained from the polar decomposition of the deformation gradient tensor [17]. It is worth noting that any part of the total strain which is not recoverable and is not directly related to stress according to equation 1.3 is called *inelastic strain*. This additional specification (relationship with stress) is important for clarity. Note e.g. that *thermal strain* causes lattice expansion or contraction (change of lattice spacing); and that the solid returns to the original shape once the external cause (temperature change) is removed. It is however convenient, for the purposes of the present analysis, to distinguish it from *elastic strain* (and, in fact, to classify it as *inelastic*).

Thus, inelastic strains include thermal strains, plastic strains, viscoelastic strains, crystallographic transformations, strains associated with cutting and pasting, lattice defects, etc. In fact, for the purposes of mechanical analysis these strains can be thought as equivalent and interchangeable (as long as only the *residual stresses* concern), as they are all inelastic strains.

The presence of inelastic strain is a necessary condition for the existence of residual stress; but not a sufficient one. Namely, fully compatible inelastic strain everywhere does not give rise to any residual stress, and can therefore be called *impotent* [18, 19]. Those non-uniformly distributed inelastic strains that create *mismatched*

displacement fields create residual elastic strain, hence residual stresses [7]. For the purposes of analysis, by following T. Mura [20] the term *eigenstrain* and notation $\boldsymbol{\varepsilon}^*$ are used to refer to inelastic strains seen as sources of residual elastic strain (hence residual stress). The total strain associated with the displacements of material points can then be expressed in the additive form $\boldsymbol{\varepsilon}_{total} = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}^*$. Using a known eigenstrain field to deduce the residual elastic strain field is termed the direct problem of eigenstrain analysis and therefore the inverse problem of eigenstrain analysis becomes using a known residual elastic strain distribution to retrieve the eigenstrain field.

In the current work, in the course of inelastic deformation analysis, the focus is on two major kinds of inelastic deformation: thermal expansion and plastic flow. The two kinds of inelastic strain account for much of the residual stress emergence. Good example for the former is the shrink-fitting technique, and shot peening surface treatment for the latter. In the case of welding, both effects (thermal and plastic deformation) are present. Both deformation mechanisms are widely used in industry to introduce residual stresses into engineering components.

Thermal strains are created when the material is subjected to a temperature change. The value is expressed as

$$\boldsymbol{\varepsilon}_{thermal} = \boldsymbol{\alpha}(T_{final} - T_{initial}), \quad (1.4)$$

where $\boldsymbol{\alpha}$ is the coefficient tensor of linear thermal expansion.

The mechanism and the mathematical description of thermal strains are particularly simple. Therefore, they are chosen to represent *all* inelastic strains by distributions of thermal strains, and study the corresponding residual stresses distributions. Naturally, a question arises whether, indeed, (a) all kinds of eigenstrain distributions can be represented by equivalent thermal strain distributions, and (b)

whether such a representation is unique. This question can be answered by considering the following equation:

$$\begin{bmatrix} \epsilon_{xx}^* & \epsilon_{xy}^* & \epsilon_{xz}^* \\ \epsilon_{yx}^* & \epsilon_{yy}^* & \epsilon_{zy}^* \\ \epsilon_{zx}^* & \epsilon_{yz}^* & \epsilon_{zz}^* \end{bmatrix} = \begin{bmatrix} \alpha_{xx} & \alpha_{xy} & \alpha_{xz} \\ \alpha_{yx} & \alpha_{yy} & \alpha_{zy} \\ \alpha_{zx} & \alpha_{yz} & \alpha_{zz} \end{bmatrix} \Delta T, \quad (1.5)$$

In equation 1.5, the dependence of the eigenstrain tensor components on the spatial coordinates is implied, and this tensor is represented by the (pseudo)thermal strain tensor. By assuming a uniform temperature change ΔT over the entire body, the suitable variation of the components of the thermal expansion coefficient tensor can be readily found.

This technique of *pseudo-thermal strains* provides a practical tool that is used to reconstruct the inelastic strain fields in different engineering components. Further details about the numerical implementation of the *eigenstrain* technique and its applications to the direct and inverse problems of residual stress analysis can be found in Chapters 4, 5 and 6.

The eigenstrain methodology described above provides a means of avoiding the challenging process modelling. The mechanisms of thermal-mechanical processes can be extremely complex, and correct modelling requires the knowledge of power input, history, material thermodynamics, material parameters, etc. In Chapter 6, the problem is addressed of residual stress distributions that arise in Linear Friction Welding (LFW). In contrast with the “lean” framework of inverse eigenstrain analysis, here a fully coupled thermal-mechanical FE process simulation is developed. Validation is provided against inverse eigenstrain analysis and experimental measurements.

Plastic deformation is the distinctive aspect of the material behaviour of

ductile materials and one of the major sources of eigenstrain and residual stresses. Therefore, a large part of the present work has been devoted to the modelling of the elasto-plastic behaviour of metallic alloys and the attendant residual stresses.

In this context it is important to note that, just as for the plastic deformation, the description and understanding of the residual stresses is lengthscale-dependant. This is due to the fact that the measurement and representation of plastic strains and their effects occurs at different length scales for different techniques and models [5]. For example, neutron diffraction is used to determine macro- to mesoscopic lattice strains, while X-Ray diffraction can provide information ranging from macro- to meso- to microscopic spatial resolution. Electron diffraction probes lattice strains (and hence stresses) at the level of a few tens inter-atomic distances. Correspondingly, the modelling tools used to interpret these measurements and to describe plasticity must show similar scale dependence: different physical models and algorithms are needed in order to describe the nonlinear material behaviour at different scales.

At the macroscopic level, continuum plasticity, or phenomenological plasticity theory is used. It is a descriptive theory based on macroscopic elasto-plastic constitutive laws. The material is treated as a homogeneous continuum and deformation behaviour is captured by a set of empirical relations between (incremental) plastic strains and other deformation parameters (stresses, temperatures, hardening parameters, and their history). Summaries of such macroscopic continuum models and their possible implementations are given by Lemaitre and Chaboche [21], Crisfield [22] and Hill [23], among others.

However, models based on continuum mechanics do not allow accounting for inhomogeneities at the meso- and micro-scale. This can be achieved by considering representative volume elements (RVE's) of material and using micro-mechanical

constitutive relations that take account of the physical mechanisms active at these scales. One such approach relies on the use of (poly) crystal plasticity theory to take into account the grain morphology and crystallographic orientation. In this way, the relationship between the macroscopic stress state and the stress state at the grain level can be investigated in detail. It is well known that the most common manifestation of plastic deformation in crystalline solids is crystal slip [24] (Figure 1.7). The constitutive theory of crystal plasticity now is a well-established framework for the analysis of slip processes at the grain level. The quantitative description of plastic flow by crystallographic slip may be traced back to the early work of Taylor and Elam [25, 26], and Taylor [26, 27]. They base their consideration on the view that crystal slip tends to occur preferentially on certain crystallographic planes and in certain specific crystal directions (Figure 1.7). Constitutive equations for elasto-plastic behaviour of ductile single crystals from the standpoint of modern continuum mechanics were formulated by Mandel [28] and Hill [29], and extended to finite deformations by Rice [30], Hill and Rice [31], Asaro and Rice [32], and Asaro [33, 34].

The slip process occurs by dislocation motion (Figure 1.8). Dislocation is an important type of defect in crystalline materials. All real crystals contain imperfections that disturb locally the regular arrangement of the atoms and that may be classified as point, line, surface or volume defects. Point defects (vacancies, - interstitial atoms), surface defects (stacking faults, grain boundaries and twin boundaries), volume defects (precipitates, voids and bubbles) all can significantly modify the properties of crystalline solids. However, it is the line defects (dislocations) and their movements that control the crystal slip, and hence plastic

deformation¹. The definition of a dislocation is given in terms of the Burgers circuit and vector. These are well-known concepts now found in most textbooks on materials, and will be omitted here for brevity. Two types of dislocations should be distinguished: screw and edge dislocations (Fig. 1.6). The Burgers vector of an edge dislocation is normal to the dislocation line, while the Burgers vector of a screw dislocation is parallel to the dislocation line.

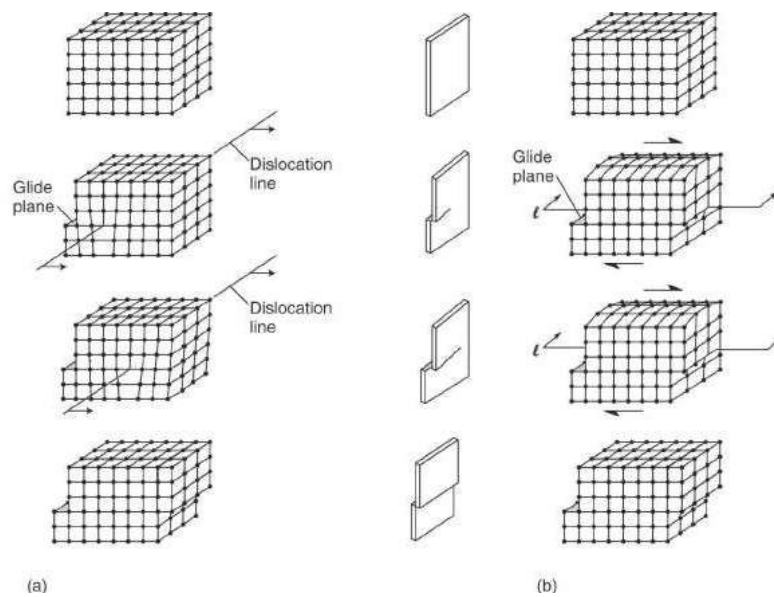


Figure 1.7: Illustration of Edge (a) and Screw (b) dislocations [24]

Two types of dislocation motion should be distinguished: glide and climb. Dislocation glide occurs by means of a dislocation moving in the plane containing both the dislocation line and the Burgers vector. Glide of many dislocations results in macroscopically observable crystal slip. Both edge and screw dislocations can glide along the slip planes. Climb occurs when the dislocation moves out of the glide surface (thus moving normally to the Burgers vector). In view of the importance of dislocations for the mechanism of plasticity, it is natural to develop a dislocation-based crystal plasticity theory. This approach was adopted in the present study,

¹ Note that time-independent plastic deformation is implied here, and must be distinguished from creep that depends on diffusion e.g. along grain boundaries.

together with the account of grain orientation and diffraction post-processing. It will be shown that, on the one hand, it can predict the macroscopic material response of (poly)crystalline materials, i.e. the monotonic and cyclic stress-strain curves; on the other hand, it can generate data related to local intra-granular deformation distributions. It even can probe the local lattice distortion (created by the presence of the dislocation) and misorientation. Therefore, it is important to develop a better understanding of the interaction between the deformation and dislocations, and the related scaling effects.

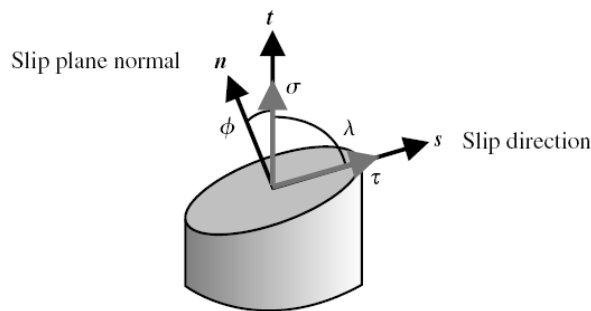


Figure 1.8: Illustration of a single slip system [35]

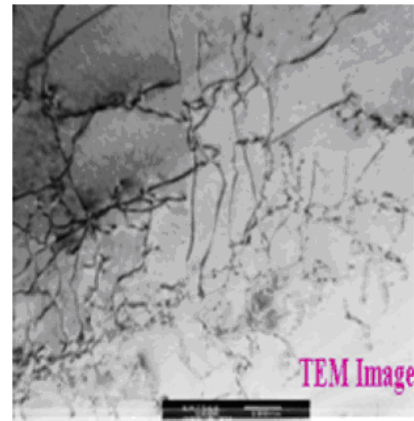


Figure 1.9: The formation of dislocation loops during plastic deformation [24]

At a finer scale of consideration (microscopic), Discrete Dislocation Dynamics (DDD) models can be employed. DDD simulations focus on the motion of individual dislocations caused by externally imposed displacements or applied stress. In order to achieve accurate description of the mechanical behaviour of ductile materials it is necessary to identify suitable parameters (e.g. dislocation mobility), to represent the mechanisms of dislocation interaction and to account for different boundary conditions of the simulation volume. A three-dimensional physically-based general framework was proposed by Arsenlis, Cai, Bulatov et al. [36, 37], and good correlation was found between their models and the experiment results.

The modelling of deformation at the atomistic scale constitutes a vast body of research. Methods such as Molecular Dynamics (MD) have been proposed and used at this scale. In our current research, electron diffraction or other similar techniques were not employed to study the residual stresses at the atomic level. Therefore, the modelling work of the plastic deformation at the atomic scale is not reviewed here.

The summary of different plasticity theories for different length scales is shown in Figure 1.9 below.

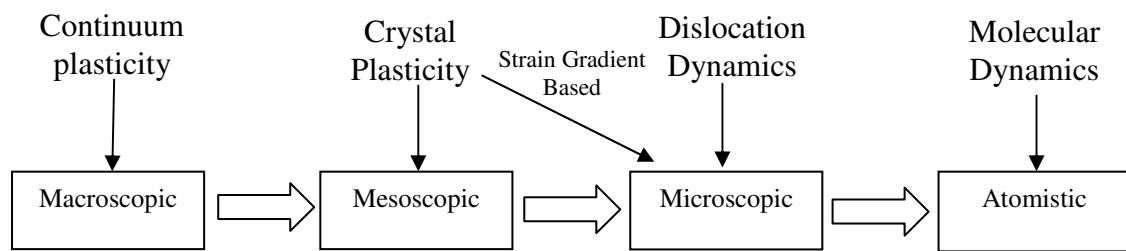


Figure 1.10: Schematic of different plasticity theories for different scales

Mechanical properties of materials also show a strong dependence on the length scale. A number of experiments have been devised and reported by various authors that demonstrate these effects, such as the application of local forces (e.g. by nano-indentation) to inclusions in particle-reinforced composites, the torsion of thin wires, the bending of thin beams, etc. In all cases the measurements show that a substantial increase in strength is observed with decreasing the particle size, the wire diameter, the beam thickness, and the indenter size, respectively. It is concluded that the material mechanical properties (such as strength or hardness) are also size-dependent, be it in simple tension, torsion, bending, or indentation testing. These effects can be observed experimentally when the characteristic dimension of the object involved is of the order of the structural scale of interest. Therefore, the representative length scale of the deformation field becomes crucial to the qualitative

and quantitative description of the size effect.

As mentioned above, the nonlinear material behaviour is well described by the continuum theories of plasticity on macroscopic scale. However, as defects localize over narrow regions, the characteristic length scale governing the variations of those defects falls far below the scale of the local state variables of classical plasticity theories. This leads to the loss of the statistical homogeneity and causes strong scale effects, since the plasticity evolution processes are statistically inhomogeneous at scales smaller than the continuum scale of interest. This suggests that the macroscopic inelastic deformations and failure are governed by mechanisms at different scale levels (nonlocality) which gives rise to the gradient-dependent effects. Thus, the gradient-dependent effect becomes important when the characteristic dimension of the plastic deformation zone is of the same order as the material intrinsic length scale, which is in the order of microns (microscopic) for commonly used structural materials.

In polycrystalline metal aggregates, grain-size strengthening is commonly observed. Hall [38] and Petch [39] first examined the grain size dependence of strength and found an empirical relationship between the average grain diameter d and the yield stress. This was extended by Armstrong et al. [40] to include the entire flow stress region $\sigma(\epsilon)$ by expressing the parameters σ_0 and k to be dependent on the strain level ϵ in a relation known as the “extended Hall–Petch relation”

$$\sigma(\epsilon) = \sigma_0(\epsilon) + k(\epsilon)d^{-n}. \quad (1.6)$$

In the literature, values for the exponent n between 0.3 and 1 show best agreement with experimental results, with $n=0.5$ being the most commonly reported value. The Hall–Petch slope k characterizes the condition of slip transfer across grain boundaries.

Three different models can be distinguished [41] to explain the strengthening effect of smaller grains. First, dislocation pile-up models state that the propagation of plastic deformation (slip) is obstructed at the crystal boundaries, causing stress concentrations due to pile-up of dislocations, which in their turn activate dislocation sources in neighbouring grains (Hall [38]; Petch [39]; Cottrell [42]; Nakanishi and Suzuki [43]; Suzuki and Nakanishi [44]). These models focus on the restricted dislocation movement across grain boundaries, which result in the flow stress dependence in Eq. 1.6 through $d^{-\frac{1}{2}}$. The main objection against this explanation is that in metals with a BCC crystal structure, no pile-ups are observed while the Hall–Petch relation remains valid.

Second, dislocation interaction models (also called work hardening models) (Ashby [45]; Hirth [46]; Conrad [47]; Dai and Parks [48]; Dai [49]; Arsenlis and Parks [50]) emphasize the increased concentration of dislocations. It is argued that, at given strain, the dislocation density accumulated within a grain becomes higher when the grain size decreases, which is inherently related to the increased inhomogeneity of deformation (i.e., strain gradient) within the grain. These models predict values for the exponent n in the entire range mentioned above.

Finally, the grain boundary source model (Li and Chou [51]) emphasizes the capacity of grain boundaries to emit dislocations under loading, which does not require a stress concentration created by a pile-up. However, until now, no clear experimental evidence has been presented able to distinguish between these models.

The dislocation interaction approach has been extended by Ashby [45]. Hardening, i.e. the increased resistance to dislocation motion, is caused by secondary dislocations piercing the slip planes. The resulting jogs and kinks multiply during plastic deformation and increase the slip resistance. Ashby [45] makes a distinction

between statistically stored dislocations (SSDs), accumulated during uniform deformation, and geometrically necessary dislocations (GNDs) which are required to preserve lattice compatibility in the case of unevenly distributed plastic slip (non-uniform plastic deformation, such as arises in the presence of lattice curvature). The introduction of these GNDs (in addition to SSDs that are inherently random) results in additional strengthening of material. Such gradient-dependent behaviour is expected to become important when deformation gradients become sufficiently large with respect to the controlling microstructural feature. Hence, polycrystals with a finer grain size develop strain gradients which extend further into the grain, exhibiting a stronger response due to the additional presence of GNDs associated with such gradients.

Strain gradient plasticity concepts are now commonly used to study length scale effects in polycrystalline metallic aggregates. A number of non-local continuum mechanics theories have been formulated to address these effects. One fruitful idea was to introduce GND and/or SSD densities as internal variables of the model. Phenomenological theories incorporating higher-order strain gradients were put forward by Fleck et al. [52], Gurtin [53] and Gudmundson [54] to predict the strain gradient dependence of strength. An alternative and more physically intuitive approach to describe the lengthscale-dependant effect without the need to include higher order strain gradients were developed by several authors (e.g., Dai and Parks [48]; Busso et al. [55]; Bassani [56]; Arsenlis and Parks [50]; Acharya and Beaudoin [57]; Huang et al. [58]). Here, strain gradient effects are introduced directly into the evolutionary laws of the internal slip system state variables. This type of strain gradient theory has been shown to be capable of providing great physical insight into the effects of microstructure on the observed macroscopic phenomena, including rate-

independent plastic deformation and visco-plasticity in both single crystal and polycrystalline materials (e.g., Busso and Cheong [59]; Meisssonier et al. [60]). They are relatively easy to implement numerically. The approach was further developed by Cheong and Busso [61], where a systematic investigation of the mesh sensitivity of the finite element (FE) results over a spectrum of length scales was carried out.

In Chapter 7 and 8, the non-local continuum rate-dependent theory proposed by Cheong and Busso [61] was adopted to investigate the effect of microstructural and deformation-related length scales on the behaviour of Ti-6V-4Al and large grain Ni polycrystals. More details can be found in corresponding chapters.

1.3 Thesis Structure

The primary aim of the present research project was to gain a better understanding of the residual stresses at different scales in engineering materials and components. Substantial part was devoted to the non-uniform inelastic deformation simulation and interpretation, as it is the origin and the cause of residual stresses. Diffraction experiments were carried out to quantify the amount of residual stresses within the volume of interest. Good correlation between models and experiments were found.

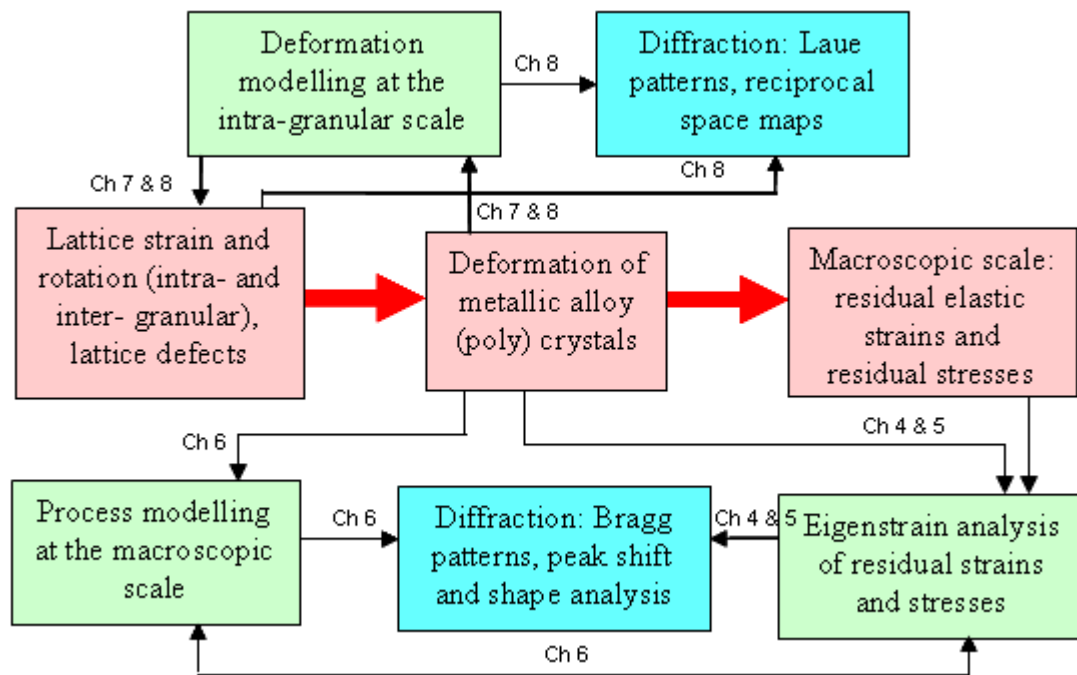


Figure 1.11: Flow Chart of information passage in the current research

Figure 1.10 shows a schematic which identifies the connections explored within the research scope reported here. In the flow chart, pink boxes with red arrows indicate the principal logical connections between cause and effect, mechanism and response. Green boxes and blue boxes are the modelling approaches and measurement techniques, respectively, employed for the investigation and cross-validation. Black arrows indicate the direction of the information flow between different techniques. The thesis chapters relevant to the exploration of these connections are labelled.

Chapter 2 & 3 provide a brief introduction to the principal tools (modelling and experimental): the Finite Element Method and subroutines for pre- and post-processing; X-Ray diffraction (XRD) and the software for interpretation of the experimental data.

Subsequent chapters are arranged in the order of increasing complexity, with progressively finer scale of consideration. The complexity of the models in the following chapters are increasing, while the scope of the problem is going down from

macro- and meso- to micro-scale. This corresponds to the reverse direction of the large red arrows in Fig. 1.10, a journey from the superficial phenomenological description to detailed analyses of deformation mechanisms. In Chapter 4, a classical 1-D macroscopic residual stress problem of a bent beam is considered. By introducing the concept of eigenstrain, the inelastic strain distribution along the middle section is reconstructed. This method is further extended to 2-D in Chapter 5, where the macroscopic residual stresses field in a worn British rail head was studied, and the inelastic strain distribution was determined. A 3-D macroscopic model was proposed in Chapter 6, but this time the whole Linear Friction Welding (LFW) process was simulated to study not only the distribution of inelastic strains, but also their cause and evolution. Chapter 7 bridges the gap between macro- and meso-scales: 3-D mesoscopic analysis of Ti-6-4 with the help of Representative Volume Element (RVE) and crystal plasticity concepts is used not only to generate the material monotonic stress-strain curve, but also to probe the inter- and intra granular mesoscopic information (e.g. grain group elastic strains and dislocation densities). Chapter 8 refines the scale further, from meso- down to the microscopic. A 3-D model of large-grained commercially pure Ni was created using strain gradient crystal plasticity theory to capture the local lattice misorientation within individual grains. It provides direct comparison and validation against diffraction data.

Chapter 9 draws the conclusions and discussed the directions for further work.

Chapter 2 Finite Element simulation technique of material mechanical behaviours

In this chapter, the Finite Element method and various related modelling tools employed in this thesis to simulate the mechanical behaviour of materials are introduced. The purpose of this description is to bridge the gap between the fundamentals of inelastic deformation modelling and the current research challenges, particularly in the context of residual stress analysis. A special focus for the present study is the development and use of bespoke tools within the commercial package ABAQUSTM that allow the introduction of user-defined non-linear material constitutive laws. Algorithms based on eigenstrain theory and two plasticity theories: Crystal Plasticity (CP) and Strain Gradient Crystal Plasticity (SGCP), both of which have already been introduced in Chapter 1, are described in details. Hereby, the whole set of numerical tools for investigating the residual stresses and deformation is presented.

2.1 The Principles of Finite Element Analysis

In structural or stress analysis, the finite element method is often used to calculate the deformation and stresses due to applied loads for the given component geometries and materials. The fundamental components required for this analysis can be classified as follows:

- 1) Equilibrium Equations: Balance of Forces acting on a solid body (stress)
- 2) Compatibility Equations: Continuity of displacements (strain)
- 3) Constitutive Equations: material response to deformation (stress $\leftrightarrow$ strain)

- 4) Boundary Conditions: i.e. prescribed displacement or load
- 5) Initial Conditions: i.e. initial velocity or temperature

But solving equilibrium equation can sometimes be very problematic. By the principle of virtual work, this equation is usually expressed:

$$\delta W = \int_{\Omega} \rho \ddot{\mathbf{u}} \cdot \delta \mathbf{u} dV + \int_{\Omega} \boldsymbol{\sigma} : \delta \boldsymbol{\varepsilon} dV + \int_{\partial\Omega} \mathbf{t} \cdot \delta \mathbf{u} dA = 0 \quad (2.1)$$

, in which $\mathbf{u}$ is the displacement vector; ρ is the density, $\mathbf{t}$ is the traction.

$\partial\Omega$ and Ω are domains of area A and volume V , respectively. This equation can be further simplified to [35]

$$\nabla \cdot \boldsymbol{\sigma} = \rho \ddot{\mathbf{u}} \quad (2.2)$$

But this equation involves a 2nd order partial differential operation on infinite number of solid body points, which is difficult to find the analytical solution (Figure 2.1). To simplify the problem, the finite element method was introduced to discretize the object into *finite* number of *elements* and equilibrium is only needed on the element nodes. The solution at all other points is obtained by interpolation instead (Figure 2.2).

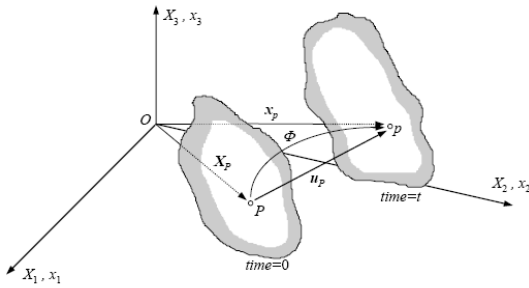


Figure 2.1: Motion of solid body [62]

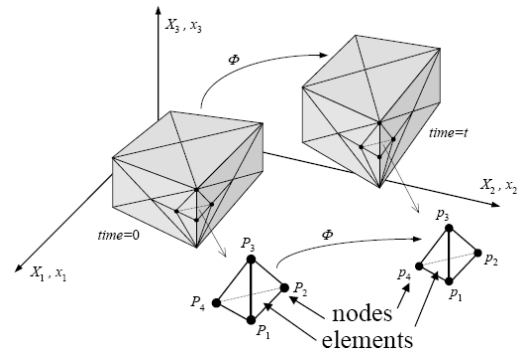


Figure 2.2: Finite Element spatial discretisation of solid body in motion [62]

By using finite element discretisation, the equilibrium equation can normally be reduced to a 2nd order ordinary differential equation:

$$\mathbf{M}\ddot{\mathbf{u}} + \mathbf{C}\dot{\mathbf{u}} + \mathbf{K}\mathbf{u} = \mathbf{F} \quad (2.3)$$

, where $\mathbf{M}$ is the mass; $\mathbf{C}$ is the damping coefficient matrix and $\mathbf{K}$ is the stiffness matrix. In a static stress analysis problem, the equation can be further reduced to:

$$\mathbf{K}\mathbf{u} = \mathbf{F} \text{ or } \mathbf{\Psi} = \mathbf{K}\mathbf{u} - \mathbf{F} \approx \mathbf{0} \quad (2.4)$$

, in which $\mathbf{\Psi}$ is the force residuals. By iterating this equation through various algorithms and checking the residual, the convergence will be reached if the residual is below certain set threshold. The simulation software (ABAQUS) then stops the current increment and moves onto the next one. The whole analysis procedure finishes when all the increments converge successfully.

To implement the equation above into the finite element code, the concept of the shape function must be introduced. Shape function interpolates the values at the element nodes to a point anywhere within the element. Therefore, the element displacements given in terms of nodal displacements $\Delta\mathbf{u}_I$ by the shape functions are

$$\Delta\mathbf{u} \approx \sum_{I=1}^{NNODE} N_I(\xi)\Delta\mathbf{u}_I \quad (2.5)$$

, where ξ is the coordinates of the point in the elements local coordinate system and NNODE denotes the number of finite element nodes. If strains, instead of displacements, are expressed in terms of the nodal displacements, it becomes:

$$\Delta\boldsymbol{\varepsilon} = \frac{d\Delta\mathbf{u}}{d\mathbf{X}} = \frac{\partial\mathbf{N}}{\partial\mathbf{X}}\Delta\mathbf{u}_I = \mathbf{B}\Delta\mathbf{u}_I \quad (2.6)$$

$$\mathbf{B} = \frac{\partial\mathbf{N}}{\partial\mathbf{X}} = \frac{\partial\mathbf{N}}{\partial\xi} \frac{\partial\xi}{\partial\mathbf{X}} = \frac{\partial\mathbf{N}}{\partial\xi} \left(\mathbf{X} \frac{\partial\mathbf{N}}{\partial\xi}\right)^{-1} \quad (2.7)$$

Then, $\mathbf{B}$ matrix is the bridge links up the strains and nodal displacements.

Hence, equation 2.4 in finite element matrix form is [35]:

$$\mathbf{f}_I = \mathbf{k}\mathbf{u}_I \quad \mathbf{f}_I = \int_A \mathbf{N}^T \mathbf{f} dA \quad \mathbf{k} = \int_V \mathbf{B}^T \mathbf{C} \mathbf{B} dV \quad (2.8)$$

Where $\mathbf{k}$ is the stiffness matrix; $\mathbf{f}_I$ is the external force. The stiffness matrix $\mathbf{k}$ can be further expressed as

$$\mathbf{k} = \int_V \mathbf{B}^T \mathbf{C} \mathbf{B} \det[\mathbf{J}] d\xi \quad \mathbf{J} = \frac{\partial \mathbf{X}}{\partial \xi} = \mathbf{X} \frac{\partial \mathbf{N}}{\partial \xi} \quad (2.9)$$

, in which $\mathbf{J}$ is the Jacobian matrix of global coordinates $\mathbf{X}$ in respect to the element local coordinates ξ .

Based on eq. 2.9 and 2.7, the stiffness matrix $\mathbf{k}$ can therefore be related to the material stiffness $\mathbf{C}$ as long as the shape function $\mathbf{N}$ and the shape function derivative $\frac{\partial \mathbf{N}}{\partial \xi}$ are known. This conclusion is very important as the work reported in chapter 7 and 8 implemented it into the ABAQUS secondary development subroutine –UEL (*User defined ELement*) to create a C3D20R element with “C” representing the continuum element and “3D” meaning three dimensional; “20” tells that it has 20 element nodes and “R” is the symbol of reduced number of integration points, in this case, it is eight. Those eight integration points form a new C3D8-like element and the shape function and derivative of that are employed to calculate variables which determine the material properties. An illustration of the C3D20R element and integration points formed C3D8 element is presented here. (Figures 2.3 & 2.4) Further details of the algorithm can be found in Chapter 7.

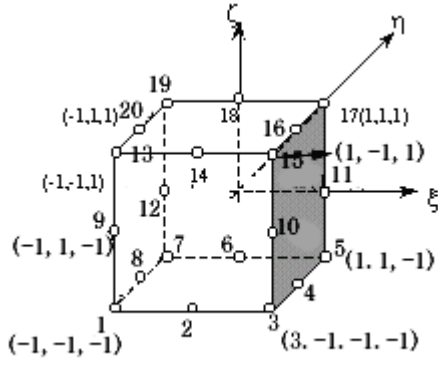


Figure 2.3 Element of C3D20R

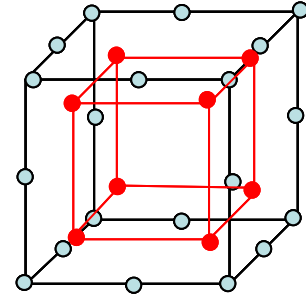


Figure 2.4 IP formed Element of C3D8 within C3D20R

In the content above, the concept of the Integration Point (IP) is used. In the element characteristics determination, it often requires integration operation, which sometimes can be very computationally expensive. Therefore, an approximate solution can be found using numerical integration procedures. If a function of single variable must be integrated over an element domain, i.e.

$$I = \int_{\Omega_e} f(\xi) dV \quad (2.10)$$

It is possible to find its approximation by

$$I \approx I_p = W_1 f(\xi_1) + W_2 f(\xi_2) + \dots + W_p f(\xi_p) \quad (2.11)$$

, where ξ_i are the positions of the integration points; W_i are the predetermined weights as in the Gauss-Legendre rules. For C3D20R element, the sampling positions and the corresponding weights are given below.

p	i	ξ_i	W_i
2	1	$1/\sqrt{3}$	1.0
	2	$-1/\sqrt{3}$	1.0
Table 2.1 Gauss-Legendre integration points for C3D20R			

2.2 Kinematics of Large Deformations

Large elastic-plastic deformations happen in many occasions during manufacturing processes, i.e. deep drawing, direct extrusion etc. Therefore, it is vital to study the material behaviours undergoing large deformations and corresponding theories. As in the present work, our samples (Ti-6Al-4V, Ni, MMC) experienced more than 1% of plastic strains, they definitely fall into the category of the large deformation theory, and no doubt it is employed in the simulation framework. A brief introduction to the large deformation theory and its implementation into the FE framework is presented here.

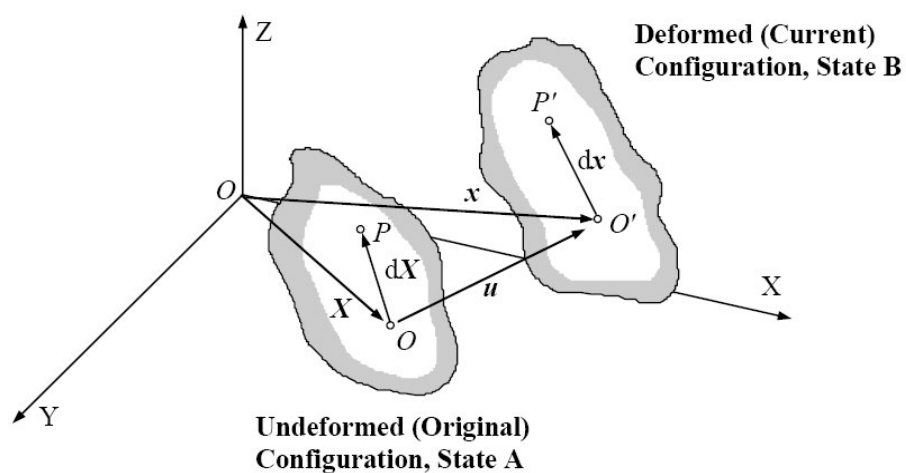


Figure 2.5 An element of material in the undeformed configuration undergoing deformation to the deformed configuration [62]

In Figure 2.5, a piece of imaginary material undergoes the deformation from the original state A to the current state B in the global material coordinate system XYZ. An infinitesimal vector $d\mathbf{X}$ (OP) embedded in the material in state A experiences the same deformation to the vector $d\mathbf{x}$ (O'P') in state B. Hereby, the *deformation gradient*, $\mathbf{F}$ is defined as

$$d\mathbf{x} = \mathbf{F}d\mathbf{X} \quad \text{or} \quad \mathbf{F} = \frac{d\mathbf{x}}{d\mathbf{X}} \quad (2.12)$$

It is well known that the deformation comprises three distinct parts: rigid body translation, rigid body rotation and stretch. In the static stress analysis, the rigid body translation does not affect stresses, hence neglected. Therefore, the deformation gradient which includes both stretch and rigid body rotation provides a complete description of deformation (excluding translations). It is the basic output of the UMAT (User defined MATerial) subroutine and the cornerstone of the secondary development in ABAQUS to define a material's mechanical behaviour. In the subroutine, the variables with names DFGRD0 and DFGRD1 give the deformation gradient in tensor form at the beginning and the end of the increment, respectively.

However, rigid body rotation does not contribute to shape or size change, or internal stress. In solving deformation problems, it is necessary to separate out the stretch from the rigid body rotation contained within $\mathbf{F}$. This can be achieved by the polar decomposition theorem. The theorem states that any non-singular, second-order tensor can be decomposed uniquely into the product of an orthogonal tensor (a rotation), and a symmetric tensor (stretch). Therefore, as a non-singular, second-order tensor, the deformation gradient can be written as

$$\mathbf{F} = \mathbf{R}\mathbf{U} = \mathbf{V}\mathbf{R} \quad (2.13)$$

, where $\mathbf{R}$ is an orthogonal rigid body rotation tensor ($\mathbf{R}\mathbf{R}^T = \mathbf{I}$); $\mathbf{U}$ and $\mathbf{V}$ are symmetric stretch tensors ($\mathbf{V} = \mathbf{V}^T$).

However, plasticity is sometimes time/rate-dependant (i.e. viscoplasticity). It is both sensible and convenient if the plasticity evolution can be expressed in rate

form (i.e. strain rate). Therefore, the concept of *velocity gradient* is introduced. The velocity gradient $\mathbf{L}$ describes the spatial rate of change of the velocity and is given by

$$\mathbf{L} = \frac{\partial \mathbf{v}}{\partial \mathbf{x}} \quad (2.14)$$

The velocity gradient can also be expressed in terms of the deformation gradient:

$$\mathbf{L} = \frac{\partial \mathbf{v}}{\partial \mathbf{x}} = \frac{\partial \mathbf{v}}{\partial \mathbf{X}} \frac{\partial \mathbf{X}}{\partial \mathbf{x}} = \frac{\partial}{\partial t} \left(\frac{\partial \mathbf{x}}{\partial \mathbf{X}} \right) \frac{\partial \mathbf{X}}{\partial \mathbf{x}} = \dot{\mathbf{F}} \mathbf{F}^{-1} \quad (2.15)$$

, which maps the deformation gradient onto the rate of change.

The velocity gradient can also be decomposed into stretch (symmetric) and rigid body rotation (anti-symmetric) parts:

$$\mathbf{L} = \text{sym}(\mathbf{L}) + \text{asym}(\mathbf{L}) \quad (2.16)$$

, where

$$\text{sym}(\mathbf{L}) = \frac{1}{2} (\mathbf{L} + \mathbf{L}^T) \quad \text{asym}(\mathbf{L}) = \frac{1}{2} (\mathbf{L} - \mathbf{L}^T) \quad (2.17)$$

The symmetric part is also denoted as $\mathbf{D}$, the *rate of deformation*; the asymmetric part is call the *continuum spin* $\mathbf{W}$, so that

$$\mathbf{L} = \mathbf{D} + \mathbf{W} \quad (2.18)$$

Most metallic materials under large deformation experience severe plasticity. In which cases, the elastic strains, though not negligible, can be assumed to be small compared with the plastic strains. Therefore, the decoupling of elastic-plastic deformation is important to obtain the elastic strain tensors and stresses. To demonstrate the decoupling of the deformation gradient, a piece of the imaginary material is employed again, but with an intermediate state, in which material only

undergoes purely plastic deformation. (Figure 2.6)

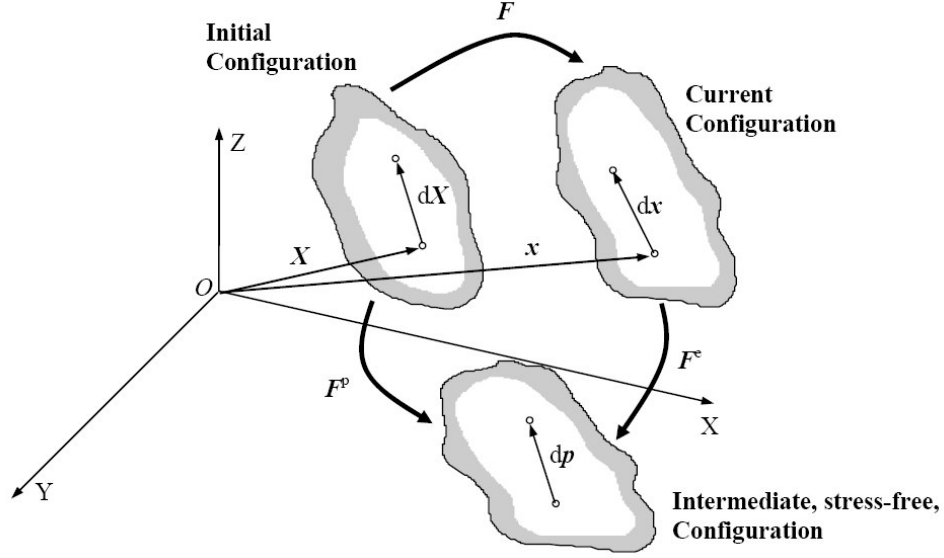


Figure 2.6 Schematic diagram showing an element of a material in the initial, intermediate and current configurations. [62]

Hence, the plastic deformation gradient can be defined via the intermediate state vector $d\mathbf{p}$ as

$$\mathbf{F}^p = \frac{d\mathbf{p}}{d\mathbf{X}} \quad (2.19)$$

And the elastic deformation gradient becomes

$$\mathbf{F}^e = \frac{d\mathbf{x}}{d\mathbf{p}} \quad (2.20)$$

The deformation gradient can then be decomposed in a multiplicative way:

$$\mathbf{F} = \frac{d\mathbf{x}}{d\mathbf{X}} = \frac{d\mathbf{x}}{d\mathbf{p}} \frac{d\mathbf{p}}{d\mathbf{X}} = \mathbf{F}^e \mathbf{F}^p \quad (2.21)$$

, which decouples the elastic and plastic effects into two deformation gradient vectors.

On top of that effect, the stretch-rotation decomposition has to be considered. By convention, all the rigid body rotation is lumped into the plastic deformation gradient, so that the elastic deformation gradient includes stretch only. In Equation 2.22, the

symmetric stretch $\mathbf{V}^e$ belongs solely to $\mathbf{F}^e$, while $\mathbf{F}^p$ contains the total rigid body rotation part $\mathbf{R}$.

$$\mathbf{F}^e = \mathbf{V}^e \quad \mathbf{F}^p = \mathbf{V}^p \mathbf{R} \quad (2.22)$$

Velocity gradient needs to be elastic-plastic decoupled as well. By defining

$$\mathbf{L}^e = \dot{\mathbf{F}}^e (\mathbf{F}^e)^{-1} = \dot{\mathbf{V}}^e (\mathbf{V}^e)^{-1} = \mathbf{D}^e + \mathbf{W}^e \quad (2.23)$$

$$\mathbf{L}^p = \dot{\mathbf{F}}^p (\mathbf{F}^p)^{-1} = \mathbf{D}^p + \mathbf{W}^p \quad (2.24)$$

, the velocity gradient can be expressed in terms of $\mathbf{L}^e$ and $\mathbf{L}^p$, but $\mathbf{L}$ is not simply the additive form of those two parts, it is derived from the decomposition of deformation gradient and given by

$$\mathbf{L} = \mathbf{L}^e + \mathbf{V}^e \mathbf{L}^p (\mathbf{V}^e)^{-1} = \mathbf{D}^e + \mathbf{W}^e + \mathbf{V}^e \mathbf{D}^p (\mathbf{V}^e)^{-1} + \mathbf{V}^e \mathbf{W}^p (\mathbf{V}^e)^{-1} \quad (2.25)$$

Remembering that $\mathbf{D}$ is the symmetric part of $\mathbf{L}$ and $\mathbf{W}$ is the asymmetric part, it gives

$$\mathbf{D} = \mathbf{D}^e + \text{sym}(\mathbf{V}^e \mathbf{D}^p (\mathbf{V}^e)^{-1}) + \text{sym}(\mathbf{V}^e \mathbf{W}^p (\mathbf{V}^e)^{-1}), \quad (2.26)$$

$$\mathbf{W} = \mathbf{W}^e + \text{asym}(\mathbf{V}^e \mathbf{D}^p (\mathbf{V}^e)^{-1}) + \text{asym}(\mathbf{V}^e \mathbf{W}^p (\mathbf{V}^e)^{-1}). \quad (2.27)$$

In the small elastic strains situation, the elastic deformation gradient $\mathbf{V}^e$ can be seen as an identity matrix, so Equation 2.26 and 2.27 can be simplified into

$$\mathbf{D} \approx \mathbf{D}^e + \mathbf{D}^p \quad (2.28)$$

$$\mathbf{W} \approx \mathbf{W}^e + \mathbf{W}^p \quad (2.29)$$

Equation 2.28 is widely used in FE plasticity model implementations. By specifying

$\mathbf{D}^p$ via a constitutive equation and taking $\mathbf{D}$ as a known, $\mathbf{D}^e$ can be determined using Equation 2.28. The stress rate can then be determined using Hooke's law. However, vector expression of the stress rate in a material undergoing large deformation in respect to a fixed coordinate system may change in value due to rigid body rotation. Therefore, a material-fixed coordinate system, or to say, material objectivity must be brought forward. The definition of material objectivity is as such that if a vector, $\mathbf{A}$, is frame indifferent or material objective, it should satisfy the following rule to get its counterpart $\mathbf{A}'$ after rotation:

$$\mathbf{A}' = \mathbf{R}\mathbf{A}\mathbf{R}^T \quad (2.30)$$

, in which $\mathbf{R}$ is the rotation matrix. It can be easily proved that the deformation rate $\mathbf{D}$ and Cauchy stress $\boldsymbol{\sigma}$ are both material objective. The stress rate $\overset{\nabla}{\boldsymbol{\sigma}}$ defined in Hooke's Law in terms of $\mathbf{D}^e$,

$$\overset{\nabla}{\boldsymbol{\sigma}} = 2G\mathbf{D}^e + \lambda \text{Tr}(\mathbf{D}^e)\mathbf{I} \quad (2.31)$$

, is also material objective, where G is the shear modulus and λ is the lamé first parameter. It is called *Jaumann stress rate*, which is the result purely from the constitutive response of the material, not from the rigid body rotation. Once the Jaumann stress rate $\overset{\nabla}{\boldsymbol{\sigma}}$ is obtained, the material stress rate $\dot{\boldsymbol{\sigma}}$ between time t and $t + \Delta t$ can be calculated from [35]

$$\dot{\boldsymbol{\sigma}} = \overset{\nabla}{\boldsymbol{\sigma}} + \mathbf{W}\boldsymbol{\sigma}_t - \boldsymbol{\sigma}_t\mathbf{W}. \quad (2.32)$$

The stress increment during Δt can therefore be calculated accordingly. Given that the total strain increment is known, the predicted stress increment is computed from

Equation 2.32. The predict-correct iteration can therefore be performed to reach a satisfying answer.

2.3 Principles and implementation of Inverse Eigenstrain Method

Measurement (evaluation) of the residual stress within the sample is often related to the measurement of the residual elastic strain distribution in certain direction(s). This applies both to the destructive slitting method, and to the non-destructive X-Ray diffraction method. Some information can then be obtained about the overall strain distribution. However, the underlying eigenstrain distribution that acts as the source of residual stress remains unknown. Therefore, the problem is posed as finding the best solution for this unknown eigenstrain field – the so-called inverse problem of eigenstrain theory, as introduced in Chapter 1. In our model, the pseudo-thermal representation of eigenstrain is used to simulate bending. The kinematics of beam bending is particularly simple. In the Kirchhoff approximation, attention can be focused on only one component of strain (longitudinal), and the longitudinal stress is supposed to be linearly dependent on this component through Young's modulus. The best possible inverse problem solution is searched in terms of the unknown linear thermal expansion coefficient variation across the beam section. In this Chapter the least squares method to minimize the mismatch between the simulation and the experimental result is introduced. Since this provides the basis for subsequent eigenstrain analysis for higher dimensional problems as well, the treatment below is sufficiently general to allow application to such cases.

Suppose that an eigenstrain distribution $\mathcal{E}_{ij}^*(x, y)$ is introduced into an elastic body. Solving this particular kind of elastic problem with a perturbation gives rise to a distribution of residual elastic strains $e_{ij}(x, y)$. Assuming that from the experiment, a

finite number of residual stress component values t_q at locations (x_q, y_q) can be obtained. The same stress components T_q computed from the numerical solution depend implicitly on the assumed eigenstrain distribution $\mathcal{E}_{ij}^*(x, y)$. In order to assess the goodness of the choice of $\mathcal{E}_{ij}^*(x, y)$ in terms of the match to the experimental data, the following measure J is introduced:

$$J[\mathcal{E}_{ij}^*(x, y)] = \sum_q w_q (T_q - t_q)^2 \quad (2.33)$$

Because of the choice of the sum of squared differences to represent the mismatch between the prediction and the experiment, the expression on the right of the above equation is non-negative, and is only equal to zero if the agreement is perfect. The problem of finding the unknown eigenstrain distribution can now be reformulated as the problem of identifying the function $\hat{\mathcal{E}}_{ij}^*(x, y)$ that delivers the minimum to J , i.e. $\hat{\mathcal{E}}_{ij}^* = \arg \min J$. To formulate a practical algorithm for finding $\hat{\mathcal{E}}_{ij}^*(x, y)$, this unknown distribution can be represented by a truncated series with unknown coefficients:

$$\mathcal{E}^*(x, y) = \sum_{k=1}^K c_k E_k(x, y) \quad (2.34)$$

Turning now to the specific case of plastically bent beam, let us denote by $s_k(x)$ the distribution of the longitudinal stress component σ_{yy} (i.e. in the same direction as the pseudo-thermal strain) arising from the eigenstrain distribution given by the k^{th} basis function $E_k(x, y)$. Note that in the case of simple bending the solution only depends on the transverse coordinate x . Evaluating $s_k(x)$ at each of the

q^{th} measurement points with coordinates x_q gives rise to predicted values $s_{kq} = s_k(x_q)$.

Now the predicted stress values at each measurement point can be expressed as the linear combination of s_{kq} with the same coefficients c_k , i.e. $\sum_k c_k s_{kq}$. Let t_q denote the values of the same stress component σ_{yy} at points x_q measured in the experiment.

The measure of goodness of the prediction introduced above has the form:

$$J = \sum_q w_q \left(\sum_k c_k s_{kq} - t_q \right)^2 \quad (2.35)$$

, where the sum in q is taken over all the measurement points. The choice of weights w_q remains at our disposal and can be made e.g. on the basis of the accuracy of measurement at different points. For simplicity it is possible to assume that $w_q = 1$.

The search for the best choice of model can now be accomplished by minimizing J with respect to the unknown coefficients, c_k i.e. by solving:

$$\text{grad}_{c_k} J = \left(\frac{\partial J}{\partial c_k} \right) = 2 \sum_{q=1}^Q s_{kq} \left(\sum_{m=1}^K c_m s_{mq} - t_q \right) = 2 \left(\sum_{m=1}^K c_m \sum_{q=1}^Q s_{kq} s_{mq} - \sum_{q=1}^Q s_{kq} t_q \right) = 0 \quad (2.36)$$

and introducing the following matrix and vector notation,

$$S = \{s_{kq}\}, \quad t = \{t_q\}, \quad c = \{c_k\}. \quad (2.37)$$

The entities appearing in last equation can be written in matrix form as:

$$A = \sum_{q=1}^Q s_{kq} s_{mq} = SS^T, \quad b = \sum_{q=1}^Q s_{kq} t_q = St. \quad (2.38)$$

Thus, the solution of the inverse problem has been reduced to a system of linear equations $Ac = b$ for the unknown vector of coefficients $c = \{c_k\}$. The entire

solution procedure was implemented within a Matlab[®] program, with S and t providing the essential input data (a matrix of influence coefficients computed either analytically or numerically, and a column of experimental data). The solution of the above linear system always exists and is unique. The result of the computation in terms of the c vector contains the optimum values of the coefficients. Once it is found, the assembly of the found eigenstrain solution and of the corresponding residual elastic fields (strains and stresses) is fairly trivial[63].

In Chapter 4, 5 and 6, this method is employed to find the best-matching eigenstrain field in different components.

2.4 Rate-independent crystal plasticity formulation

The crystal plasticity formulation used here is based on the kinematics of large deformations theory described in last section. The aim of it is to not only capture the metal macroscopic deformation behaviours, but also mesoscale grain level slip and rotation, which leads to the deformation inhomogeneity. To prescribe the phenomenon in the finite element context, the crystal plasticity theory is created by Asaro[34], Anand and Kothari[64]. The implementation of it is achieved by Manonukul and Dunne[65], with modifications described in Korsunsky et al[66]. Here a detailed summary of the formulation is provided to explain the implementation so that its application on the simulation of Ti-6V-4V deformation in Chapter 7 can be understood.

When a load is applied, the total deformation and rotation of a crystal is given by the deformation gradient $\mathbf{F}$, which can be written in terms of elastic and plastic parts. Recalling Eq. 2.21,

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^p. \quad (2.39)$$

The material undergoes plastic slip in the α^h slip system, γ^α , through the ‘undeformed’ crystal lattice given by

$$\mathbf{F}^p = \mathbf{I} + (\mathbf{s}^\alpha \mathbf{n}^{\alpha T}) \gamma^\alpha \quad (2.40)$$

, where $\mathbf{s}^\alpha$ and $\mathbf{n}^\alpha$ are the vector which represent the slip system (slip direction and normal, respectively). The term $\mathbf{F}^e$ includes both the elastic deformation and rigid body rotation. Vectors $\mathbf{s}^\alpha$ and $\mathbf{n}^\alpha$ always remain perpendicular. This is one of the core assumptions made in crystal plasticity theory, which assumes that plastic deformation is solely created by crystal slip.

The velocity gradient in the current configuration can be introduced as

$$\mathbf{L} = \dot{\mathbf{F}} \mathbf{F}^{-1} = \dot{\mathbf{F}}^e (\mathbf{F}^e)^{-1} + \mathbf{F}^e \dot{\mathbf{F}}^p (\mathbf{F}^p)^{-1} (\mathbf{F}^e)^{-1} \quad (2.41)$$

, and decomposed into deformation rate, $\mathbf{D}$, and spin tensor, $\mathbf{W}$, as in Eq. 2.18.

The terms $\mathbf{D}$ can be also decomposed into parts due to plastic slip ($\mathbf{D}^p, \mathbf{W}^p$) and lattice deformation ($\mathbf{D}^e, \mathbf{W}^e$). Since the plastic deformation occurs by dislocation slip, in the current state

$$\mathbf{L}^p = \mathbf{D}^p + \mathbf{W}^p = \sum_{\alpha=1}^n \dot{\gamma}^\alpha \mathbf{s}^\alpha \mathbf{n}^{\alpha T}. \quad (2.42)$$

Here the sum runs over all active slip systems and $\dot{\gamma}^\alpha$ is the shearing rate on the α^h slip system measured relative to the lattice. Furthermore, the plastic deformation rate $\mathbf{D}^p$ and the plastic spin tensor $\mathbf{W}^p$ can also be derived from the symmetric and skew parts, respectively, of the plastic velocity gradient $\mathbf{L}^p$.

Assuming that crystal elasticity is unaffected by slip, then following Hill and Rice[31], the elastic law can be written as

$$\overset{\nabla}{\boldsymbol{\sigma}} + \boldsymbol{\sigma} \operatorname{tr}(\mathbf{D}^e) = \mathbf{C} : \mathbf{D}^e. \quad (2.43)$$

Here $\mathbf{C}$ is the elastic moduli tensor and $\overset{\nabla}{\boldsymbol{\sigma}}$ is the Jaumann rate of Cauchy stress based on the axes which spin together with the lattice and is given, in terms of the Cauchy stress rate. Recalling Eq. 2.32

$$\overset{\nabla}{\boldsymbol{\sigma}} = \dot{\boldsymbol{\sigma}} - \mathbf{W}^e \boldsymbol{\sigma} + \boldsymbol{\sigma} \mathbf{W}^e. \quad (2.44)$$

Manipulation of Eq. 2.44 using 2.43 allows us to write

$$\overset{\nabla}{\boldsymbol{\sigma}} = \mathbf{C} : \mathbf{D} - \mathbf{C} \sum_{\alpha=1}^n \mathbf{P}^{\alpha} \dot{\gamma}^{\alpha} - \boldsymbol{\sigma} \operatorname{tr}(\mathbf{D}), \quad (2.45)$$

Equations (2.44) and (2.45) can be now rearranged and simplified to give

$$\dot{\boldsymbol{\sigma}} = \mathbf{C} : \mathbf{D} - \boldsymbol{\sigma} \operatorname{tr}(\mathbf{D}) - \mathbf{W} \boldsymbol{\sigma} + \boldsymbol{\sigma} \mathbf{W} - \sum_{\alpha=1}^n (\mathbf{C} : \mathbf{P}^{\alpha} + \boldsymbol{\beta}^{\alpha}) \dot{\gamma}^{\alpha}, \quad (2.46)$$

, where

$$\boldsymbol{\beta}^{\alpha} = \boldsymbol{\Omega}^{\alpha} \boldsymbol{\sigma} - \boldsymbol{\sigma} \boldsymbol{\Omega}^{\alpha} \quad (2.47)$$

$$\mathbf{P}^{\alpha} = \frac{1}{2} (\mathbf{s}^{\alpha} \mathbf{n}^{\alpha T} + \mathbf{n}^{\alpha} \mathbf{s}^{\alpha T}) \quad (2.48)$$

$$\boldsymbol{\Omega}^{\alpha} = \frac{1}{2} (\mathbf{s}^{\alpha} \mathbf{n}^{\alpha T} - \mathbf{n}^{\alpha} \mathbf{s}^{\alpha T}) \quad (2.49)$$

In order to obtain the Cauchy stress rate, it is necessary to determine the shearing rate $\dot{\gamma}^{\alpha}$ on the α^h active slip system. The conditions under which a slip system is active or inactive are based on the yield and loading–unloading criteria. The magnitude of $\dot{\gamma}^{\alpha}$ can be determined using the constitutive equation for plastic slip on each slip system

$$\dot{\tau}_c^\alpha = \sum_{\alpha=1}^n \mathbf{h}_{\alpha\beta} \dot{\gamma}^\beta \quad (2.50)$$

, where $\dot{\gamma}^\beta$ is the shearing rate on slip system, and the matrix is $\mathbf{h}_{\alpha\beta}$ describes the rate of increase of the deformation resistance on slip system α due to shearing on slip system β ; it describes both self-hardening (same slip system, $\mathbf{h}_{\beta\beta}$) and latent-hardening (different slip systems, $\mathbf{h}_{\alpha\beta}$, $\alpha \neq \beta$). Each element $\mathbf{h}_{\alpha\beta}$ depends on the deformation history. The instantaneous hardening moduli remain the least well-characterized part of the constitutive equations for crystal elasto-plasticity. An α^h slip system is considered to slip, or flow plastically, when the resolved shear stress on the slip system τ^α exceeds a critical resolved shear stress τ_c^α . The critical resolved shear stress τ_c^α is determined by the current dislocation density and substructure. The planes $\tau^\alpha = \tau_c^\alpha$ represent the facets of the current pyramidal yield surface in stress space. The outward unit normal to the yield facets is $\mathbf{P}^\alpha$. A slip system is considered inactive if $\tau^\alpha < \tau_c^\alpha$, or $\tau^\alpha = \tau_c^\alpha$ and a trial stress rate $\mathbf{P}^\alpha : \mathbf{C} : \mathbf{D}$ points inside the yield surface, i.e. the system is under the condition of unloading. On the other hand, a slip system is considered active if $\tau^\alpha = \tau_c^\alpha$ and a trial stress rate $\mathbf{P}^\alpha : \mathbf{C} : \mathbf{D}$ points outside the yield surface, i.e. the system is under the condition of loading:

$$\begin{aligned} \dot{\gamma}^\alpha &= 0, & \tau^\alpha &< \tau_c^\alpha, \\ \dot{\gamma}^\alpha &= 0, & \tau^\alpha &= \tau_c^\alpha \cap \mathbf{P}^\alpha : \mathbf{C} : \mathbf{D} \leq 0, \\ \dot{\gamma}^\alpha &\geq 0, & \tau^\alpha &= \tau_c^\alpha \cap \mathbf{P}^\alpha : \mathbf{C} : \mathbf{D} > 0. \end{aligned} \quad (2.51)$$

The resolved shear stress, or Schmid stress, on the α^h slip system is defined (Asaro and Rice[32],)

$$\boldsymbol{\tau}^\alpha = \mathbf{s}^\alpha (\boldsymbol{\sigma} \mathbf{n}^\alpha) = \mathbf{P}^\alpha : \boldsymbol{\sigma}. \quad (2.52)$$

Using the rate of change of the resolved shear stress on the α^h slip system that can be obtained by taking the material time derivative of Equation 2.52, Equation 2.45 together with Asaro's formulation for the co-rotational rate of the symmetrical part of velocity gradient, the rate of change of the shear stress can be written as

$$\dot{\boldsymbol{\tau}}^\alpha = \mathbf{P}^\alpha : \left(\mathbf{C} : \mathbf{D} - \mathbf{C} : \sum_{\alpha=1}^n \mathbf{P}^\alpha \dot{\boldsymbol{\gamma}}^\alpha - \boldsymbol{\sigma} \operatorname{tr}(\mathbf{D}) \right) + \boldsymbol{\beta}^\alpha : \left(\mathbf{D} - \sum_{\alpha=1}^n \mathbf{P}^\alpha \dot{\boldsymbol{\gamma}}^\alpha \right) \quad (2.53)$$

To satisfy the consistency condition during plastic slip, $\dot{\boldsymbol{\tau}}^\alpha = \dot{\boldsymbol{\tau}}_c^\alpha$, Eq. 2.53 can be rewritten, using Eq. 2.50, as

$$\sum_{\alpha=1}^n \mathbf{h}_{\alpha\beta} \dot{\boldsymbol{\gamma}}^\beta = \mathbf{P}^\alpha : \left(\mathbf{C} : \mathbf{D} - \mathbf{C} : \sum_{\alpha=1}^n \mathbf{P}^\alpha \dot{\boldsymbol{\gamma}}^\alpha - \boldsymbol{\sigma} \operatorname{tr}(\mathbf{D}) \right) + \boldsymbol{\beta}^\alpha : \left(\mathbf{D} - \sum_{\alpha=1}^n \mathbf{P}^\alpha \dot{\boldsymbol{\gamma}}^\alpha \right). \quad (2.54)$$

The above equation can now be rewritten in the form

$$\sum_{\alpha=1}^n \mathbf{A}^{\alpha\beta} \dot{\boldsymbol{\gamma}}^\beta = \mathbf{b}^\alpha. \quad (2.55)$$

Here the matrix $\mathbf{A}^{\alpha\beta}$ is singular and Equation 2.55 has a solution but it is non-unique. This is a well-known problem with time-independent crystal plasticity, which results from the non-uniqueness of the solutions for $\dot{\boldsymbol{\gamma}}^\alpha$ when more than five slip systems are active at the same time. Anand and Kothari[64] overcame this problem by using a singular-value decomposition to obtain a pseudo-inverse of a singular matrix. Although this is clearly primarily a numerical ploy, and does not necessarily have a physical explanation, it is adopted here as a matter of expedience.

In Chapter 7, this crystal plasticity formulation is used to describe the deformation of α phase Ti-6Al-4V and capture the grain group stresses.

2.5 A physically-based, time-dependent strain gradient crystal plasticity formulation

The initial motive for adopting a strain gradient crystal plasticity formulation is to gain knowledge of the meso to micro scale intra-granular deformation information which crystal plasticity theory can not access. Besides individual crystal slip, this type of plasticity theory enable the dislocation evolution feature which controls the material hardening behaviour, lattice rotation and misorientation etc. Therefore, it is an ideal tool for us to probe the microscopic grain level deformation. The formulation framework employed here is adopted from Cheong and Busso [61], a detailed description of the algorithm is presented here for clarity.

2.5.1 The flow rule- Kinetics of the deformation

The flow rule is based on two fundamental assumptions made by Busso and McClintock: [67]

1. The lattice resistance is thermally activated.
2. Bypassing of forest dislocations by gliding dislocations is mainly a stress-activated process.

Therefore, in our work, to look for an expression for the shear strain rate of a generic slip system α under a given temperature, structure and resolved shear stress τ^α is to determine the rate at which individual dislocations can overcome the lattice friction. In an energy approach to establish the link, the energetic path between two dislocation states can be characterized by a peak Gibbs free energy barrier ΔG^α . The probability of an energy fluctuation at a temperature T that could allow the dislocation to overcome the this barrier is given by the theory of kinetics in terms of Boltzmann constant k ,

$$P_T^\alpha = \exp\left(-\frac{\Delta G^\alpha}{kT}\right) \quad (2.56)$$

The rate of activation can then be found by multiplying P_T^α by a pre-exponent term $\dot{\gamma}_0$.

$$\dot{\gamma}^\alpha = \dot{\gamma}_0^\alpha P_T^\alpha = \dot{\gamma}_0^\alpha \exp\left(-\frac{\Delta G^\alpha}{kT}\right) \quad (2.57)$$

As the activation energy is far too complex to be obtained in closed form for the mechanisms of interest, a more phenomenological relation was proposed to account for the actual activation energy. As the stress dependence of $\dot{\gamma}_0$ is expected to be small, [68] important information about ΔG^α can be obtained from experimental measured relations between strain rate and stress for the slip system. A convenient form for ΔG^α proposed by Kocks [68] is given in terms of the driving stress τ^α , the strength $\hat{\tau}$ at which dislocations can be mobilized without the assistance of thermal activation, the total free energy of activation under a vanishingly small applied stress F_0 , and two exponents p and q chosen to best fit the stress dependence of the activation energy,

$$\Delta G^\alpha = F_0 \left\{ 1 - \left(\frac{\tau^\alpha}{\hat{\tau}} \right)^p \right\}^q. \quad (2.58)$$

The strength $\hat{\tau}$ can be approximated by the product of the lattice friction stress at 0 K, $\hat{\tau}_0$, with the ratio of the shear modulus at the temperature of interest to that at 0 K to reduce all elastic interactions to 0 K:

$$\hat{\tau} = \hat{\tau}_0 \frac{\mu}{\mu_0}. \quad (2.59)$$

The shear strain rate then becomes

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \exp \left\{ -\frac{F_0}{kT} \left[1 - \left(\frac{\tau^{\alpha}}{\hat{\tau}_0 \mu / \mu_0} \right)^p \right]^q \right\}. \quad (2.60)$$

Since the model assumes that only the lattice resistance can be thermally activated, the driving stress $\hat{\tau}$ for the thermal activation energy can be replaced by the lattice resistance stress $\hat{\tau}_1$. Knowing that there are two dominant mechanisms contributing to the strengthening of the material: the thermally activated lattice resistance to dislocation motion and the discrete obstacle resistance produced by forest dislocations, the lattice resistance stress $\hat{\tau}_1$ can be obtained by subtracting the athermal component (obstacle resistance produced by forest dislocation) of the flow stress, S_0^{α} , from the overall flow stress τ_R^{α} :

$$\tau^{\alpha} \equiv \tau_1^{\alpha} = \tau_R^{\alpha} - S_0^{\alpha} \frac{\mu}{\mu_0}. \quad (2.61)$$

Hence, the final expression for the shear strain rate is

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \exp \left\{ -\frac{F_0}{kT} \left[1 - \left(\frac{\tau_R^{\alpha} - S_0^{\alpha} \mu / \mu_0}{\hat{\tau}_0 \mu / \mu_0} \right)^p \right]^q \right\} \text{sgn}(\tau_R^{\alpha}) \quad (2.62)$$

, where $\text{sgn}(\tau_R^{\alpha})$ is the sign function, accounting for either positive or negative slip in the system.

2.5.2 Kinematics of dislocation motion

In last session, the flow rule is presented. The flow rule is built on the shear strain rate $\dot{\gamma}$ on a particular slip system α , which is thermally dependent with a Boltzmann type exponential thermal activation expression and the unknown athermal discrete obstacle resistance produced by forest dislocations S_0^{α} . The dislocations contribution to the resistance is quantified by

$$S_0^\alpha = [(S_S^\alpha)^2 + (S_G^\alpha)^2]^{\frac{1}{2}} = \lambda_S \mu b_S^\alpha \sqrt{\sum_{\beta=1}^N \mathbf{h}_S^{\alpha\beta} \rho_S^\beta} + \lambda_G \mu b_G^\alpha \sqrt{\sum_{\beta=1}^N \mathbf{h}_G^{\alpha\beta} \rho_G^\beta} . \quad (2.63)$$

Here, λ is a statistical coefficient which accounts for the deviation from regular spatial arrangements of the dislocations, b^α represents the magnitude of the Burgers vector, and $h^{\alpha\beta}$ is the interaction function defined as

$$\mathbf{h}^{\alpha\beta} = w_1 + (1 - w_2) \delta^{\alpha\beta} . \quad (2.64)$$

The term w_1 and w_2 in Eq. 2.64 are the interaction coefficients and $\delta^{\alpha\beta}$ is the Kronecker Delta. The subscription S, G represents the two different dislocation types: Statistically Stored Dislocations (SSD) and Geometrically Necessary Dislocations (GND). Here, the total dislocation density is assumed to comprise edge and screw types of SSDs and three types of GNDs: $\rho_{G_{sw}}^\alpha$ screw type which is parallel to the slip direction, $\rho_{G_{en}}^\alpha$ edge type which is parallel to the slip normal and $\rho_{G_{et}}^\alpha$ to $\mathbf{t}^\alpha = \mathbf{m}^\alpha \times \mathbf{n}^\alpha$, respectively (Eq. 2.65).

$$\rho_T^\alpha = \rho_S^\alpha + \rho_G^\alpha = (\rho_{S_e}^\alpha + \rho_{S_{sw}}^\alpha) + (\rho_{G_{sw}}^\alpha + \rho_{G_{et}}^\alpha + \rho_{G_{en}}^\alpha) \quad (2.65)$$

The evolutionary equations for both screw and edge type of the SSDs are developed here, with dislocation multiplication and annihilation forming the bases of their evolutionary behaviours.

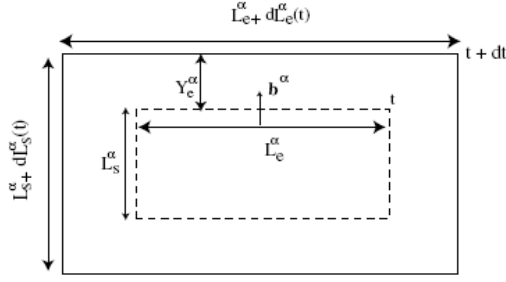


Figure 2.7 A schematic diagram of dislocation multiplication of an idealised, expanding dislocation loop during a time interval dt [69]

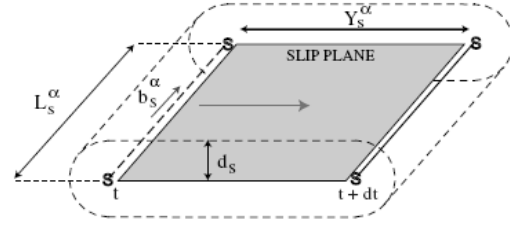


Figure 2.8 A schematic diagram of dislocation annihilation of the annihilation region (dashed line) for a screw dislocation after a time interval dt [69]

In this work, dislocation generation is assumed to be associated with the expansion of dislocation loops originated from existing Frank-Read sources. Figure 2.7 shows an idealised, expanding dislocation loop on an arbitrary active slip system α during a time interval dt . The loop is assumed to be rectangular, with straight edge and screw sides of lengths L_e^α and L_s^α , respectively. The change in dislocation densities ($d\rho_i^\alpha$), where the subscription i refers to either edge (e) or screw (s) dislocations, is attributed to the increase in length of the individual dislocation segments (dL_i^α) expanding simultaneously within a control volume V ,

$$d\rho_i^\alpha = \frac{dL_i^\alpha(t)}{V}. \quad (2.66)$$

Considering an edge segment of the dislocation loop, its contribution to the plastic increment after a time interval dt is

$$d\gamma_e^\alpha = b^\alpha Y_e^\alpha \left[\frac{L_e^\alpha + dL_e^\alpha(t)}{V} \right]. \quad (2.67)$$

Here, Y_e^α is the mean free path of the edge dislocation segment, defined to be the distance travelled by the segment before its motion is arrested by forest dislocations

(Figure 2.7). Differentiating Eq. 2.66 with respect to time yields the rate of generation of the edge dislocation density,

$$\dot{\rho}_{e,gen}^{\alpha} = \frac{C_e}{b^{\alpha} Y_e^{\alpha}} \dot{\gamma}^{\alpha} \quad (2.68)$$

, and similarly for the generation of screw dislocations,

$$\dot{\rho}_{s,gen}^{\alpha} = \frac{C_s}{b^{\alpha} Y_s^{\alpha}} \dot{\gamma}^{\alpha} \quad (2.69)$$

In Eq. 68 and 69, C_s and Y_s^{α} are parameters which scale the magnitudes of the slip rate contributions from the edge and screw segments, respectively.

In this work, the predominant annihilation mechanism is assumed to be the mutual annihilation between parallel dislocations of the same character but opposite sign (herein defined as anti-parallel dislocations). An annihilation event occurs when two dislocations are drawn towards each other by their attractive forces in order to reduce their line energies. Through this combination process, the opposing dislocations mutually annihilate. The probability of such an event occurring is determined by the cross-sectional area for annihilation. Such a region is illustrated by the dashed line in Figure 2.8 around a gliding screw dislocation, which moves from the position at time “ t ” to “ $t + dt$ ”. Here, the symbol ds represents the critical distance for mutual annihilation between two anti-parallel screw dislocations to take place. Based on the region outlined in the figure, the annihilation area A_s^{α} for a screw segment gliding on an arbitrary slip system α is:

$$A_s^{\alpha} = \left[2d_s Y_s^{\alpha} + \pi d_s^2 \right]. \quad (2.70)$$

By combining Eq. 2.66 and 2.70, the probability of an annihilation event is:

$$P_{\text{ann}} = \frac{1}{2} \left[\frac{A_s^\alpha L_s^\alpha}{V} \right] = \frac{A_s^\alpha \rho_s^\alpha}{2}. \quad (2.71)$$

, where the factor of $\frac{1}{2}$ in Eq. 2.71 assumes an equal density of anti-parallel screw dislocations. From the Orowan relationship [70], the rate of annihilation can be expressed as

$$\dot{\rho}_{\text{s,ann}}^\alpha = P_{\text{ann}} \left[\frac{C_s \dot{\gamma}_s^\alpha}{b^\alpha Y_s^\alpha} \right]. \quad (2.72)$$

It should be noted that the factor of $\frac{1}{2}$ is eliminated since two screw dislocations are annihilated in every event. With Eq. 2.70-72, the screw dislocation density annihilation rate is

$$\dot{\rho}_{\text{s,ann}}^\alpha = \frac{C_s}{b^\alpha} \left[\frac{\pi d_s^2}{Y_s^\alpha} + 2d_s \right] \rho_s^\alpha \dot{\gamma}^\alpha. \quad (2.73)$$

A similar expression obtained for edge dislocations does not include the additional term $\frac{\pi d_s^2}{Y_s^\alpha}$ as due to its inability to cross-slip. Therefore, the edge dislocation annihilation rate is,

$$\dot{\rho}_{\text{e,ann}}^\alpha = \frac{C_e}{b^\alpha} [2d_e] \rho_e^\alpha \dot{\gamma}^\alpha \quad (2.74)$$

Noting that the critical edge annihilation distance d_e is smaller than the screw (i.e. $d_e < d_s$). To express the evolutionary laws for edge and screw dislocations in terms of their dislocation densities, ρ_s^α and ρ_e^α must be linked to the mean obstacle spacing l_m^α ,

where the dominant obstacles are forest dislocations. A relationship between Y_i^α and l_m^α can be written as,

$$Y_i^\alpha = \frac{l_m^\alpha}{K_i} \quad (2.75)$$

, in which K_i is a dimensionless proportionality constant controlling the mobility of dislocations. Since a moving dislocation will be affected by the nature of the forest obstacle, i.e. edge and screw dislocations, the mean obstacle spacing l_m^α should be a function of the total dislocation density ρ_T^α . Here, l_m^α follows the inverse-square root relationship obtained from geometric considerations:

$$l_m^\alpha = \frac{1}{\sqrt{\sum_{\beta=1}^N \rho_T^\beta}} \quad (2.76)$$

The dislocation density evolutionary equations are formulated as balance equations (i.e. $\dot{\rho}_i^\alpha = \dot{\rho}_{i,gen}^\alpha - \dot{\rho}_{i,ann}^\alpha$). From Eq. 68, 69 and 73-76, the final expression of the evolution of edge and screw SSDs can be obtained as:

$$\dot{\rho}_{S_e}^\alpha = \frac{C_e}{b_s^\alpha} [K_e \sqrt{\sum_{\beta=1}^N \rho_T^\beta} - 2d_e \rho_{S_e}^\alpha] |\dot{\gamma}^\alpha| \quad (2.77)$$

$$\dot{\rho}_{S_{sw}}^\alpha = \frac{C_{sw}}{b_s^\alpha} [K_{sw} \sqrt{\sum_{\beta=1}^N \rho_T^\beta} - \rho_{S_{sw}}^\alpha \{K_{sw} \pi d_{sw}^2 \sqrt{\sum_{\beta=1}^N \rho_T^\beta} + 2d_{sw}\}] |\dot{\gamma}^\alpha| \quad (2.78)$$

The determination of the time rate change of the geometrically necessary dislocation densities $\rho_{G_i}^\alpha$ in Eq. 2.65 is based on the relationship between inelastic strain gradients and dislocation densities originally proposed by Busso. [55] Here,

Nye's dislocation tensor [71] is used to define a tensorial measure of the GND densities which can be related to the resultant Burger's vector of all GNDs.

Let $d\mathbf{Y}$ be a material line element. Following the multiplicative decomposition of the total deformation gradient, Eq. 2.21, assume that this material line element first undergoes an inelastic deformation into an intermediate configuration, $d\mathbf{Y}^*$, followed by an elastic deformation which takes it into its final (or current) configuration, $d\mathbf{y}$. Thus,

$$d\mathbf{y} = \mathbf{F}^e \mathbf{F}^p d\mathbf{Y} = \mathbf{F}^e d\mathbf{Y}^* \quad (2.79)$$

, where $d\mathbf{Y}^* = \mathbf{F}^p d\mathbf{Y}$.

By definition, the density of the GNDs is related to the net Burger's vector of all dislocations piercing an infinitesimal surface S with normal $\mathbf{r}$, and enclosed counter-clockwise by a circuit $\mathbf{G}$ in the intermediate configuration associated with $\mathbf{F}^p$. The resulting discontinuity on completion of a Burger's circuit around the path $\mathbf{G}$ can then be defined as

$$\mathbf{G} = -\oint_{\eta} \mathbf{F}^p d\mathbf{Y} \quad (2.80)$$

An expression for the plastic deformation gradient can be obtained by integrating

$$\dot{\mathbf{F}}^p = \left\{ \sum_{\alpha} \dot{\gamma}^{\alpha} \mathbf{m}^{\alpha} \otimes \mathbf{n}^{\alpha} \right\} \mathbf{F}^p \quad (2.81)$$

, which gives

$$\mathbf{F}^p = \int_{\zeta=0}^{\zeta=t} \left\{ \sum_{\alpha} \dot{\gamma}^{\alpha} \mathbf{m}^{\alpha} \otimes \mathbf{n}^{\alpha} \right\}^{-1} \dot{\mathbf{F}}^p d\zeta. \quad (2.82)$$

Furthermore, from Stokes' generalized theorem, Eq. 2.80 can be rewritten in terms of Nye's dislocation density tensor $\mathbf{\Lambda}$ as

$$\mathbf{G} = \int_S \mathbf{\Lambda} \mathbf{r} dS \quad (2.83)$$

, with

$$\mathbf{\Lambda} \equiv \text{curl} \{ \mathbf{F}^p \} = \varepsilon (\mathbf{F}^p \otimes \nabla) \quad (2.84)$$

, and where ε is the permutation tensor.

The evolutionary equation for the GNDs can be obtained by differentiating Eq. 2.83,

$$\dot{\mathbf{G}} = \int_S \dot{\mathbf{\Lambda}} \mathbf{r} dS = \int_S \sum_{\alpha} \dot{\mathbf{\Lambda}}^{\alpha} \mathbf{r} dS \quad (2.85)$$

Where, from Eq. 2.82 and 2.84,

$$\dot{\mathbf{\Lambda}}^{\alpha} = \text{curl} \{ (\dot{\gamma}^{\alpha} \mathbf{m}^{\alpha} \otimes \mathbf{n}^{\alpha}) \mathbf{F}^p \} \quad (2.86)$$

Let $\mathbf{G}^{\alpha}$ be the contribution to the tensor from the slip system α . Then, Eq. 2.85 becomes

$$\dot{\mathbf{G}} = \sum_{\alpha} \dot{\mathbf{G}}^{\alpha} \quad (2.87)$$

, with

$$\dot{\mathbf{G}}^{\alpha} = \int_S \dot{\mathbf{\Lambda}}^{\alpha} \mathbf{r} dS \quad (2.88)$$

From the work of Nye [71], $\dot{\mathbf{\Lambda}}^{\alpha}$ can be related to the evolution of individual dislocation groups within the crystal as follows. Consider a set α of dislocations with an equivalent GND vector ρ_G^{α} and Burger's vector $\mathbf{b}_G^{\alpha}$. The density of these

dislocations crossing a unit area S with normal $\mathbf{r}$ is given by $\int_S \boldsymbol{\rho}_G^\alpha \mathbf{r} dS$, and the

associated Burger's vector discontinuity can then be defined as

$$\mathbf{G}^\alpha = \int_S (\boldsymbol{\rho}_G^\alpha \mathbf{r}) \mathbf{b}_G^\alpha dS = \int_S (\mathbf{b}_G^\alpha \otimes \boldsymbol{\rho}_G^\alpha) \mathbf{r} dS. \quad (2.89)$$

The associated rate of change of the net Burger's vector discontinuity crossing the unit area S is obtained by differentiating Eq. 2.89,

$$\dot{\mathbf{G}}^\alpha = \int_S (\mathbf{b}_G^\alpha \otimes \dot{\boldsymbol{\rho}}_G^\alpha) \mathbf{r} dS \quad (2.90)$$

, where

$$\dot{\boldsymbol{\rho}}_G^\alpha = \dot{\boldsymbol{\rho}}_{G_{sw}}^\alpha \mathbf{m}^\alpha + \dot{\boldsymbol{\rho}}_{G_{et}}^\alpha \mathbf{t}^\alpha + \dot{\boldsymbol{\rho}}_{G_{en}}^\alpha \mathbf{n}^\alpha \quad (2.91)$$

represents the time rate of change of the vector field of GND densities. Hence, the tensor relation, from which the evolutionary equations for the individual set of GNDs can be extracted, is obtained by combining Eq. 2.86 and 2.91, and equating Eq. 2.88 and 2.90,

$$\begin{aligned} & \dot{\boldsymbol{\rho}}_{G_{sw}}^\alpha (\mathbf{b}_G^\alpha \otimes \mathbf{m}^\alpha) + \dot{\boldsymbol{\rho}}_{G_{et}}^\alpha (\mathbf{b}_G^\alpha \otimes \mathbf{t}^\alpha) + \dot{\boldsymbol{\rho}}_{G_{en}}^\alpha (\mathbf{b}_G^\alpha \otimes \mathbf{n}^\alpha) \\ &= \mathbf{curl} \left\{ (\dot{\gamma}^\alpha \mathbf{m}^\alpha \otimes \mathbf{n}^\alpha) \mathbf{F}^p \right\} \end{aligned} \quad (2.92)$$

When rewritten in vector form in terms of the magnitude of the GNDs' Burger's vector $\mathbf{b}_G^\alpha$, Eq. 2.92 can be simplified to

$$b_G^\alpha (\dot{\boldsymbol{\rho}}_{G_{sw}}^\alpha \mathbf{m}^\alpha + \dot{\boldsymbol{\rho}}_{G_{et}}^\alpha \mathbf{t}^\alpha + \dot{\boldsymbol{\rho}}_{G_{en}}^\alpha \mathbf{n}^\alpha) = \mathbf{curl}(\dot{\gamma}^\alpha \mathbf{n}^\alpha \mathbf{F}^p) \equiv \dot{\boldsymbol{\Lambda}} \quad (2.93)$$

It determines fully the evolutionary behaviour of each set of GND densities in terms of the gradient of slip rates. Once the values of the individual $\dot{\boldsymbol{\rho}}_{G_i}^\alpha$ are determined, the

rate of change of the corresponding slip resistances can readily be calculated from Eq. 2.63.

2.5.3 Implicit finite element implementation

The determination of the density of GNDs from Eq. 2.93 requires knowledge of the spatial gradients of the plastic deformation gradients, which in turn necessitates knowledge, at any given finite element increment, of non-local plastic deformation. In order to determine this, a user-defined twenty-noded, reduced integration element (UEL), which is alike C3D20R, has been developed within ABAQUS. For the UEL, it is necessary to specify the internal and external force vectors together with the material Jacobian required for the implicit finite element integration. With quadratic interpolation, a typical shape function is of the form

$$n_1 = -\frac{1}{8}(1-\eta)(1-\xi)(1-\zeta)(\eta+\xi+\zeta+2) \quad (2.94)$$

, and the internal force vector is

$$\begin{aligned} \mathbf{f}^{\text{int}} &= \int \mathbf{B}^T \boldsymbol{\sigma} dV = \iiint \mathbf{B}^T \boldsymbol{\sigma} \det(\mathbf{J}) d\eta d\xi d\zeta \\ &\approx \sum_{i=1}^2 \sum_{j=1}^2 \sum_{k=1}^2 H_i H_j H_k \mathbf{B}^T \boldsymbol{\sigma} \det(\mathbf{J}) \end{aligned} \quad (2.95)$$

, where η, ξ and ζ are the element local coordinate directions, $\mathbf{J}$ the Jacobian transformation, H are Gauss integration weighting values and the $\mathbf{B}$ matrix is determined from

$$\boldsymbol{\varepsilon} = \mathbf{B}\mathbf{u} \quad (2.96)$$

, in which $\boldsymbol{\varepsilon}$ is the elemental strain and $\mathbf{u}$ is the nodal displacement. In a implicit scheme, it is necessary to specify a residual $\mathbf{r}$, such that

$$\mathbf{r} = \mathbf{f}^{\text{int}} - \mathbf{f}^{\text{ext}} = \mathbf{0} \quad (2.97)$$

, and Newton iteration is performed until a specified residual tolerance is achieved where the updated displacements, $\mathbf{u}^{n+1}$ are obtained from

$$\mathbf{r} + \frac{\partial \mathbf{r}}{\partial \mathbf{u}} \Delta \mathbf{u} = \mathbf{0} \quad \Delta \mathbf{u} = - \left[\frac{\partial \mathbf{r}}{\partial \mathbf{u}} \right]^{-1} \mathbf{r} \quad \mathbf{u}^{(n+1)} = \mathbf{u}^{(n)} + \Delta \mathbf{u}. \quad (2.98)$$

The finite element Jacobian $\frac{\partial \mathbf{r}}{\partial \mathbf{u}}$ is required which, in the absence of externally applied loading, can be determined as follows. In the implicit scheme, the internal force vector can be written in terms of the elastic-plastic tangent stiffness matrix $\mathbf{C}^{\text{ep}}$ and the stress $\boldsymbol{\sigma}_t$ at the beginning of a given time increment, as

$$\mathbf{f}^{\text{int}} = \int \mathbf{B}^T \boldsymbol{\sigma} dV = \int \mathbf{B}^T [\boldsymbol{\sigma}_t + \mathbf{C}^{\text{ep}} \Delta \boldsymbol{\varepsilon}] dV \quad (2.99)$$

Applying the differential operator to this end using Eq. 2.96 gives

$$\delta \mathbf{f}^{\text{int}} = \int \mathbf{B}^T \delta \boldsymbol{\sigma} dV = \int \mathbf{B}^T [\delta \boldsymbol{\sigma}_t + \mathbf{C}^{\text{ep}} \delta \Delta \boldsymbol{\varepsilon}] dV = \int \mathbf{B}^T \mathbf{C}^{\text{ep}} \mathbf{B} dV \delta \mathbf{u} \quad (2.100)$$

, so that the Jacobian is given by

$$\mathbf{J} = \frac{\partial \mathbf{f}^{\text{int}}}{\partial \mathbf{u}} = \int \mathbf{B}^T \mathbf{C}^{\text{ep}} \mathbf{B} dV. \quad (2.101)$$

Therefore the consistent elastic-plastic tangent stiffness matrix $\mathbf{C}^{\text{ep}}$ is needed to carry on the implicit calculation.

In the implicit scheme, all quantities are written at the end of the time increment, at $t + \Delta t$, unless stated explicitly otherwise, and the stress can be written in terms of a trial stress $\boldsymbol{\sigma}_{\text{tr}}$, and the plastic corrector term, as

$$\boldsymbol{\sigma} = \mathbf{D}\boldsymbol{\varepsilon}^e = \mathbf{D}(\boldsymbol{\varepsilon}_i^e + \Delta\boldsymbol{\varepsilon}^e) = \mathbf{D}(\boldsymbol{\varepsilon}_i^e + \Delta\boldsymbol{\varepsilon}) - \mathbf{D}\Delta\boldsymbol{\varepsilon}^p = \boldsymbol{\sigma}^{\text{tr}} - \mathbf{D}\Delta\boldsymbol{\varepsilon}^p \quad (2.102)$$

, in which $\mathbf{D}$ is the global elastic stiffness matrix determined from the local stiffness $\mathbf{C}$ by

$$\mathbf{D} = \mathbf{T}_\sigma^{-1} \mathbf{C} \mathbf{T}_\varepsilon \quad (2.103)$$

, where $\mathbf{T}_\sigma$ and $\mathbf{T}_\varepsilon$ are the rotation matrices mapping the reference crystal coordinate system into the local one for the particular grain orientation specified. A vector stress residual $\boldsymbol{\psi}$ is defined as

$$\boldsymbol{\psi} = \boldsymbol{\sigma} - \boldsymbol{\sigma}^{\text{tr}} + \mathbf{D}\Delta\boldsymbol{\varepsilon}^p = \mathbf{0} \quad (2.104)$$

, and the differential operator applied to give

$$\delta\boldsymbol{\psi} = \delta\boldsymbol{\sigma} - \delta\boldsymbol{\sigma}^{\text{tr}} + \mathbf{D}\delta\Delta\boldsymbol{\varepsilon}^p = \mathbf{0}. \quad (2.105)$$

Now the differential of the strain tensor increment is

$$\begin{aligned} \delta\Delta\boldsymbol{\varepsilon}^p &= \delta\text{sym}(\mathbf{L}^p)\Delta t = \delta\text{sym}\left(\sum_\alpha \dot{\gamma}^\alpha \mathbf{m}^\alpha \otimes \mathbf{n}^\alpha\right)\Delta t = \\ &\text{sym}\left(\sum_\alpha \dot{\gamma}_0 \exp\left\{-\frac{F_0}{kT}\left[1 - \left(\frac{\tau_R^\alpha - S_0^\alpha \mu / \mu_0}{\hat{\tau}_0 \mu / \mu_0}\right)^p\right]^q\right\}\left(-\frac{F_0}{kT}\right)\right. \\ &\left. q\left[1 - \left(\frac{\tau_R^\alpha - S_0^\alpha \mu / \mu_0}{\hat{\tau}_0 \mu / \mu_0}\right)^p\right]^{q-1}(-1)p\left(\frac{\tau_R^\alpha - S_0^\alpha \mu / \mu_0}{\hat{\tau}_0 \mu / \mu_0}\right)^{p-1}\right. \\ &\left.\frac{1}{\hat{\tau}_0 \mu / \mu_0} \Delta t \mathbf{m}^\alpha \otimes \mathbf{n}^\alpha \delta\tau_R^\alpha\right) = \text{sym}\left(\sum_\alpha Q^\alpha \Delta t \mathbf{m}^\alpha \otimes \mathbf{n}^\alpha \delta\tau_R^\alpha\right) \end{aligned} \quad (2.106)$$

, in which Q is just grouping of the material properties together, and $\delta\tau_R^\alpha$ is given by

$$\delta\tau_R^\alpha = \delta(\boldsymbol{\sigma} \mathbf{n}^\alpha) \cdot \mathbf{m}^\alpha \equiv (\mathbf{n}^\alpha \otimes \mathbf{m}^\alpha) : \delta\boldsymbol{\sigma}. \quad (2.107)$$

Substituting Eq. 2.107 into 2.106 and writing all tensor quantities in Voigt Notation gives

$$\delta \Delta \boldsymbol{\varepsilon}^p = \sum_{\alpha} Q^{\alpha} \Delta t \mathbf{A}^{\alpha} \otimes \mathbf{A}^{\alpha} \delta \boldsymbol{\sigma} = \mathbf{P} \delta \boldsymbol{\sigma} \quad (2.108)$$

, where $\mathbf{A}^{\alpha}$ are slip system-dependant vectors given by

$$\mathbf{A} = (\mathbf{m} \otimes \mathbf{n})_i = \begin{pmatrix} m_1 n_1 & m_2 n_2 & m_3 n_3 & m_1 n_2 + m_2 n_1 & m_2 n_3 + m_3 n_2 & m_3 n_1 + m_1 n_3 \end{pmatrix}^T. \quad (2.109)$$

Substituting Eq. 2.108 into 2.105 gives

$$\delta \boldsymbol{\psi} = \delta \boldsymbol{\sigma} - \delta \boldsymbol{\sigma}^{\text{tr}} + \mathbf{D} \mathbf{P} \delta \boldsymbol{\sigma} = [\mathbf{I} + \mathbf{D} \mathbf{P}] \delta \boldsymbol{\sigma} \quad (2.110)$$

, so that a Newton iterative scheme gives

$$\boldsymbol{\psi} + \frac{\partial \boldsymbol{\psi}}{\partial \boldsymbol{\sigma}} \delta \boldsymbol{\sigma} = [\boldsymbol{\sigma} - \boldsymbol{\sigma}^{\text{tr}} + \mathbf{D} \Delta \boldsymbol{\varepsilon}^p] + [\mathbf{I} + \mathbf{D} \mathbf{P}] \delta \boldsymbol{\sigma} = \mathbf{0} \quad (2.111)$$

, such that the stress can be updated iteratively by

$$\delta \boldsymbol{\sigma} = [\mathbf{I} + \mathbf{D} \mathbf{P}]^{-1} [\boldsymbol{\sigma} - \boldsymbol{\sigma}^{\text{tr}} + \mathbf{D} \Delta \boldsymbol{\varepsilon}^p] \quad \boldsymbol{\sigma}^{(n+1)} = \boldsymbol{\sigma}^{(n)} + \delta \boldsymbol{\sigma} \quad (2.112)$$

Until a specified tolerance on the stress residual is obtained

$$|\boldsymbol{\psi}| = |\boldsymbol{\sigma} - \boldsymbol{\sigma}^{\text{tr}} + \mathbf{D} \Delta \boldsymbol{\varepsilon}^p| \leq \text{tol}(10^{-12}) \text{MPa} \quad (2.113)$$

As mentioned above, it is necessary to determine the consistent tangent stiffness

matrix $\mathbf{C}^{\text{ep}}$ in Eq. 2.101. From Eq. 2.102,

$$\delta \boldsymbol{\sigma} = \delta \boldsymbol{\sigma}^{\text{tr}} - \mathbf{D} \delta \Delta \boldsymbol{\varepsilon}^p. \quad (2.114)$$

For determining the material Jacobian within the increment, the differential operator applied to the trial stress gives

$$\delta \boldsymbol{\sigma}^{\text{tr}} = \delta [\mathbf{D}(\boldsymbol{\sigma}_t + \Delta \boldsymbol{\varepsilon})] = \mathbf{D} \delta \Delta \boldsymbol{\varepsilon} \equiv \mathbf{D} \delta \boldsymbol{\varepsilon} \quad (2.115)$$

, and substituting Eq. 2.108 and 2.115 into 2.114 and re-arranging gives

$$\delta\boldsymbol{\sigma} = [\mathbf{I} + \mathbf{D}\mathbf{P}]^{-1} \mathbf{D}\delta\boldsymbol{\varepsilon} \quad (2.116)$$

, so that the Jacobian, or consistent elastic-plastic tangent stiffness is given by

$$\mathbf{C}^{\text{ep}} = \frac{\partial\boldsymbol{\sigma}}{\partial\boldsymbol{\varepsilon}} = [\mathbf{I} + \mathbf{D}\mathbf{P}]^{-1} \mathbf{D} \quad (2.117)$$

With the consistent elastic-plastic tangent stiffness matrix, the description of the model implementation is almost completed. The one last issue which must be addressed before leaving this section is the calculation of the spatial gradient of plastic deformation. In order to determine $\text{curl}(\dot{\gamma}^\alpha \mathbf{n}^\alpha \mathbf{F}^{\text{p}})$ in Eq. 2.93, the spatial derivatives of the plastic deformation gradient must be obtained. Within a 20-noded, reduced integration element (with 8 Gauss integration points), an internal, 8-noded, linear element is introduced such that its nodes coincide with the Gauss points of the 20-noded element, which is shown in Figure 2.4. With linear shape functions N , for the 8-noded internal element, the spatial derivatives of the plastic deformation gradient can then be determined from

$$\frac{\partial \mathbf{F}^{\text{p}}}{\partial \mathbf{x}} = \frac{\partial (\mathbf{N} \mathbf{F}_i^{\text{p}})}{\partial \mathbf{x}} = \frac{\partial \mathbf{N}}{\partial \mathbf{x}} \mathbf{F}_i^{\text{p}} = \frac{\partial \mathbf{N}}{\partial \boldsymbol{\alpha}} \mathbf{J}^{-1} \mathbf{F}_i^{\text{p}} \quad (2.118)$$

In which $\mathbf{F}_i^{\text{p}}$ are the Gauss point plastic deformation gradients and $\mathbf{J}$ is the appropriate Jacobian transformation mapping from the external to the internal elements.

This algorithm is employed to simulate the elasto-plastic deformation of α phase Ti-6Al-4V in Chapter 7 and pure large grain Ni in Chapter 8.

Chapter 3 Diffraction measurement techniques and interpretation

As explained in Chapter 1, to a large part of the residual stresses measurement carried out in the present project was realized by diffraction methods. In this context, Bragg's Law provides a key relationship between the experimental parameters.

In order to understand each specific diffraction setup utilised, it is important to consider three aspects of the mode used: 1) where the incident beam comes from; 2) how the experimental setup is arranged so that the Bragg condition is satisfied; 3) how the patterns obtained are interpreted so that the sample lattice information is extracted. In this chapter, these three aspects will be addressed in order to illuminate the experimental and interpretation procedures used for residual stress evaluation by diffraction. The focus here is placed on the X-Ray Diffraction (XRD) method, although a very brief introduction is also given to neutron diffraction. Due to their importance for the present study, two kinds of X-ray diffraction setup involving white beam are highlighted in particular: the energy dispersive powder diffraction with multiple peak pattern refinement (using GSAS software), and micro-beam single crystal Laue diffraction with pattern fitting (using XMAS software).

3.1 Generation of synchrotron X-ray and neutron beams

3.1.1 Synchrotron X-ray beams

X-rays are a kind of electromagnetic wave formed by the propagation of mass-less quantum particles called photons. X-rays are produced by excitation and relaxation of atoms that results in the emission of characteristic radiation (e.g. within

an X-ray tube) or whenever charged particles (e.g. electrons) are accelerated or decelerated (e.g. by the process of Bremsstrahlung within an X-ray tube, or due to the application of magnetic field in a synchrotron bending magnet or insertion device). Here, the interest is placed on the latter mechanism employed at synchrotron facilities.

The synchrotron principle of X-ray generation is usually implemented at large multi-purpose laboratories, such as the European Synchrotron Radiation Facility (ESRF, Grenoble, France) and Diamond Light Source (DLS, Oxfordshire, UK). In a typical synchrotron, the electrons are produced by an *electron gun* and accelerated to large energies of a few GeV by *linac* and *booster*. The electrons are then injected into a *storage ring* and continue to travel at almost the speed of light. As they pass areas of high magnetic field (within bending magnets or insertion devices, such as wigglers or undulators), they emit pulses of X-rays with a wide spectrum. Since the process involves loss of energy, additional acceleration is applied to electron bunches within RF (Radio Frequency) cavities, so that the energy of the stored beam is maintained constant. In the conventional regime the storage ring is re-filled typically every 12 hours or so. However, in recent years the method of continuously injecting electrons has been developed, so that now continuous top-up mode is operated routinely without affecting beam stability.

The X-rays emitted into a small horizontal fan are guided to individual *beamlines*, which are branch-outs of the storage ring. A schematic of the synchrotron layout is shown in Figure 3.1.

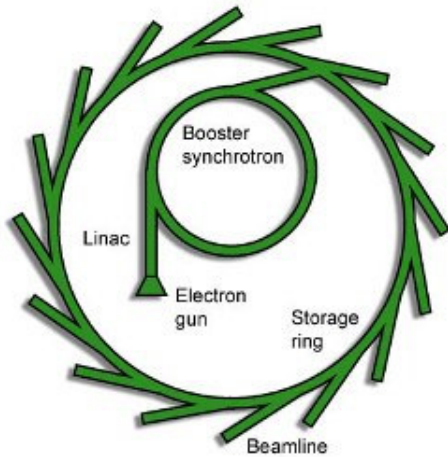


Figure 3.1 Schematic of a typical synchrotron layout [72]

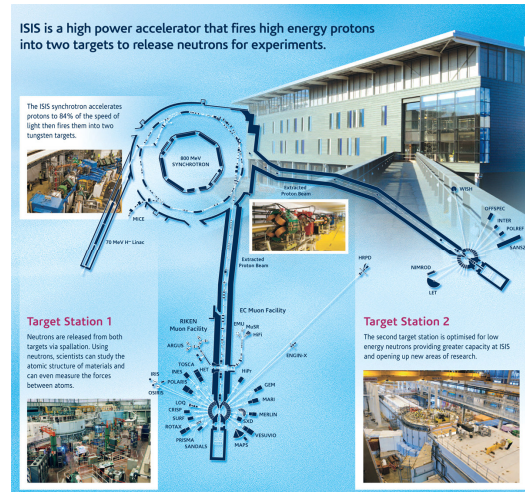


Figure 3.2 Illustration of spallation neutron source ISIS [73]

At the beamline, the X-ray beam that enters through the port is filtered and/or focused by the optical elements such as mirrors and monochromators. They modify the properties of the entering beam to suit the beamline's specification. The character of the beam can be categorised in many ways, e.g. by the energy range (high/low/medium, and monochromatic, pink, or white), divergence (focused or unfocused), polarization, time structure, etc.

3.1.2 Neutron beams

Neutron is a subatomic particle which has no net electric charge but large rest mass in comparison with the photon. The nature of neutrons provides a distinct advantage over X-rays: they do not interact with the electron clouds, and their interaction with the nucleus of an atom is relatively weak, but not negligible. As a consequence, neutron beams form a highly penetrating and non-destructive probe. This allows the investigation of the interior of materials rather than the surface layers without damaging the samples, including complex and delicate biological or polymeric systems.

Due to their fundamentally different nature, neutrons can not be produced in the same way as X-rays. There are two principal types of neutron sources: fission reactors and spallation sources. A reactor neutron source relies on the fission chain reaction, which is initiated, controlled, and sustained at a steady rate, to generate neutron flux. A spallation neutron source requires a high energy proton beam, usually produced by a synchrotron, which bombards a metal target and generates neutrons by the process known as nuclear spallation (Figure 3.2). The neutrons produced by spallation have a distribution of energies that is further affected by passing the beam through a moderator that “cleans up” the spectrum. Since neutrons have mass, their energy is related to speed, so that if neutrons of different energies start their travel at the same instant, they arrive at the experimental hutch and ultimately at the detector after different time delays. The neutron time-of-flight (TOF) is inversely related to their speed and linearly proportional to the wavelength of the de Broglie wave:

$$\lambda = \frac{h}{mv} = \frac{h}{mL} \text{TOF}, \quad (3.1)$$

where h is Planck’s constant, m is the neutron rest mass, and L is the flight length. It follows that a suitably accurate time-resolving detector can register neutron diffraction patterns in the form of intensity (counts) vs. time. Using the above relationship, the diffraction pattern can then be converted to intensity vs. wavelength, or lattice spacing. The systematic interpretation of neutron diffraction patterns proceeds in the same way as the conventional synchrotron X-ray diffraction. Since neutron diffraction experimental details lie beyond the scope of the current study, they are omitted from further discussion. It is worth noting that both polychromatic and monochromatic neutron beams can be obtained and utilised. The interpretation of neutron measurements used in the present study was carried out using beamline

software that was user-friendly and relatively easy to understand. The interpretation procedures will not be discussed here in any more detail. Further information concerning neutron measurement experiments and results are given in the corresponding chapters.

3.2 Diffraction Modes

Based on the character of the beam (monochromatic or polychromatic) and the sample (single or polycrystal), the diffraction setups can be categorized into four different modes: θ - 2θ scanning mode; energy dispersive powder mode; reciprocal space mapping mode and white beam, single crystal Laue mode. Note has to be taken that single or polycrystalline setup does not necessarily signify the entire sample under investigation, but rather the portion of the sample occupying the X-ray gauge volume formed by the intersection of the incident and diffracted beams. For example, in micro-beam Laue setup, the sample used in the present study was a dog-bone shaped pure Ni polycrystal. However, the ability of focusing the beam to reduce the gauge volume down to (sub)micron level allows the X-ray beam to interact with a single grain within the polycrystal, so that the corresponding diffraction mode is single crystal polychromatic Laue diffraction.

Below, a brief introduction is given to all the experimental modes and their applications used in the present study. A special focus is placed on the interpretation procedure for two particular modes: the energy dispersive whole pattern powder refinement for elastic strain measurement, and (micro-beam) single crystal Laue diffraction pattern indexation for the determination of grain orientation and deformation structure analysis.

1) In the single crystal monochromatic setup, the diffraction condition requires both

the crystal and a point detector to be set at precise angles for the reflection to be measured. Sample tilting within the diffraction plane allows the rocking curve to be determined (the variation of scattered intensity with sample mis-orientation with respect to the Bragg condition). This method is capable of providing very high resolution maps of the details of the reciprocal space around individual reflections. However, sample rotation causes gauge volume variation, and sample alignment becomes progressively challenging for very small beams. The measurements themselves are also time intensive, since tilting around two angles is required for the collection of 2-D reciprocal space maps.

- 2) In the single crystal polychromatic (Laue) setup, a white beam is used to illuminate the sample. A film or an area detector spanning a certain solid angle can be placed at the nominal 2θ angles of 0° , 90° or 180° and used to collect the diffraction pattern consisting of point peaks. The method allows very fast measurements and does not require sample tilting. However, since no resolution in energy is available, in the pure Laue setup the radial dimension in the reciprocal space can not be probed.
- 3) In the polycrystal monochromatic setup, the key assumption is that each scattering volume contains a large number (> 2500) of crystallites, such that there are always some of the crystallites to satisfy the diffraction condition for any given orientation of the sample. A point detector counting photons is then scanned in 2θ to collect a pattern of counts versus angle corresponding to a section through the so-called Debye-Scherrer cones. The method provides excellent diffraction profiles with little instrumental broadening contribution particularly suitable for line profile analysis; although the data collection is relatively slow due to the lower flux of the monochromated beam.

- 4) In the polycrystal polychromatic setup, a white beam with a smooth energy spectrum is used to illuminate the sample. The energy dispersive point detector is mounted at a fixed 2θ angle to collect the pattern of counts versus energy. This method is characterised by larger instrumental broadening contribution due to the resolution of the solid state detector. However, very quick measurements of lattice cell parameters are possible, making the technique ideal for fast elastic strain measurement or mapping.

3.3 Pawley pattern refinement of energy dispersive diffraction data (GSAS)

For each diffraction peak, the profile can usually be fitted by Gaussian or pseudo-Voigt peak functions, allowing the peak position, amplitude and width (Full Width Half Maximum, FWHM) to be obtained. The single peak fitting routine analyzes the individual hkl reflections to extract the elastic lattice strain value corresponding to diffraction from a particular set of lattice planes sharing common indices and orientation in the laboratory coordinate system. However, the utility of single peak strain determination may be limited when using it to interpret the macroscopic strain, as the inhomogeneity of elasto-plastic deformation between grains may cause individual peak strain to be different from the macroscopic average [74]. In this case, whole pattern refinement is preferred, as it has been shown to provide a better correlation with the macroscopic average elastic strain [75].

Rietveld refinement [76] is the first of example of interpretation of this kind. Given a known crystal structure, the positions of the observed lattice reflections can be predicted. They are then refined (i.e. adjusted in accordance with small lattice distortions until best fit is achieved). This is the Rietveld refinement method. Pawley

refinement is a similar approach, but with the merit that it accommodates the variation in peak intensities by allowing the intensity of individual reflections to change freely, while the peak positions are determined in the usual manner from the unit cell dimensions. This approach provides an empirical average of the different reflections and potentially includes physics that describes the overall deformation of the polycrystal.

The General Structure Analysis System (GSAS) [77] is a powerful tool for powder diffraction analysis. It incorporates Rietveld and Pawley refinement procedures and is capable of performing full-pattern refinement for angle dispersive, time-of-flight neutron and white beam (energy dispersive) data. The GSAS software only requires the instrument parameter and measurement data files (in standard GSAS format) as the input, and outputs the least-square-fitted grain-group average lattice parameters. Here, a brief introduction to the GSAS algorithm for energy dispersive analysis is presented to clarify the refinement procedure that it employs. Firstly, the peak profile is assumed to be given by the Gaussian function:

$$I(\Delta T) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{\Delta T^2}{2\sigma^2}\right], \quad (3.3)$$

where $\sigma^2 = AT^2 + BT + C$, and T is the X-ray photon energy in KeV.

$$\Delta T = (T - T_{\text{ph}}) - [\varepsilon_a d \cos \phi + \varepsilon_A \frac{(hk)^2 + (hl)^2 + (kl)^2}{h^2 + k^2 + l^2}]T. \quad (3.4)$$

Here, T_{ph} is the peak center position (in terms of energy) defined by Bragg's Law:

$$T_{\text{ph}} = hc / 2d \sin \theta. \quad (3.5)$$

In Eq. 3.4, ϕ is the angle between the hkl plane normal and the c axis. Hence, there are five coefficients to be refined in GSAS: A , B , C , $\mathcal{E}_a$ and $\mathcal{E}_A$.

The relationship between the d -spacing and lattice parameters is represented by

$$1/d^2 = \mathbf{hgh}^T \quad (3.6)$$

, while $\mathbf{h} = (h, k, l)$ and $\mathbf{g}$ is the reciprocal metric tensor:

$$\mathbf{g} = \begin{pmatrix} a^{*2} & a^*b^* \cos \gamma^* & a^*c^* \cos \beta^* \\ a^*b^* \cos \gamma^* & b^{*2} & b^*c^* \cos \alpha^* \\ a^*c^* \cos \beta^* & b^*c^* \cos \alpha^* & c^{*2} \end{pmatrix}. \quad (3.7)$$

Equation 3.6 and 3.7 can be found in most crystallography books. The quality of structural analysis is characterized by the residuals R defined as

$$R_p = \sum |I_o - I_c| / \sum I_o, \quad (3.8)$$

and

$$R_{wp} = \sqrt{\sum w(I_o - I_c)^2 / \sum wI_o^2}, \quad (3.9)$$

where I_o and I_c are the observed and calculated intensities respectively. The weighing factor w is given by $w = 1/\sigma^2$, where σ is the estimated statistical error for the intensity. Figure 3.3 and Figure 3.4 show examples of refinement result from the diffraction data of the silicon powder and Ti-6Al-4V alloy samples respectively.

The data refinement operation with GSAS is fairly straight-forward. It requires only two major steps before the lattice parameters can be outputted. The first step is the calibration of the detector, or the determination of the Channel-to-Energy

conversion. When an X-ray photon arrives at the energy dispersive solid state detector, it creates a number of electron-hole pairs. This number controls the pulse height in the amplifier, and is found to be proportional to the photon energy. The multi-channel analyzer (MCA) in the detector discriminates the pulse height and puts the pulses into different channels (performs “binning”). The detector output data is presented in the form of intensity vs. channel histogram. It is crucial to calibrate the Channel-to-Energy conversion coefficients before attempting the full pattern refinement: the relationship is only approximately linear. Although this can be obtained from the detector manufacturer-, more precise calibration is needed, since small deviations may lead to large strain error. The channel number n to energy E conversion is assumed to be quadratic:

$$E = A + Bn + Cn^2. \quad (3.10)$$

The way to determine A , B and C is to take a diffraction pattern from a standard material, normally silicon powder, and compare it with the prediction (without changing the lattice parameter). By altering the values of A, B, C and finding the minimum of the fitting error, their best values can be obtained. Figure 3.3 shows the GSAS refinement pattern of Si powder data using the quadratic Channel-to-Energy conversion.

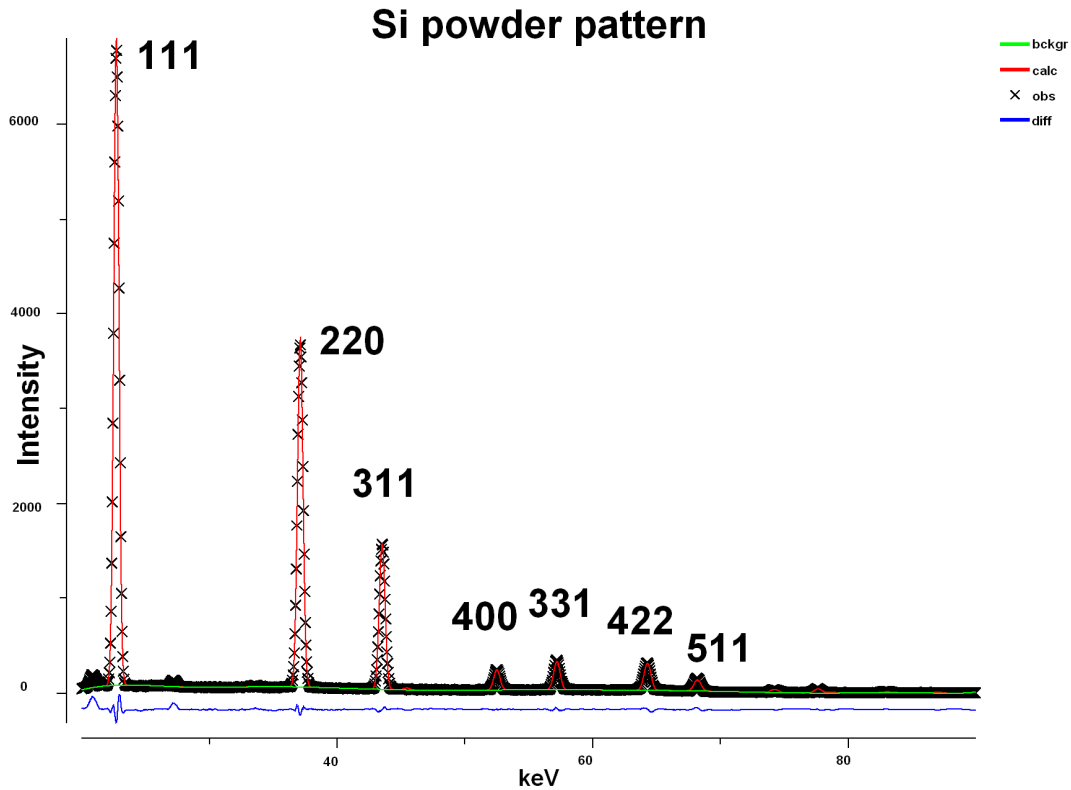


Figure 3.3 Pattern of Si powder data using the quadratic channel-to-energy conversion

The second step of GSAS data interpretation is the full pattern refinement of strained samples. This is carried out in the batch mode, since strain measurements are made not at one point, but along a line, over an area or in a volume. In this case, a typical or representative data file is selected for initial refinement using manual GSAS fitting, with the procedure similar to that for the silicon powder refinement. Importantly, the “refine cell” function in the program must be selected, indicating that the lattice parameters are varied to seek for the best fit values. The Channel-to-Energy conversion coefficients, on the contrary, are fixed to the values found in the calibration step.

Once a “template” data file is obtained in this way, the remaining data points are interpreted using a batch analysis Matlab routine, which uses variables from the template refinement, and calls GSAS repeatedly to perform lattice parameter refinement; then stores the results in an output file. Figure 3.4 shows the GSAS

refinement result for a Ti-6Al-4V dog-bone sample.

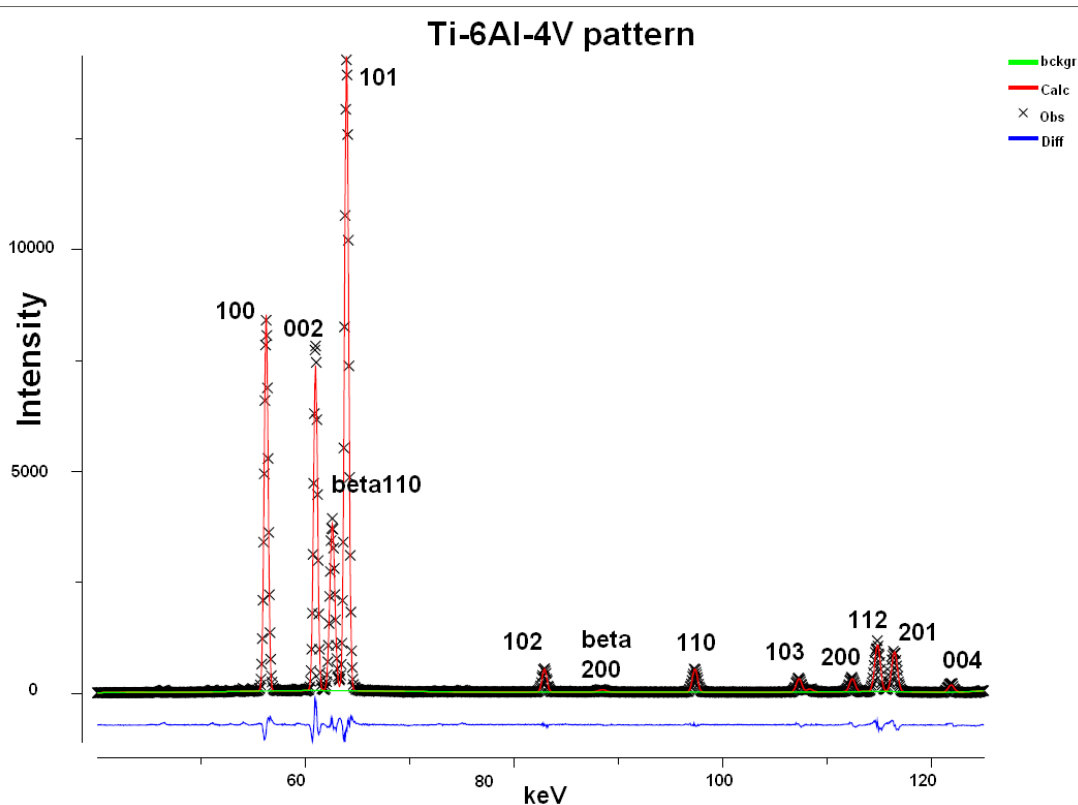


Figure 3.4 Pattern of Ti-6Al-4V data using batch refinement

In Chapter 7, the GSAS refinement procedure described here is employed to analyse the *in situ* loading data for a Ti-6Al-4V alloy dog-bone shaped sample. The details about the residual strain results and interpretation can be found in that Chapter.

3.4 Micro beam Laue diffraction and XMAS interpretation for grain orientations

Micro-beam Laue is a technique developed in recent years allowing probing the crystal structure and deformation at the meso- to micro-scale. Its principle is similar to the classical Laue diffraction, except that in micro-beam Laue small beamsizes are used (from a few microns down to sub-micron). In micro-beam Laue diffraction, a small polychromatic beam illuminates a single crystal (grain) within the sample, and the scattered beams fall on a high resolution CCD area detector to form the Laue diffraction spot pattern. Figure 3.5 shows a Laue diffraction pattern from a

Si single crystal wafer.

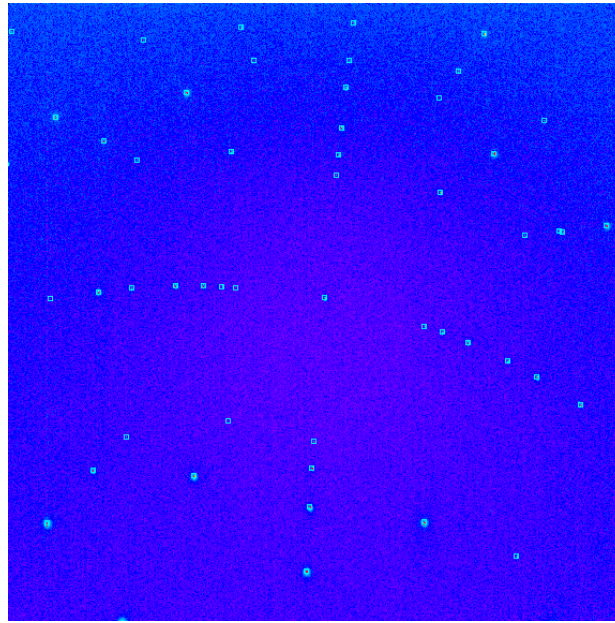


Figure 3.5 Laue diffraction pattern from a Si single crystal wafer

From the collected patterns, lattice orientation and deviatoric elastic strain of the crystal can be determined.

There are two conventional Laue setups: back-reflection Laue, and transmission Laue. Illustrations of these setups are shown in Figure 3.6& 3.7

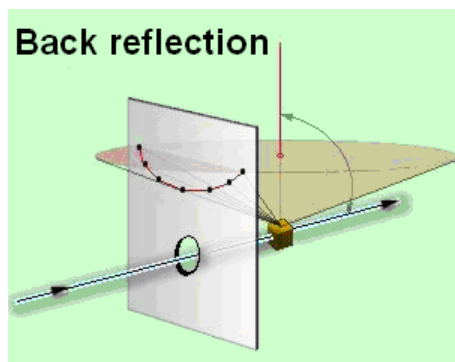


Figure 3.6 Back reflection Laue setup [78]

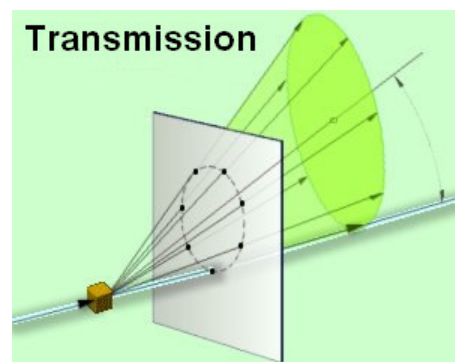


Figure 3.7 Transmission Laue setup [78]

In the back-reflection method, the 2D detector is placed between the x-ray source and the crystal. The beams which are diffracted in a backward direction are recorded. In the transmission Laue method, the detector is placed behind the crystal to record beams which are transmitted through the crystal.

Based on the geometries of different setups, the indexation of Laue spots can be carried out. The indexation procedure starts with computing the 2θ position and the

Bragg plane normal for each reflection. Then a list of possible indexes is assigned to each reflection based on the range of energies contained within the incoming white beam. Next, a search is performed for reflection pairs coming from the same grain. Once a pair is successfully found, other reflections for this given grain are predicted. If a match is found between the prediction and the collected Laue spots for several other reflections, they are assigned to the grain under consideration and labelled with corresponding indexes. Once all the reflections in the pattern have been indexed, a search is performed for the remaining reflections in the pattern, as a means of identifying the reflections belonging to another grain. This loop of search-and-find is carried on until as many as possible Laue spots have been indexed.

The found grain orientation(s) are expressed in the form of the rotation matrix. The above indexation routine has been implemented in XMAS (X-ray Micro-diffraction Analysis Software) by Tamura et al. [79]. The availability of this software offers the capability of automated Laue diffraction analysis for large numbers of Laue patterns.

For successful XMAS analysis of Laue patterns, two calibration steps need to be carried out before the collection of patterns from the real samples. First, the detector to diffracting volume (detector-to-sample) distance must be calibrated via the triangulation method. The detector is moved towards or away from the sample so that the Laue spot pairs have different inter-spot distances at different detector-to-sample positions. When the travel distance for the detector is known, the sample-to-detector distance then can be determined. Then, the detector misorientation angles (pitch, roll, and yaw) as well as the detector centre position can be refined by measuring Laue reflections from a known crystal with negligible strain. Single crystal silicon is used for this purpose.

Figure 3.5 shows a Laue pattern from a Si single crystal wafer. Once the calibration steps are successfully finished, grain orientation analysis can be carried out on real experiment samples. In Chapter 8, the micro-beam Laue technique and XMAS are used to analyse the deformation of a large grained pure Ni sample. Details about the experimental and simulation results can be found in that Chapter.

Chapter 4 1-D macroscopic analysis of a residual stress state: Al/SiCp bent bars

4.1 Introduction

The initial state and subsequent evolution of residual stress and strain during service life of engineering components are critically important for reliable performance and structural integrity. The need for the knowledge and control of residual strains is especially acute for safety critical components in the aerospace and automotive industries. Performance optimisation in these applications is frequently associated with weight reduction that naturally leads to increased service stresses under applied loads. On many occasions it has been demonstrated that the introduction of compressive residual stresses of sufficient magnitude and durability at key locations within components can result in significant fatigue life extension.

Metal matrix composites form a class of attractive light-weight, high stiffness and strength materials often built on the base of light metallic alloys, such as aluminium or titanium. The incorporation of stiff and hard (usually ceramic) reinforcement in the form of fibres or particles leads to a significant increase in the overall elastic modulus. Strength is also improved due to a variety of mechanisms, including grain refinement, creation of additional obstacles to dislocation movement, etc. However, one of the challenges to the application of metal matrix composites often encountered in practice is their relatively low resistance to fatigue crack initiation and propagation.

Residual stresses in metal matrix composites exist on a variety of scales, from microscopic (at the characteristic length scale of alloy crystallites and diameters of

particles or fibres, to macroscopic, associated with the overall deformation or thermal history of the entire sample or component [80, 81]. Thorough understanding of these stresses is required in order to modify and control them by deformation and thermal processing, and to be able to predict their evolution in service. To achieve this goal, the combination of theoretical and numerical models and experimental measurement techniques is needed.

In this chapter, eigenstrain theory has been used in several different ways in order to model the observed (measured by high energy synchrotron diffraction) and predict the expected variation of residual stresses due to machining. Inverse eigenstrain theory [63] then has been used in combination with the strain gauge record obtained during electric discharge machining (EDM) of a slot in the bent composite bars. Although the experimental configuration was similar to that of Cheng et al. [82], it is the author's belief that the inverse eigenstrain interpretation methodology used possesses a much broader range of applicability, and can be applied to a variety of other more complex sample shapes and sectioning procedures.

4.2 Experiment

The material used in the experiment had the manufacturer's denomination AMC225xe and was a particulate composite based on the matrix of aluminium alloy AA2124, with the nominal composition (in wt %) Cu – 3.8, Mn – 0.5, Mg – 1.4, Zn < 0.25, Al balance. Reinforcement consisted of fine (<3 μ m) particles of SiC. The metal matrix composite shows a good combination of mechanical properties, e.g. stiffness ($E_{Al} = 72$ GPa, $E_{SiC} = 450$ GPa, $E_{comp} = 115$ GPa) and strength (composite yield stress of 480 MPa, UTS of 650 MPa) without an appreciable change in density ($\rho_{Al} = 2.77\text{g}\cdot\text{cm}^{-3}$, $\rho_{SiC} = 3.2\text{ g}\cdot\text{cm}^{-3}$). Square cross-section bars of dimensions 10×10×55

mm³ were machined from the billet, and then 4 point (A, B, C and D in Figure 4.1a) bending was applied to the sample with Maximum applied moment of 125 N·m. The resulting lateral force and bending moment distribution in the bar were plotted in Figure 4.1a. This level of bending moment caused partial plastic deformation along the central cross section PQ (partial plastic deformation indicates plastic deformation near both ends P and Q, but no plasticity in the middle), which left residual curvature in the bar after unloading. Figure 4.1b gave the illustration of the bentbar sample and theoretical residual strain (x-axis) distribution along the central cross section PQ. It is worth noting that this distribution remains unchanged along any vertical line between B and C due to the constant bending moment, and in the current study, focus will be placed only on this section as well. The residual strain distribution in AB or CD section would not affect the result obtained from PQ either in X-Ray diffraction or slitting method, hence omitted.

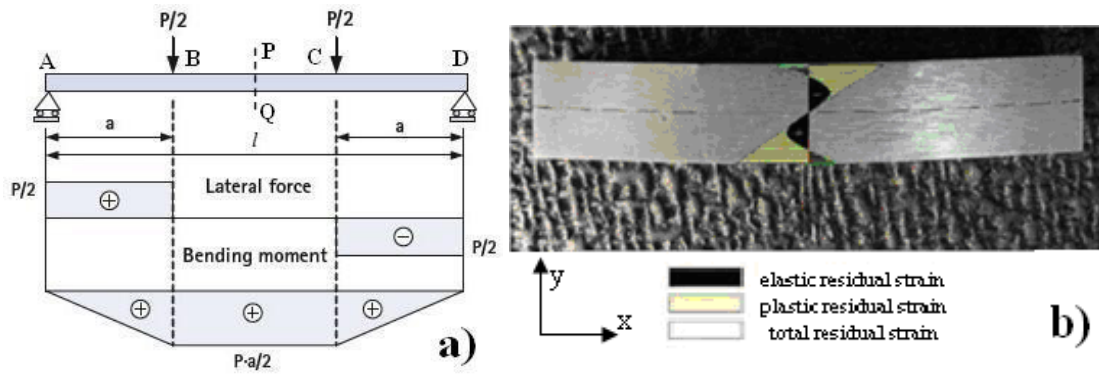


Figure 4.1 (a) Schematic of 4-point bending (b) Illustration of the bentbar sample and residual strain distribution along the middle cross section

Synchrotron X-ray diffraction was performed to deduce the residual stress profile in the central section of the bar. The specimens were then subjected to incremental slitting using wire EDM (electric discharge machining) with continuous strain gauge monitoring. EDM parameters chosen were: wire spool speed of 150mm min⁻¹ and potential difference of 100V. Since wires of 0.1mm were liable to breaking, copper wire of 0.25mm diameter was used in the final experimental setup,

producing a slot of 0.4mm width. Slow cutting advance rate (feed) of about $20\mu\text{m min}^{-1}$ was deliberately chosen to minimize damage and ensure the collection of sufficient number of data points by the data-logging system. The complete slitting experiment lasted 8 hours; giving about 300 data points for each strain gauge mounted on the front (entry) and back faces of the sample. Afterwards, the X-ray diffraction and incremental slitting results were analyzed using the direct and inverse eigenstrain methods mentioned above.

4.3 Eigenstrain modelling analysis

In order to use the eigenstrain method to analyze the experimental data, a 2-D beam model was set up with the geometry identical to that is used in the experiment. The model was pinned at a single point on the bottom face of the sample to avoid numerical instability and eigenstrain was introduced using anisotropic thermal expansion to mimic the permanent plastic strain (Figure 4.2).

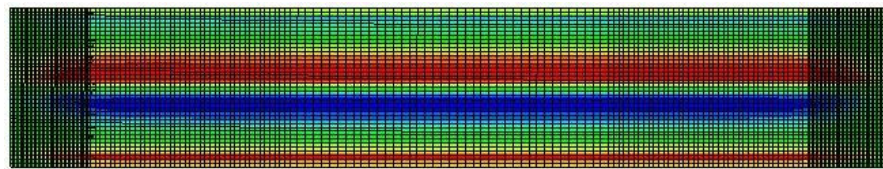


Figure 4.2 Illustration of the finite element mesh used in the inverse eigenstrain analysis, and the residual elastic strain distribution created by eigenstrain using the pseudo-thermal expansion method.

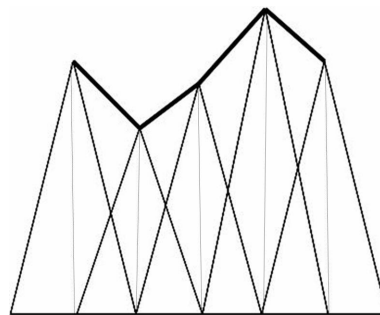


Figure 4.3 Illustration of the representation of an unknown eigenstrain distribution (bold lines) by the superposition of triangular basis functions (thin solid lines) at equally distributed positions spanning the beam cross-section.

The unknown eigenstrain distribution was represented using the linear superposition of overlapping triangular pulse basis functions, illustrated in Figure 4.3 (triangular pulse, or “tent” functions). Although inelastic strains are introduced into the model, it is important to note that the superposition principle still applies, as in any thermo-elastic problem. Therefore, the resulting residual stresses and residual elastic strains are given by the sum, with appropriate coefficients, of the readily obtainable by FE individual solutions for each basis function.

Figure 4.4 shows the comparison between experimentally determined equivalent macroscopic residual elastic strain profile and the eigenstrain-based reconstruction. It is apparent that the inverse eigenstrain-based procedure captures well the general trend of the residual elastic strain (r.e.s.) distribution.

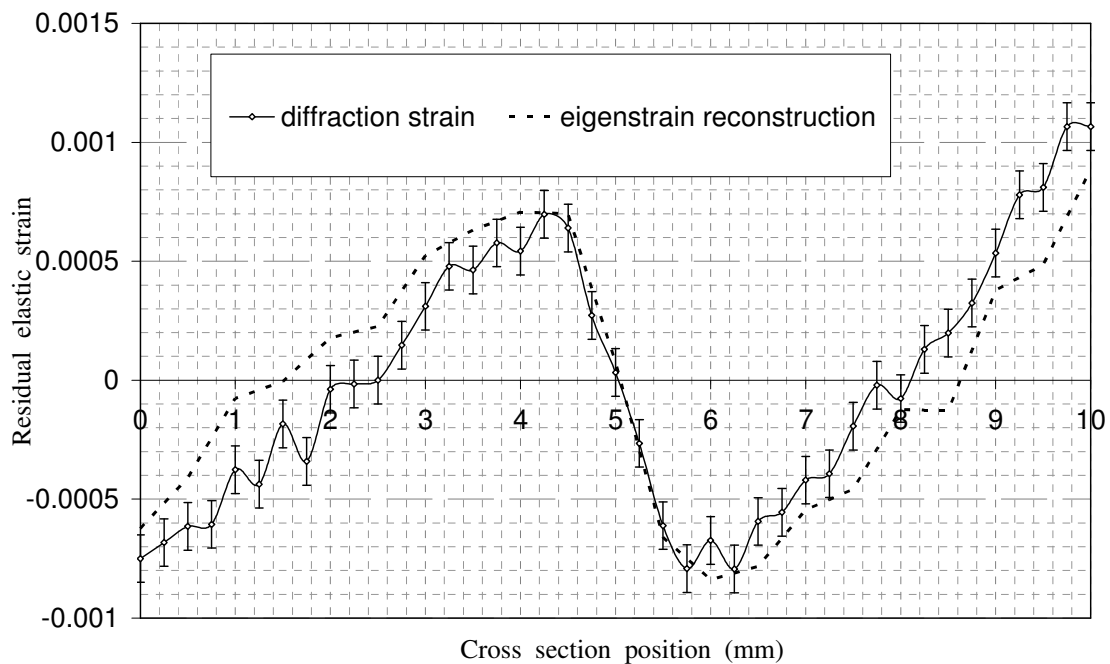


Figure 4.4 Diffraction-based equivalent macroscopic average residual elastic strains (markers) and their eigenstrain-based reconstruction using triangular pulse functions (dashed curve).

Eigenstrain-based modelling was next used for further study of the EDM slitting experiment. Modelling this experiment required simulating the procedure of material removal within the FE framework. This was achieved by deactivating selected elements within the model. This causes the modification of the strain

distribution in the bar, leading to the surface strain changes that are monitored by the strain gauges experimentally. The size of deactivated elements was carefully chosen to match the slitting width and depth increments considered. Figure 4.5 illustrates the slitting procedure within the model for depths of 2.5mm and 5mm, respectively.

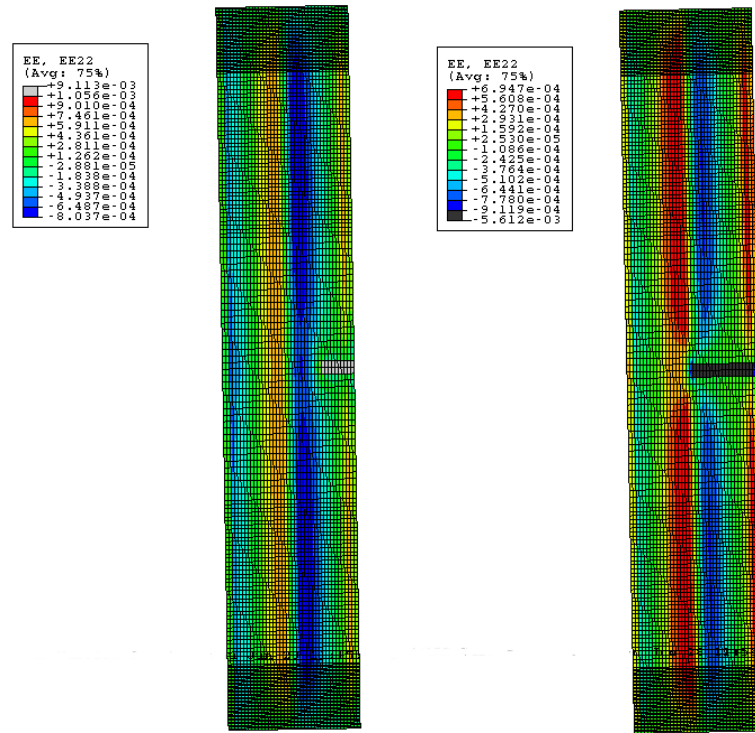


Figure 4.5 FE simulations of EDM slitting, showing the residual strain re-distribution caused by the process (2.5mm and 5mm deep slits are shown on the left and right respectively).

The model was set up to incorporate the eigenstrain distribution deduced from the inverse analysis of diffraction data. The slitting simulation was then run successively for different cut-in depths, and strain changes were extracted at the locations corresponding to the strain gauges used. The predictions were compared with the experimental results (Figure 4.6). It is apparent that in this case very good agreement was obtained between the slitting model predictions and the experimental data from strain gauges mounted on the front face (cut-in surface) and back face.

Of course, in a typical EDM slitting experiment the strain distribution along the cross section is unknown a priori. In other words, a way to deduce the underlying

eigenstrain profile (and with it the residual strain and stress distribution) from the results of the slitting experiments is needed.

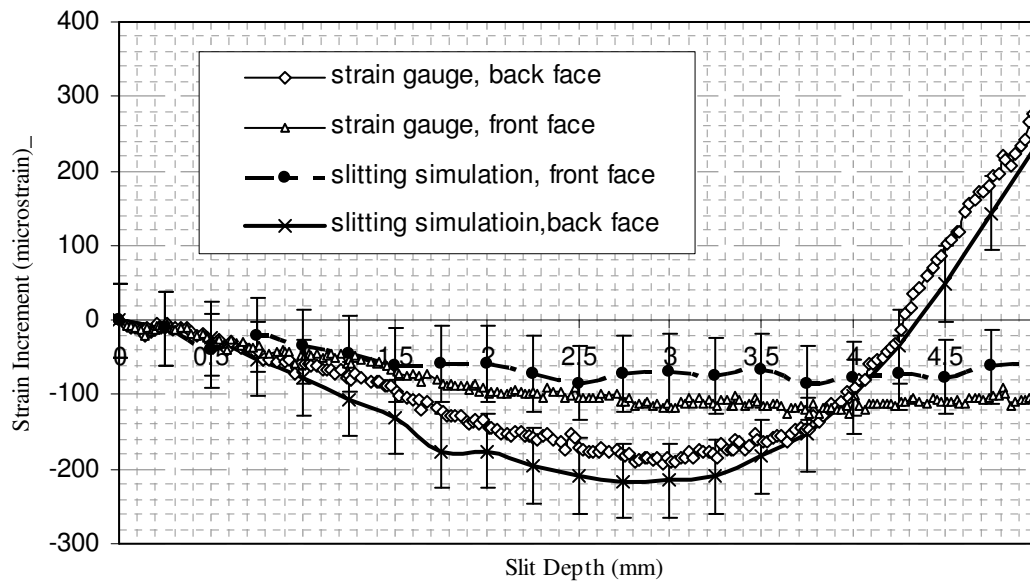


Figure 4.6 Comparison of strain increments at sample surfaces measured experimentally by strain gauges during the EDM slitting experiment (markers) with slitting simulation predictions made using diffraction-based eigenstrain distribution.

Noting from Figure 4.6 that the front face strain gauge shows relatively little sensitivity to the cut-in depth beyond the first 1.5mm of slitting, it was concluded that the front face strain gauge was unlikely to provide useful input to the procedure. The attention was therefore focused on the signal recorded by the back face strain gauge. This was used to develop an inverse eigenstrain problem formulation and solution procedure. A simple approximation chosen was to introduce two independent linearly varying functions to represent the inelastic strain distributions within the compressive and tensile plastic zones, respectively. In order to obtain the best values of the unknown parameters, the least squares method was again employed. Figure 4.7 shows that excellent agreement was achieved in this way between the slitting-based eigenstrain model prediction and the back face strain gauge signal recorded during the EDM slitting experiment.

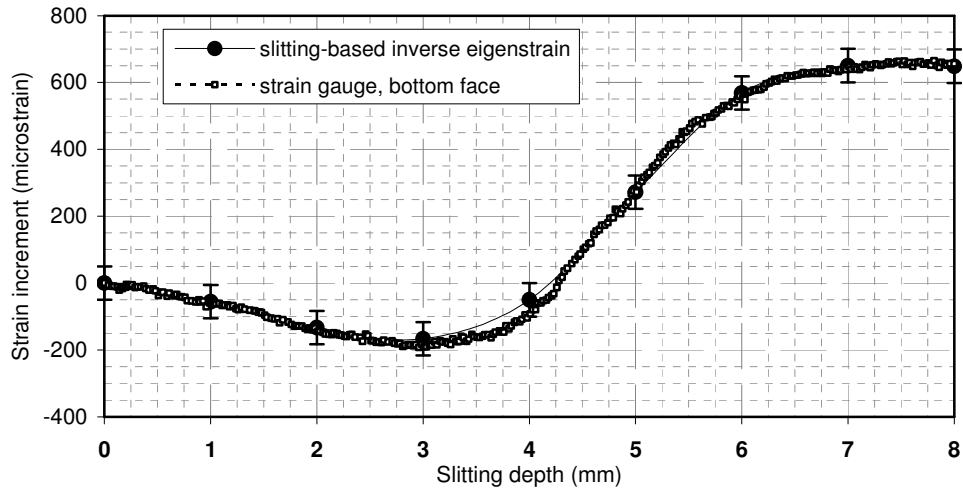


Figure 4.7 Comparison of strain increments at sample surfaces measured by strain gauges during the EDM slitting experiment (markers) with slitting-based simulation predictions.

Figure 4.8 shows the comparison between the residual elastic strain profile deduced from the slitting-based inverse eigenstrain analysis (dashed lines) and the profile deduced from the analysis of high energy synchrotron X-ray diffraction data. It is apparent that although the general trends of both two plots are the same, some degree of discrepancy persists between the results obtained by these two techniques.

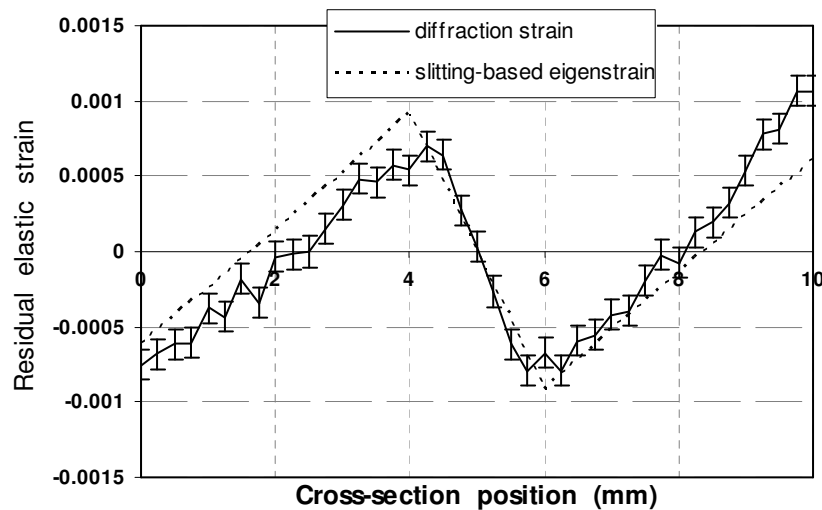


Figure 4.8 The prediction of the slitting-based inverse eigenstrain procedure (continuous curve and large solid circles) vs. back face strain gauge readings measured experimentally during EDM slitting.

The following conclusions can be drawn from the results presented in this

Chapter:

- (a) The framework presented for the solution of eigenstrain inverse problems appears to be both efficient and robust. The sum-of-squares measure of the mismatch between model and experiment provides a good means of problem regularisation, and ensures existence and uniqueness of approximate solutions.
- (b) The discretised version of the eigenstrain basis functions provides excellent flexibility and should be extended to higher dimensions.
- (c) Further regularisation may be required in order to treat such problems like, e.g, incremental slitting.

Chapter 5 2-D macroscopic residual stress state: inverse eigenstrain analysis of worn railway rail head

5.1 Introduction

One of the challenges for the development of eigenstrain-based approaches to residual stress analysis is that the information about eigenstrain distributions is not always readily accessible in practice. For most cases, it is the residual elastic strains, or increments of the total strains, that can be measured directly via various destructive and non-destructive experimental techniques [5]. Therefore, the inverse problem of eigenstrain analysis becomes the key step towards understanding and quantifying the RS sources, that is, using a known residual elastic strain (or total strain increment) information to retrieve the underlying eigenstrain field.

A range of inverse eigenstrain studies have been carried out in recent years. They can be categorized conveniently by their dimensionality. Note, however, that this requires careful specification of the aspect of the problem being referred to: the dimension of the numerical (FE) model; the dimension of the eigenstrain (components) being reconstructed; and finally, the dimension of the spatial variation of eigenstrain that is being considered. In previous studies reported in the literature, the dimension of the simulation was either 2D or 3D, with various shapes considered [63, 83]. Multiple components of eigenstrain were also considered [84, 85]. However, their spatial variations have been mostly limited to 1D (i.e. representable as a line plot). So far, no fully two-dimensional discrete inverse eigenstrain analysis has been carried out (meaning simultaneously 2D sample geometry, 2D eigenstrain components and 2D eigenstrain variation). In real engineering components the

residual stress distribution variation is always multi-axial. Therefore, it is necessary to develop a novel method capable of dealing with the multi-dimensionality of the strain variation.

5.2 Methodology – the ‘tent’ base function

In previous chapter the situation was considered when the mechanical model was 2D, but only 1D strain variation was allowed. Then, the base function was selected in the form of an equilateral triangle corresponding to a localised ramp up and down, or a triangular “pulse”. By generalising this idea to the 2D case, it is natural to propose a base function in the form of a pyramidal “pulse” above a triangular element (Figure 5.1). Due to the shape that arises above the plane, we propose to call it the “tent” function. Figure 5.1 illustrates two pulses defined by point 5 (directly above point 1 in the plane) and point 6 (directly above point 3 in the plane). Together with the parallelogram 1234, these points form two base “tents”, 5-1234 and 6-3412, respectively. Note that the sum of them gives rise to a generalised “tent” (note the dashed line), and provides an illustration of the piecewise linear 2D approximation to an arbitrary surface above the 2D plane.

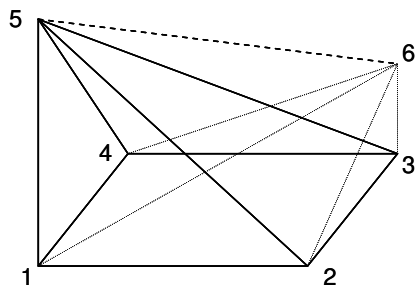


Figure 5.1 Illustration of two tent functions.

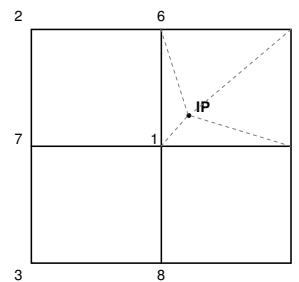


Figure 5.2 Experimental data grid points (numbered) and the interpolation of data to IP point P.

5.3 Modelling technique

The 2D eigenstrain distribution must be simulated by the linear superposition of 2D base functions, e.g. of the “tent” type described above. Obtaining the set of base function solutions for residual elastic strains requires a large number of computational runs for the generation of base-solutions. For efficient implementation, the computational process must be fully automated. In other words, once the configuration is specified, the multiple simulations must run automatically without manual input, with all the data needed for subsequent analysis being automatically stored and prepared for the optimization step.

In order to clarify the data flow within the simulation, here we introduce three different types of grids (information layers): the experimental data grid, the FE mesh grid and the “tent” grid. At the discretisation level, the integration point (IP) of the FE mesh appears to be the best choice for data localisation, since it allows smooth communication and connection between different information layers (experimental, Finite Element, and “tent”). This also means that FE mesh IP points can be chosen as collocation points, i.e. the positions over which the summation is taken in equation 2.35 for the calculation of the sum-of-squares measure J . For the residual elastic strain experimental data set, the grid is determined by the choice of experimental gauge volumes. Due to the nature of the scan (the use of mutually orthogonal linear stages for sample positioning), the experimental grid is likely to be regular and rectangular, resembling the regular mesh arising from the use of CPS4 elements (Figure 5.2 & 5.3). This observation means that the experimental data can be readily interpolated to FE mesh IP points with the help of the CPS4 shape functions. The implementation of this procedure is illustrated in Figure 5.2, where the numbered points represent the experimental data grid, and point **P** indicates the FE IP point.

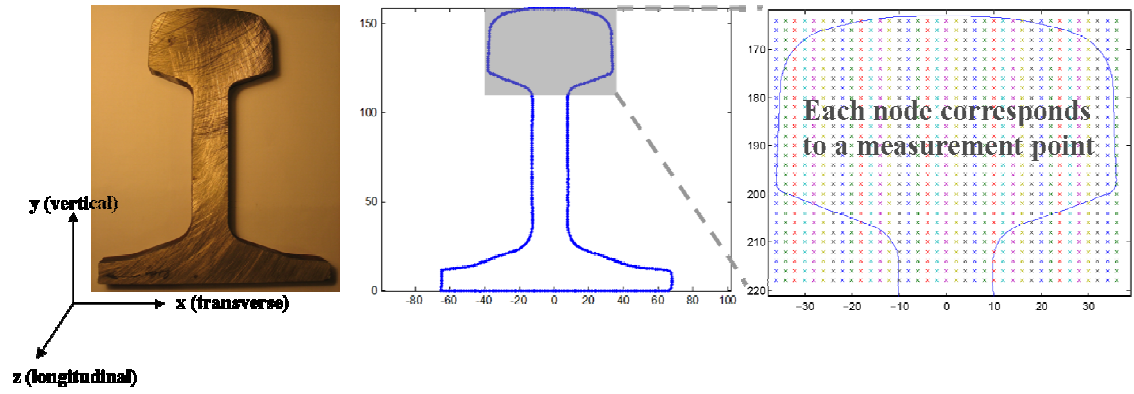


Figure 5.3 Image of the rail head sample, its contour obtained by CMM analysis, and the experimental data grid. Each point corresponds to the centre of the gauge volume used for neutron diffraction strain measurement.

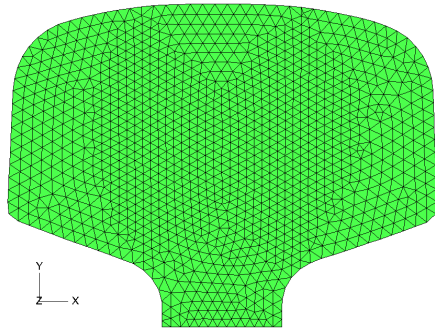


Figure 5.4 Illustration of a typical FE mesh used for simulation.

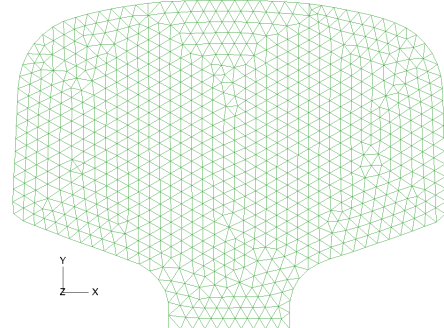


Figure 5.5 Illustration of the tent grid used.

The FE mesh grid employed could be any standard mesh used by the ABAQUSTM software. To simplify the analysis at this stage it was assumed that the elements used were CPE6M (6-node modified quadratic plane strain triangles with hourglass control), which allow linear strain variation within elements. However, the approach described below could be generalised to allow any kind of element to be used. Generally, to ensure the success of the inverse eigenstrain analysis, it is expected that the FE mesh should be denser than the tent grid, so that the eigenstrain variation can be properly represented. Figure 5.6 illustrates the two scenarios. The situation on the left corresponds to under-sampling, where there are too few IPs to capture the eigenstrain variation (red line) correctly. The situation on the right corresponds to the case when sampling is sufficient to provide a reasonable

approximation of the underlying eigenstrain variation. Figure 5.4 provides an example of an FE mesh grid, and Figure 5.5 illustrates the eigenstrain tent grid used.

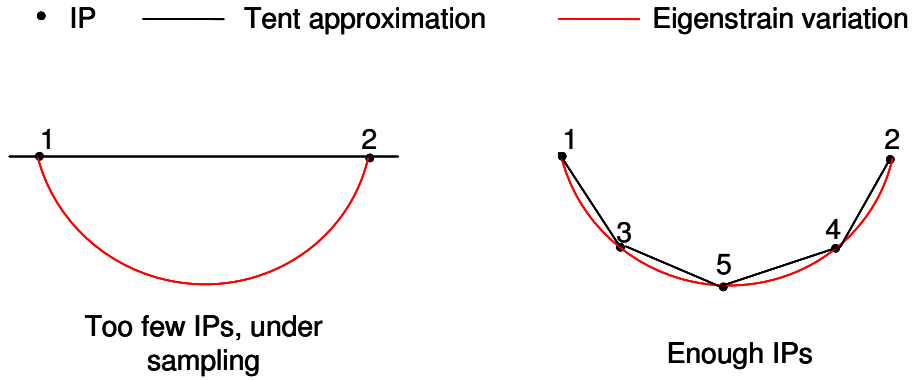


Figure 5.6 The continuous curve in the above figure illustrates the spatial variation of an eigenstrain component that needs to be determined. The IP points numbered 1, 2 on the left lead to under-sampling of this distribution. The denser mesh with IP points numbered 1, 2, 3, 4 and 5 in the right figure provides better sampling.

The tent grid is the grid that defines the discrete tent functions used in the reconstruction. Each neighbourhood of several nodes in the grid (Figure 5.5) represents a “tent” peak, as follows. If a particular point is chosen to correspond to the peak of the “tent”, then all triangular elements containing this point need to be identified, and the tent function value prescribed to be unity at the chosen point, and zero at all other nodes. This, in combination with appropriate shape functions, creates the desired “tent” shape. It is natural to use a coarse FE mesh input file as the template to form the tent grid. The element data in the coarse FE mesh input file is also useful, since it contains the point-wise connectivity information on points belonging to the same element and therefore forming together a “tent” peak.

Using the tent grid structure it is also possible to interpolate the values to the FE mesh IPs. In order to accomplish this, it is first necessary for each IP to establish to which triangle it belongs. This can be achieved easily by checking the following approach. Let points A , B and C be the vertices of a triangle and P the point being tested. Then if $\angle APB + \angle BPC + \angle CPA = 2\pi$, then point P must reside in the triangle (Figure 5.7); otherwise outside.

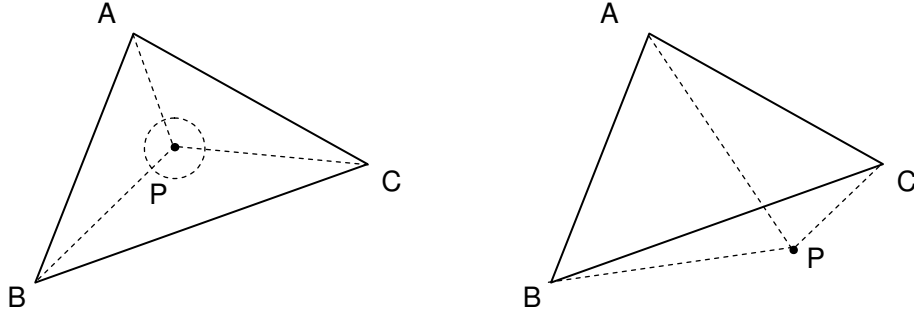


Figure 5.7 Illustration of the criterion for point P belonging to the inside of a triangular element.

Knowing the x and y coordinates of triangle ABC and point P , it is easy to calculate the vectors between P and the vertices and to calculate the angles using the dot product operation. Once it has been established that an IP lies within the triangle, the value of the “tent” function corresponding to it can be easily expressed by the corresponding values on the vertices and their coordinates using the shape function of element type CPS3. An explicit expression of the relationship between the IP coordinates (x, y) and its “tent” value z is presented below to reduce the implementation effort.

Assume that triangle ABC is to be mapped from x - y space to a canonical ζ - η space, the choice of which will become clear below. By finding the relationship between (x, y) and (ζ, η) , an algebraic function can also be found for the height (“tent” function value) at point P that is defined by its position relative to the vertices (with one vertex value set to unity and the other two to zero). Let the linear mapping sought be described by the functions $\zeta = ax + by + c$, $\eta = dx + ey + f$. These functions are found by writing the mapping equations for mapping the corners to the respective positions: $(x_A, y_A) \rightarrow (0, 1)$, $(x_B, y_B) \rightarrow (0, 0)$ and $(x_C, y_C) \rightarrow (1, 0)$. Imposing these conditions in the above definitions of ζ and η , six simultaneous equations are obtained.

In the matrix form the equations are:

$$\begin{bmatrix} x_A & y_A & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & x_A & y_A & 1 \\ x_B & y_B & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & x_B & y_B & 1 \\ x_C & y_C & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & x_C & y_C & 1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \\ e \\ f \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \quad (5.1)$$

Let the “tent” height at (0, 1) be set to unity ($z_A=1$). Then the height at point (ζ, η) corresponding to point (x, y) must be equal to η . Therefore, only the coefficients are required which relate η to the real spatial coordinates (x, y). These are:

$$\begin{aligned} d &= \frac{y_C - y_B}{x_C(y_B - y_A) + x_B(y_A - y_C) + x_A(y_C - y_B)} \\ e &= \frac{x_B - x_C}{x_C(y_B - y_A) + x_B(y_A - y_C) + x_A(y_C - y_B)} \\ f &= \frac{x_C y_B - x_B y_C}{x_C(y_B - y_A) + x_B(y_A - y_C) + x_A(y_C - y_B)} \end{aligned} \quad (5.2)$$

By employing the above procedure, all information needed for the analysis can now be collocated on FE mesh IPs. It is therefore possible to carry out the interpretation program with the help of FE state variables (SDVs). Each step in the pre-processing program involves one tent pulse centred at a certain point in the tent grid. The information is stored for post-processing regarding the experimental data (via SDV, for both xx and yy components of measured average residual elastic lattice strain) and the simulated elastic strain components (EE11, EE22 and EE12, corresponding respectively to elastic strain components xx , yy and xy). Figure 5.8 illustrates an example tent eigenstrain distribution, and Figure 5.9 shows the corresponding residual elastic strain response to that eigenstrain.

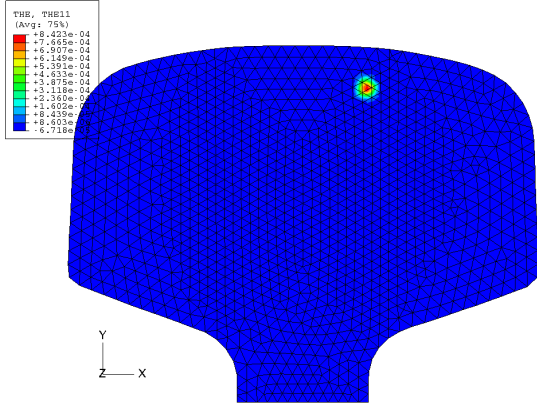


Figure 5.8 An example of an eigenstrain “tent” base function introduced in the FE model.

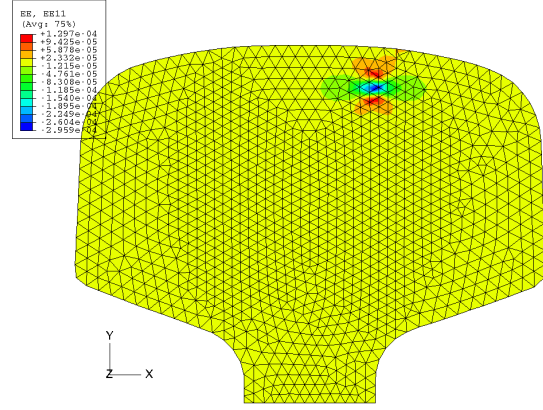


Figure 5.9 The elastic strain response (horizontal component) to a single eigenstrain “tent” base function.

In the post-processing program, the optimization process is carried out by solving the linear problem mentioned above:

$$\mathbf{A}\mathbf{c} = \mathbf{b} , \quad (5.3)$$

where

$$\mathbf{A} = \sum_{q=1}^Q s_{kq} s_{mq} = \mathbf{S}\mathbf{S}^T , \quad \mathbf{b} = \sum_{q=1}^Q s_{kq} t_q = \mathbf{S}\mathbf{t} . \quad (5.4)$$

The solution consists of finding from Eq. 5.3 such vector of coefficients $\mathbf{c}$ that corresponds to the set of “heights” of the tents that delivers the minimum of $\mathbf{J}$ in Eq. 2.35.

The conventional 1D eigenstrain problem [9] only involves one eigenstrain component (and the corresponding elastic strain component) to form the $\mathbf{S}$ matrix. In the 2D problem, the in-plane direct strain components (EE11 and EE22) are *coupled*, in the sense that eigenstrain ε_{11}^* affects elastic strain e_{22} , and *vice versa*. Capturing this coupling correctly is very important for formulating the appropriate matrix $\mathbf{S}$ from Eq. 5.4. The shear component (EE12, equal to EE21) must also be taken into consideration. Let us denote by S_{11} and S_{22} the matrices that arise due to the separate consideration of x - or y -direction elastic strains for all tents. For the consideration of fully two-dimensional problems, the coupled form should be used,

$$\mathbf{S} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix},$$

where e.g. S_{12} represents the y -direction elastic strain matrix due to the x -direction eigenstrain, and conversely for S_{21} .

The procedures described above outlines the operations performed by the post-processor: the extraction of eigenstrain influence coefficients, s_{kq} , from individual base function simulations; the assembly of the S -matrix, as well as the A -matrix and the b -vector for Eq. 5.3; and the solution of Eq. 5.4. Once the coefficients c_k are determined by the post-processor, they are written to a text file and provide the input for the final simulation that performs the one-step elastic equilibration, and displays the reconstructed eigenstrain and elastic fields.

5.4 Results and discussion

5.4.1 The neutron diffraction experiment

The neutron diffraction experiment was carried out on the STRESS-SPEC instrument at FRM-II research reactor, TU München (Germany). The details of the experimental setup and analysis are described in [86]. A regular rectangular grid of measurement points was used to cover the entire rail head area, providing information about the fully two-dimensional variation of the three-dimensional residual elastic strain (three mutually orthogonal direct strains were measured). The contour shape of the sample was previously determined by CMM (Coordinate Measuring Machine). The experimentally measured strain distributions provide the input that is required to carry out the 2D inverse eigenstrain construction described above. The results of

experimental measurements by neutron diffraction are plotted in Figures 5.10, 5.11 and 5.12.

5.4.2 Eigenstrain reconstruction results

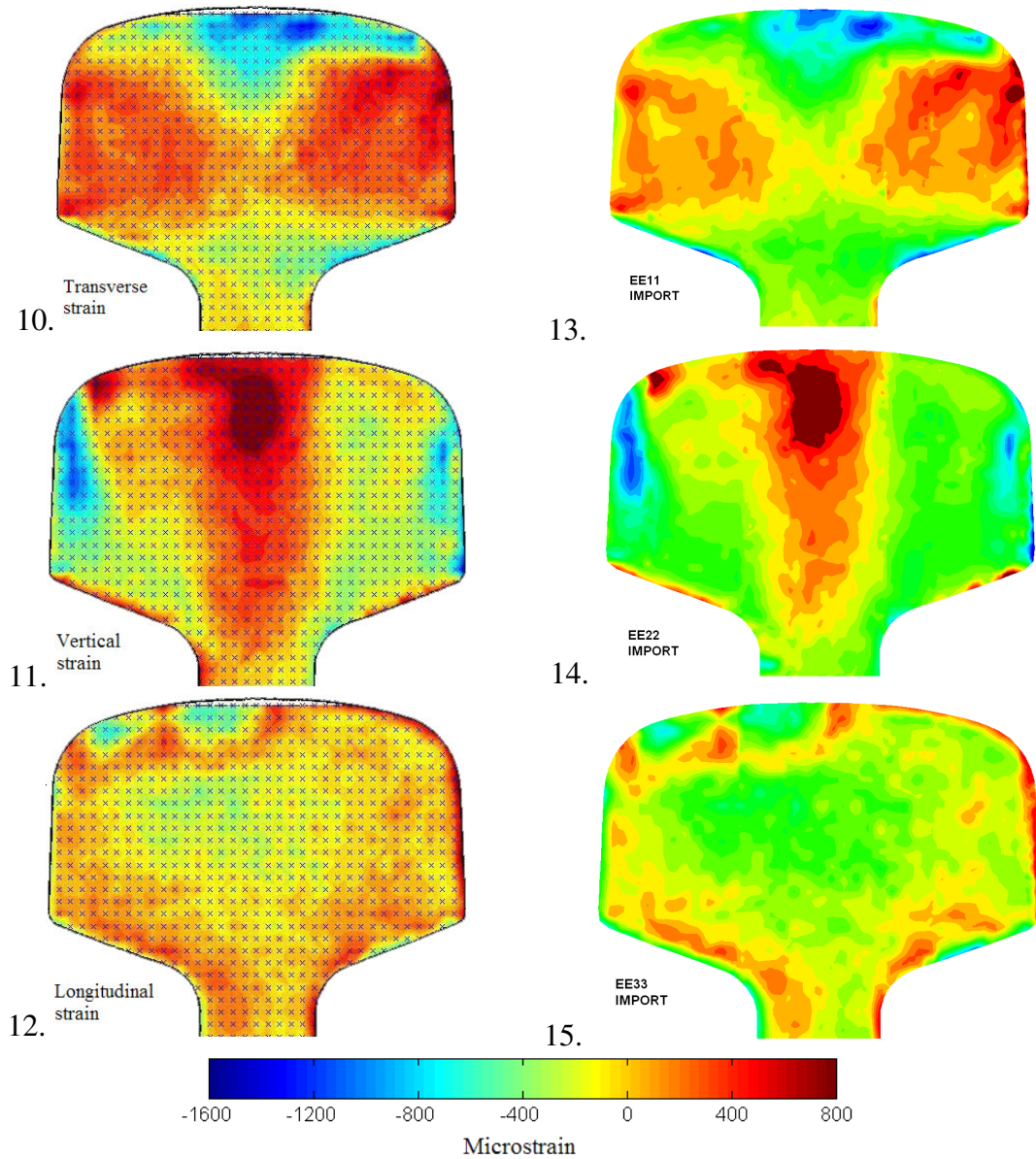


Figure 5.10, Figure 5.11 and Figure 5.12 represent the experimental data for transverse (x), vertical (y) and longitudinal (z) residual elastic strain distributions; Figure 5.13, Figure 5.14 and Figure 5.15 represent the data imported from the experiment into the FE model.

The experimental results were imported into ABAQUS using the procedure described above. The inverse eigenstrain reconstruction was carried out using the least squares matching of the imported data [63]. Figures 5.13, 5.14 and 5.15 show the

imported three elastic strain components. Note that the same colour scales were used to plot the experimental data (based on a regular rectangular grid of points, the left column) and the data imported into the FE simulation (the right column). No significant loss of accuracy occurs at this stage.

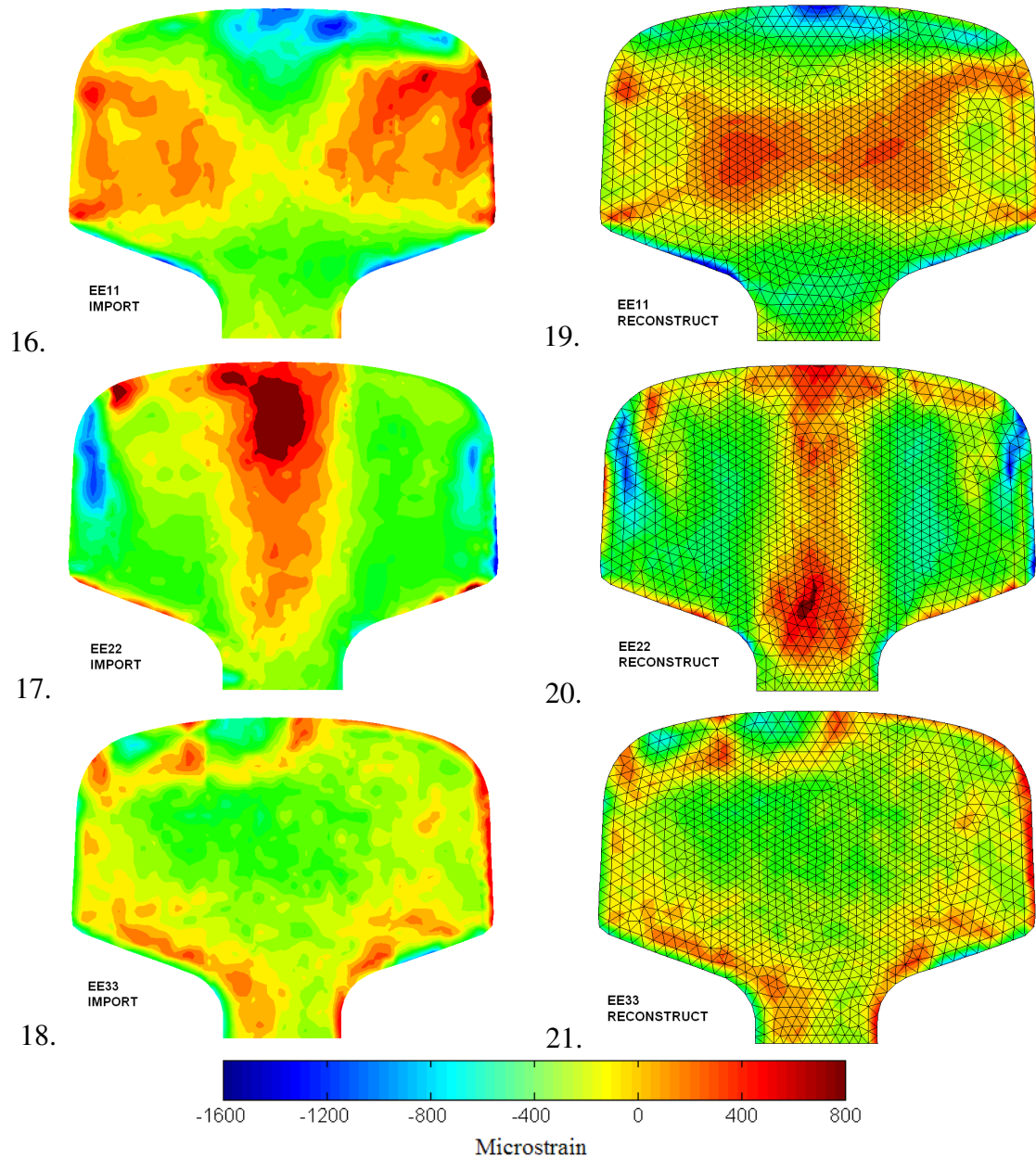


Figure 5.16, Figure 5.17 and Figure 5.18 are the data imported into the FE model; Figure 5.19, Figure 5.20 and Figure 5.21 are the reconstructed residual elastic strain distributions for the transverse (x), vertical (y) and longitudinal (z) directions.

In Figures 16, 17 and 18, the imported residual elastic strain results are plotted again to compare with the reconstructed elastic strain fields (the right column: Figures 19,

20 and 21). It is apparent that the quality of reconstruction (match to the experimental data) is excellent for the longitudinal (z) strain component. This component is practically de-coupled from the other components, and therefore matching in this case is essentially reduced to piecewise linear approximation of the experimental data by the combination of tent functions.

The quality of the match is not as satisfactory for residual elastic strain components in the transverse (x) and vertical (y) directions (Figures 5.16, 5.19 and 5.17, 5.20, respectively). Qualitatively the strain distributions are captured correctly, but quantitative agreement may be improved. In the case of in-plane strain components, coupling between the two distributions is observed, making the matching problem more challenging. Apart from the coupling issue, the boundary condition may also be a contributing factor of the mismatch. (In the model, self-balance is assumed for the railhead, but in the experiment, the railhead is connected with the rest of the flat-bottomed rail by the web and clamped for diffraction measurement)

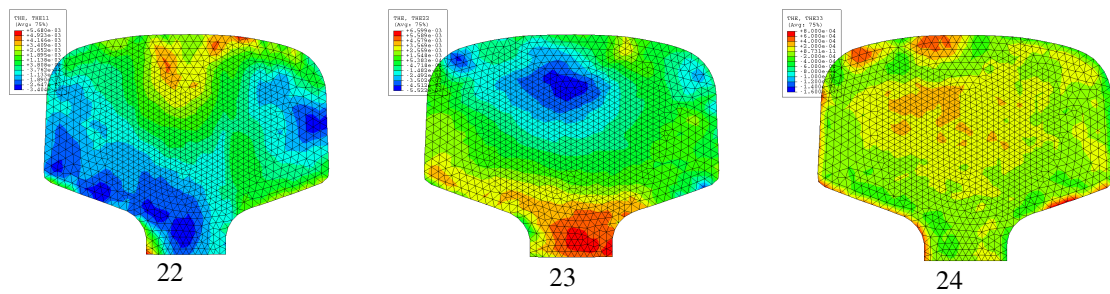


Figure 5.22, Figure 5.23 and Figure 5.24 represent the reconstructed eigenstrain distributions for transverse (x), vertical (y) and longitudinal (z) directions.

The underlying eigenstrain (inelastic strain distributions) are shown in Figures 5.22, 5.23 and 5.24. There is clear evidence of eigenstrain localisation in areas that experienced plastic deformation, either in service or during production of the rail profile by rolling. There is evidence of plastic deformation under the contact between

the wheel tyre and the rail head. There also appears to be some plastic deformation present on the bottom of the rail head on the left hand side, and also in the web.

It is concluded that the discrete inverse 2D eigenstrain method allows the model to identify correctly the eigenstrain regions and the associated stress concentration points. The new reconstruction technique allows the determination and visualisation of inelastic strain distributions. This offers an improved level of insight into the sample stress state, and hence into its deformation history. Another measure of plasticity is the diffraction peak broadening that is quantified using the full width at half-maximum (FWHM). However, this parameter is known to be only an indirect indicator of plastic deformation and to have a non-linear relationship with the dislocation density. It is, however, incapable of providing information about multi-directional inelastic strains.

In order to provide further quantitative assessment of the accuracy of the 2D inverse eigenstrain method, three lines running across the sample in the horizontal direction were sampled to examine the quality of reconstruction (Figure 5.25). Figures 5.26-31 show the horizontal and vertical components of the elastic strains along the lines running across the rail head at the nominal heights (distances to the foot of the rail) of 124, 138 and 150mm, respectively.

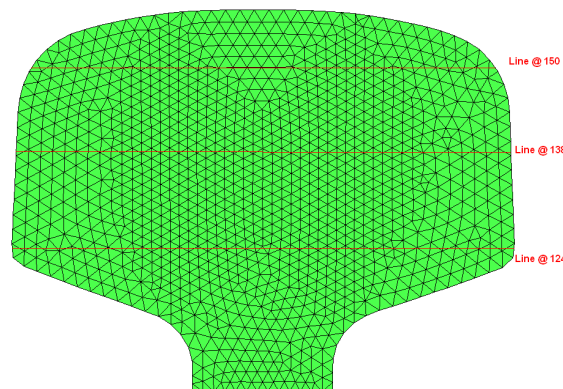


Figure 5.25 Relative positions of the three lines used for plotting.

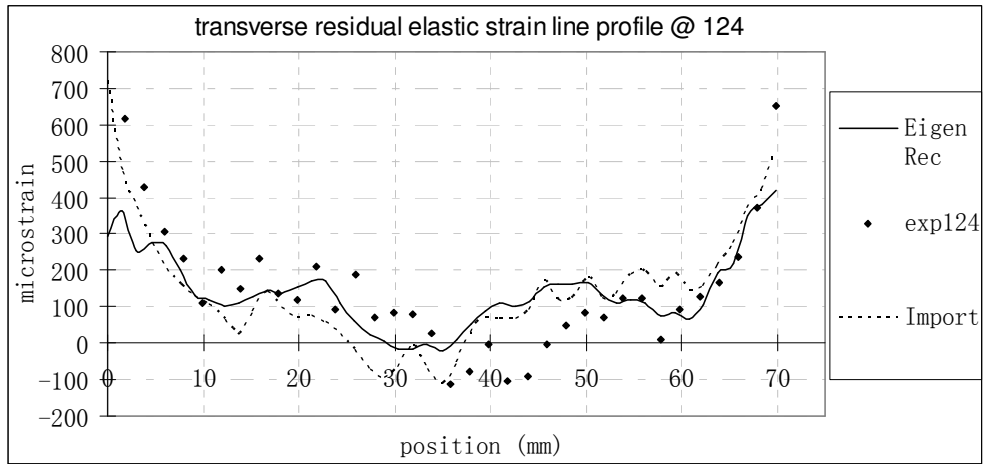


Figure 5.26 Transverse residual elastic strain (ϵ_{11}) profiles from eigenstrain reconstruction, experiment and FE direct import at line 124.

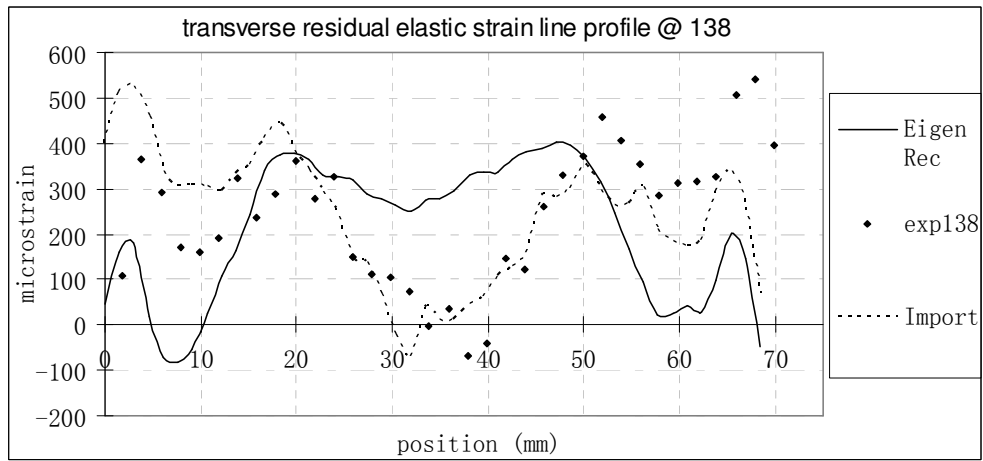


Figure 5.27 Transverse residual elastic strain (ϵ_{11}) profiles from eigenstrain reconstruction, experiment and FE direct import at line 138.

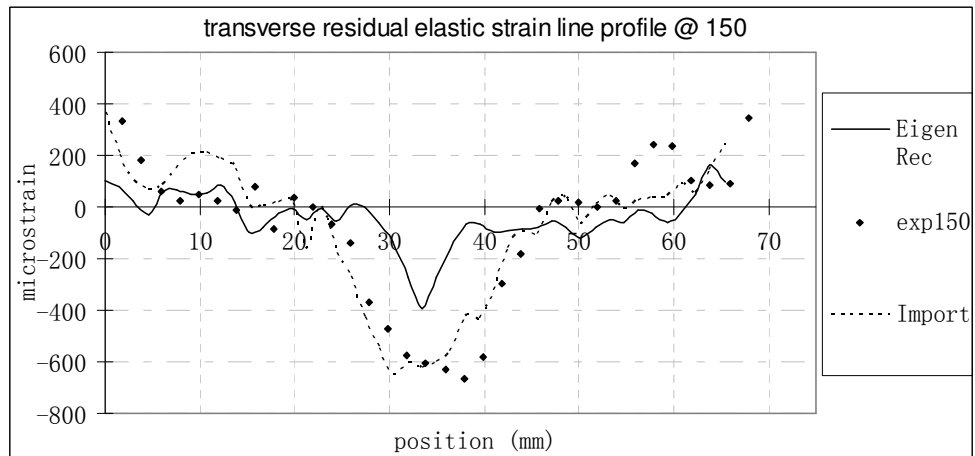


Figure 5.28 Transverse residual elastic strain (ϵ_{11}) profiles from eigenstrain reconstruction, experiment and FE direct import at line 150.

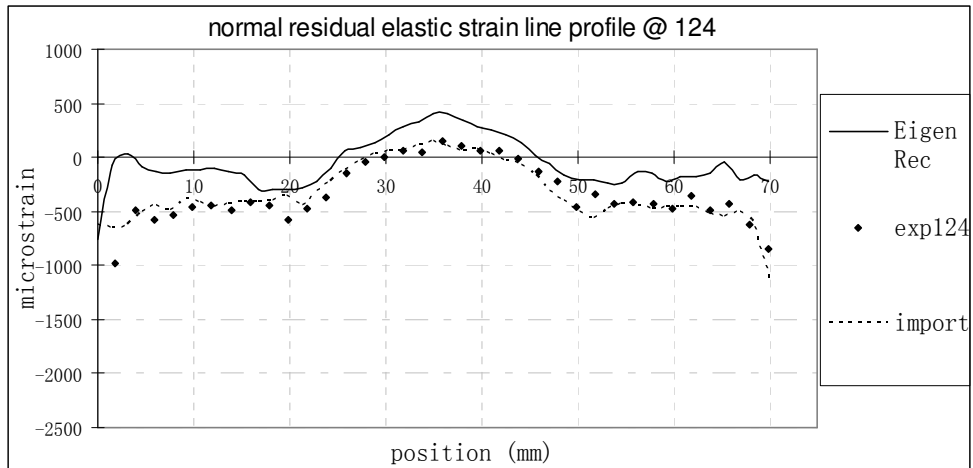


Figure 5.29 Normal residual elastic strain (ϵ_{22}) profiles from eigenstrain reconstruction, experiment and FE direct import at line 124.

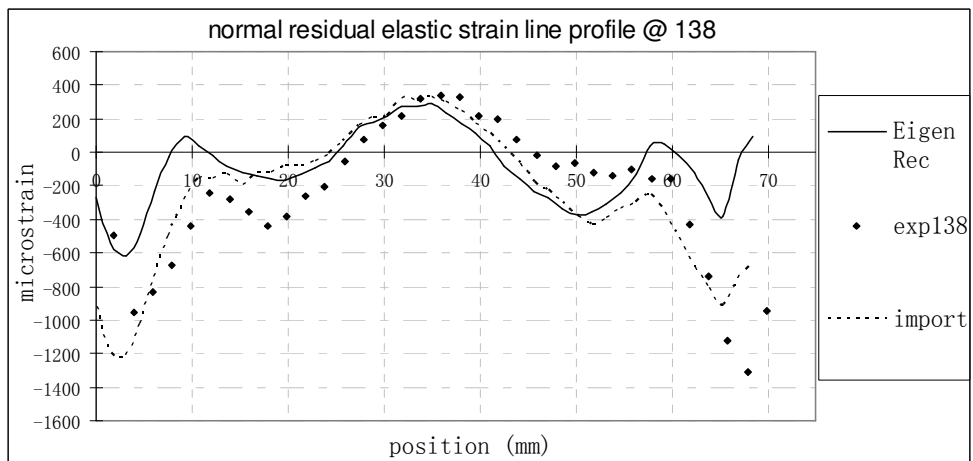


Figure 5.30 Normal residual elastic strain (ϵ_{22}) profiles from eigenstrain reconstruction, experiment and FE direct import at line 138.

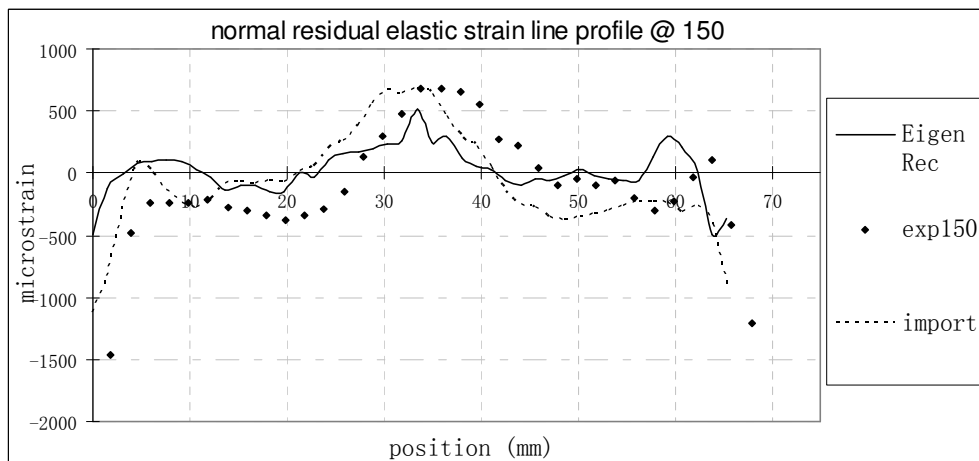


Figure 5.31 Normal residual elastic strain (ϵ_{22}) profiles from eigenstrain reconstruction, experiment and FE direct import at line 150.

In Figures 5.26-31 shown above, “Eigen Rec” refers to the eigenstrain reconstruction result, and “exp124”, etc. refers to the experimental data. The label

“import” refers to the elastic strain values imported into the FE model by 2D interpolation.

The line plots confirm that the import operation does not introduce any significant errors. The comparison between the imported data lines and the reconstruction suggests that the eigenstrain reconstruction captures the elastic strain variation reasonably well, although there are some considerable discrepancies remaining. As mentioned before, the origin of these discrepancies is likely to be associated with simulation approach of the coupling in-plane strain components and different boundary conditions applied. Further investigation is warranted on the above subjects, and a mesh sensitivity study would also be performed.

5.5 Conclusions

In the current study a fully two-dimensional, discrete inverse method for the reconstruction of eigenstrain fields within samples of arbitrary shape was proposed, developed and validated. It is believed that this method can be applied widely in the context of residual stress studies. The particular aspect of the reconstruction procedure is the ability to identify and quantify the source of residual stress – the underlying incompatible inelastic strain field (eigenstrain). Provided this distribution is found, together with the knowledge of the sample shape, the full residual stress-strain state can be reconstructed. An efficient framework for the analysis is built around an FE package (ABAQUS in the present study) that performs the mechanical computations, but also includes the pre-processor and post-processor. Once launched, the complete reconstruction can be performed automatically without any operator interference.

Chapter 6 3-D macroscopic residual stress state and process modelling: linear friction welds in Al-SiCp composite

6.1 Introduction

Metal Matrix Composites (MMCs) are a class of material that contain reinforcement phase(s) dispersed in a continuous metallic matrix. Over the past few decades, significant effort has been dedicated to developing MMCs with better physical and mechanical properties compared to monolithic metals. The synergic interaction between the matrix, usually a light alloy (Al, Ti or Mg) and the reinforcement, usually a ceramic (oxides, carbides, nitrides), allows MMCs to exceed the parent material's mechanical properties [80]. Among the MMCs, aluminium matrix composites (AMCs) form a class of attractive light-weight materials possessing a good combination of high stiffness and strength. The incorporation of stiff and hard (usually ceramic) reinforcement in the form of fibres or particles leads to a significant increase in the overall elastic modulus. Strength is also improved due to a variety of mechanisms, including grain refinement and the creation of additional obstacles to dislocation movement. Despite the several advantages over conventional alloys, a significant limitation to the industrial application of AMCs is posed by the problems that arise in conventional joining techniques, such as segregation and degradation of the reinforcement phase.

Recently, linear friction welding has been successfully applied to join the AMCs materials, since the method avoids melting and solidification that cause those

defects [87]. Linear friction welding is a solid state joining process in which the bonding of two flat-edged components is completed by their relative reciprocating motion under axial (compressive) forces. During the process, significant heat is generated by a friction at the component interface, resulting in the continued displacement of plastically deformed material [88-91]. The interaction between thermal and mechanical behaviour of the component makes the problem of modelling the process rather complicated, as the process still has not been fully understood yet.

The LFW process of titanium alloys has been characterised using 4 distinct phases in terms of shear force and displacement history [88, 92]. However, in the present study it was found that for AMCs the process did not appear to contain the same distinct phases. This required the introduction of a new descriptive structure for the stages of the LFW process, as described below.

The linear friction welding of an aluminium alloy matrix composite AMC225xe was performed at TWI (The Welding Institute, Cambridge, UK). AMC225xe is a high quality aerospace grade aluminium alloy reinforced with 25% by volume of ultra-fine particles of silicon carbide, manufactured by Aerospace Metal Composites Ltd (Farnborough, UK). The schematic illustration of the weldment can be seen in Figure 6.1 and the details of the material can be found in [87].

In order to extend our knowledge of the complex LFW process, different approaches to the RS analysis after the process were investigated, including neutron diffraction measurement, whole process simulation and eigenstrain reconstruction. This chapter will concentrate on the process modelling and its verification against the neutron diffraction measurement result.

6.2 Experimental Technique and Residual Strain Measurement

Residual strain measurement was carried out by neutron diffraction on the EXGIN-X instrument (ISIS, Rutherford Appleton Laboratory, UK). A tantalum target is bombarded with pulses of highly energetic protons from a powerful accelerator, driving (“spalling”) neutrons from the nuclei of the target atoms. Each collision leads to an extremely intense neutron pulse, delivered with only modest heat production in the neutron target. The neutron beam is then guided to the experimental station, and collimated so that a particular location within the sample is illuminated.

Figure 6.2 illustrates the neutron scattering experimental setup. The diffraction patterns were collected as time-of-flight data by two detectors mounted perpendicularly to the incident beam. Due to the lower interaction of neutrons with matter in comparison with X-rays, the absorption is relatively weak, allowing deeper penetration into bulk samples. However, the relatively small particle flux (compared to synchrotron X-ray beams) requires larger gauge volume and longer counting time. The beam size of 2×2mm and counting time of about 30 minutes for each point were adopted. Steps of 1mm were used near the bond line, providing overlapping measurements and thus allowing more precision in the strain profile reconstruction. Increasing steps were used to measure strains further from the bond line.

The data analysis was carried out on the entire diffraction spectra obtained at each measurement position, using the Open Genie software for the display and analysis of data from the neutron scattering instruments at the ISIS facility[93].

Due to the absence of reference strain-free samples, the unstrained lattice parameters d_{hkl}^0 were obtained from pattern collected by placing the beam at the very

corner of the plate, which was assumed to carry no or little residual macroscopic strain. A different reference was used for each half of the component, due to the fact that different parts came from slightly different production routes. The reference at central point ($x=0$) was taken to be the average value of the two far-field references.

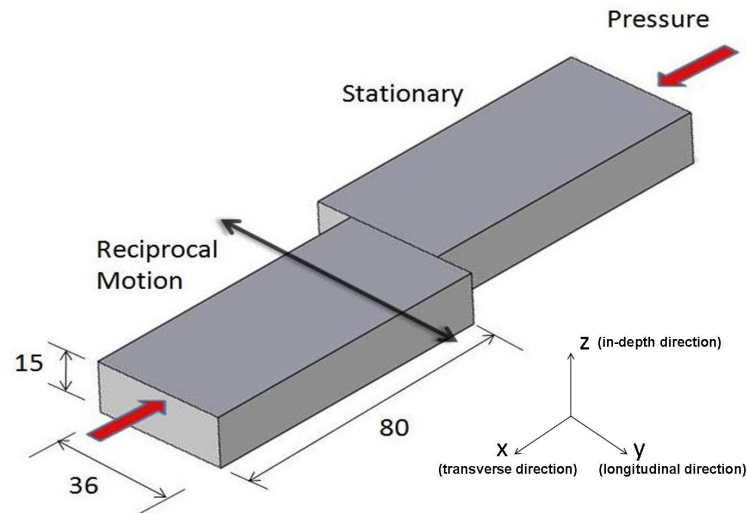


Figure 6.1 Illustration of the AMCs linear friction weldments, and coordinates used.

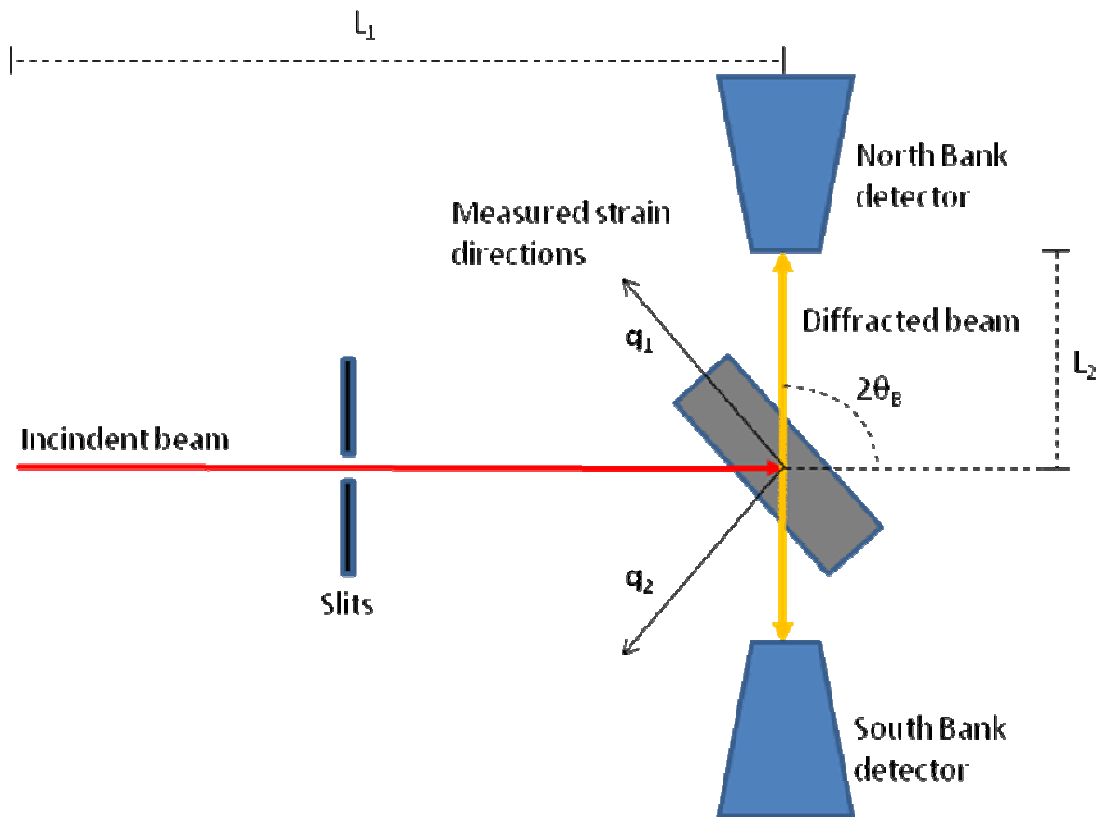


Figure 6.2 Schematic setup of the ENGIN-X diffractometer at ISIS.

Figure 6.3 shows the residual elastic y -strain distribution as a function of x position across the bond line. The y -strain exhibits a large tensile region in the vicinity of the weld zone as a consequence of the plastic deformation and cooling process involving flash extrusion of material, turning to residual compression.

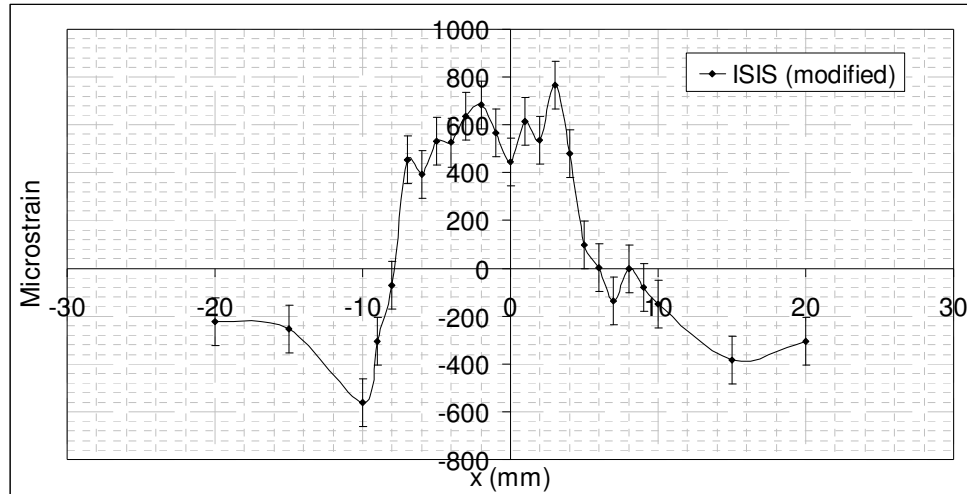


Figure 6.3 Residual elastic y -strain distribution in the welds as a function of x - position

6.3 Process simulation and residual stress analysis

For the purpose of building a process model, the FE analysis procedure initially needs to be defined. In this case, the heat for the welding was generated via the oscillation and friction between two components. The consequent plasticization, joining and bonding arise not only due to the frictional heat but also due to the forging force which makes two parts approach and deform. Therefore, it is quite clear that the process is governed by the interaction between the temperature-displacement analysis, heat transfer and strain field. The relationship between the phenomena related to heat, strain and microstructure can be illustrated as shown in Figure 6.4.

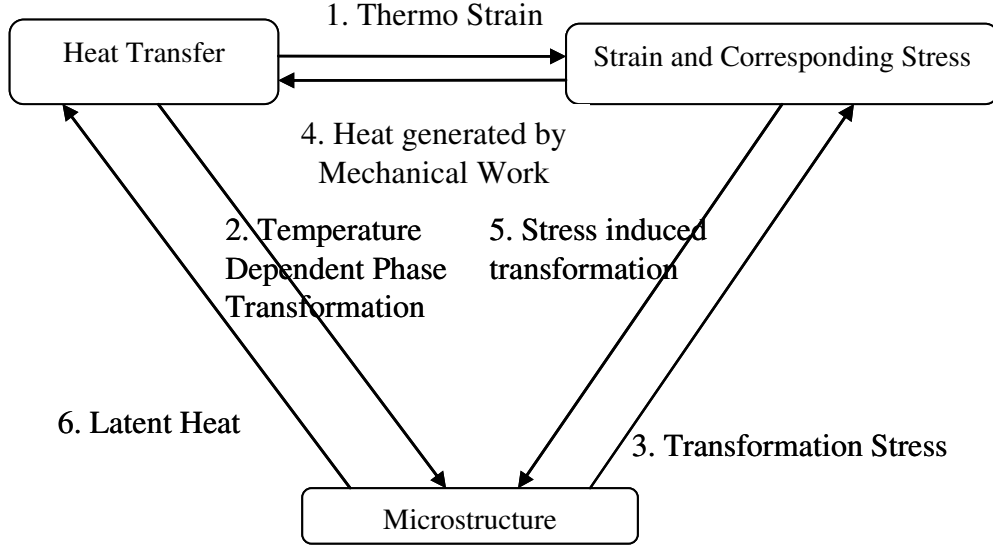


Figure 6.4 Schematic showing the interactions of the mechanism involved during thermo-mechanical processing

In the present model, the AMCs material was simulated using continuum plasticity theory. There was no significant melting or re-crystallization taking place during the welding process. Therefore, we make an approximation that the heat generated by mechanical work (Arrow 4 in Fig. 6.4) causes plasticity in the Heat Affected Zone (HAZ), but does not induce any phase change or transformation. The focus is therefore placed on the two key effects: the evolution of heat from the frictional mechanical work, and the simultaneous heating and thermal expansion and the externally applied forging force, that cause deformation by temperature-dependent plasticity. The governing constitutive equations within the framework of thermo-elasto-plastic analysis are well known, e.g. [94]:

$$\begin{aligned}
 & h(T_w - T_\infty) + \frac{\partial[k(\partial T / \partial x_i)]}{\partial x_i} + \hat{\sigma} F_{ab}(T_w^4 - T_\infty^4) + \dot{q}\hat{u} - \rho c_p \frac{\partial T}{\partial t} \\
 & = \frac{ET}{1-2\nu} \frac{\partial \epsilon_{ij}^0}{\partial T} \frac{\partial \epsilon_{ij}^e}{\partial t} - \kappa \sigma_{ij} \frac{\partial \epsilon_{ij}^p}{\partial t} - \frac{\partial \zeta}{\partial t}
 \end{aligned} \tag{6.1}$$

where the terms on the left describe the heat transfer by convection, conduction, and radiation between the solid and the environment, the internal heat generation and the

energy stored in the domain over time. In our simulation, the radiation term was omitted, given the fact that it accounts for a small fraction of the heat loss comparing with conduction and convection. The first two terms on the right-hand side describe the thermo-elastic and thermo-inelastic (thermo-plastic) heat evolution respectively, due to the work done during deformation. The variable κ in the above equation is the so-called inelastic heat fraction typically varying between 0.85 and 0.95. These two terms on the right-hand side are generally accepted to be small in comparison with others, and for this reason neglected in the analysis. The last term on the right-hand side accounts for the heat generated during phase transformation which in the present simulation of the LFW process are ignored. Therefore, the energy equation in the present case becomes.

$$h(T_w - T_\infty) + \frac{\partial[k(\partial T / \partial x_i)]}{\partial x_i} + \dot{q}\hat{u} - \rho c_p \frac{\partial T}{\partial t} = 0 \quad (6.2)$$

In the equation above, h is the heat transfer coefficient with a value of 100 W/m²K. This value is chosen taking into consideration that oscillatory motion improves the heat exchange. Parameter k is the thermal conductivity coefficient with the constant value of 150W/m K. This assumption is valid for AMCs as long as the temperature remains below 350°C, which holds in this case. The density of the material was 2880kg/m³, and the heat capacity was set to 836J/kg K. There is one final assumption that was made, and that is that the heat generated in the frictional rubbing process was distributed evenly between the two components' contact surfaces.

Material mechanical parameters were set to be temperature-dependent, except for the Poisson's ratio that was thought to stay constant at 0.3. The temperature-dependent material mechanical properties are listed in Table 6.1. The plastic deformation was assumed to be linear kinematic to account for reverse yielding.

Temperature	Elastic Modulus (GPa)	thermo expansion coefficient (ppm)	Yield stress (MPa)	Elongation	UTS (MPa)
20	115	16.026	480	5%	650
25	115	16.166	480	5%	650
150	110	19.653	321	9%	428
200	104	21.048	276	18%	358
260	95	22.722	102	34%	200
350	76	25.233	48	45%	65
Table 6.1 Temperature-dependent material mechanical behaviour parameters [95].					

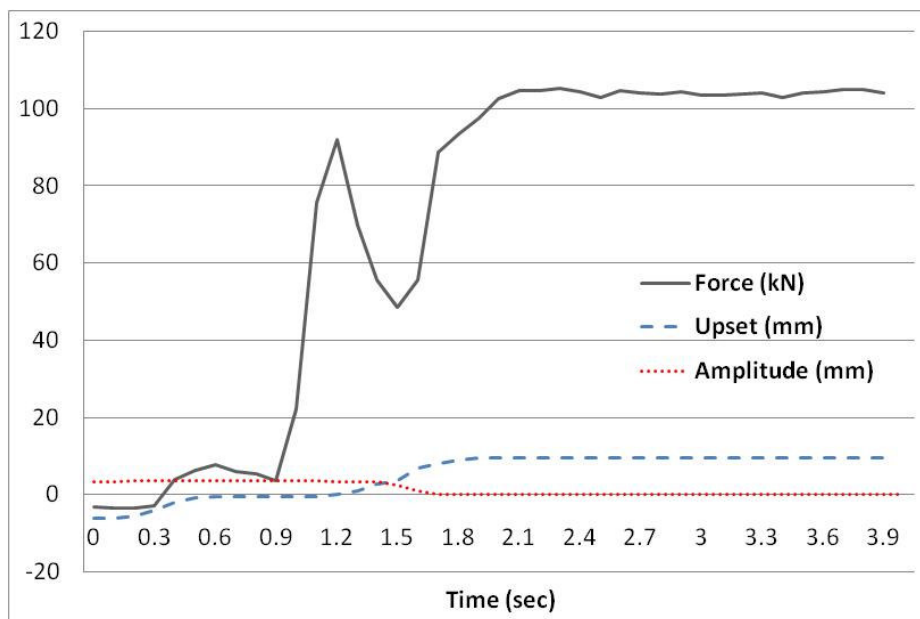


Figure 6.5 The variation of the weld parameters with time.

The LFW process itself can be divided into four distinct stages based on the four characteristic parameters of the process, namely: the oscillation amplitude, the oscillation frequency, the axial force and the burn-off. In the present study, the LFW conditions for AMC225xe/AMC225xe were set to be: 2mm in amplitude, 50Hz in frequency, 100kN in axial compressive force and 2mm burn-off. The time variation of these parameters during the process can be found in Figure 6.5. The schematic diagram of the process is shown in Figure 6.6 and the details of each stage are described as follows:

Stage 1 (0.0-1.0 sec): Warm-Up

Two materials are aligned in the machine and clamped. Oscillating motion of material A begins, whilst material B is kept static. Then the two components are brought together. Once in contact, considerable heat is generated by the solid friction due to the reciprocal motion under low force (or pressure). The wear and the creation of new metallic surfaces leads to the increase of the real contact area and of the friction coefficient. It is crucial that enough heat be generated to attain plasticization of the interface. The process has to overcome the heat losses via conduction to the parent material and radiation and convection to the atmosphere. No weld penetration is experienced in this part.

Stage 2 (1.0-1.5 sec): Osci-Forging

In this stage, whilst material A continues the oscillatory motion as in stage 1, the axial force is applied to the joint. The force is steeply increased (in a ramp) to about 90kN till 1.2 seconds and maintained. However, due to the onset of plastic flow in the work pieces, a sudden load drop occurs in the following 0.3 seconds. This phenomenon is related to the initial setting in of the “burn-off” process. Once the axial shortening starts, the force displays a sharp drop. In the meanwhile, the interface rubbing removes the oxide layer and reveals fresh surfaces suitable for bonding, creating an extrusion known as “flash”. The “flash” has different shapes depending on the material being subjected to the linear friction welding. Note here that the actual shortening exceeds the initial setting slightly due to inertia. The oscillatory motion ends when the axial shortening reaches the set burn-off. The Heat Affected Zone (HAZ) forms under the action of the frictional heat generated by the reciprocal motion.

Stage 3 (1.5-2.0 sec): Forging

This stage resembles the conventional forging process in many ways. The force increases up to about 100kN whilst the two parts continue to be pressed against each other. As a result, a large amount of “flash” of the plasticised material is expelled from the bond line resulting in the consolidation of the weld and further axial shortening, which increases approximately linearly with time, till about 2 seconds. Afterwards no further axial shortening can be obtained unless force is increased.

Stage 4 (2.0- sec): Cool-Down

With the force being maintained constant, the newly joint piece is cooled down to the room temperature. Once the process is completed, the total upset can be evaluated. In the present experiments it was 9.37mm, with the total length of welds changed from 160mm to 150.63mm.

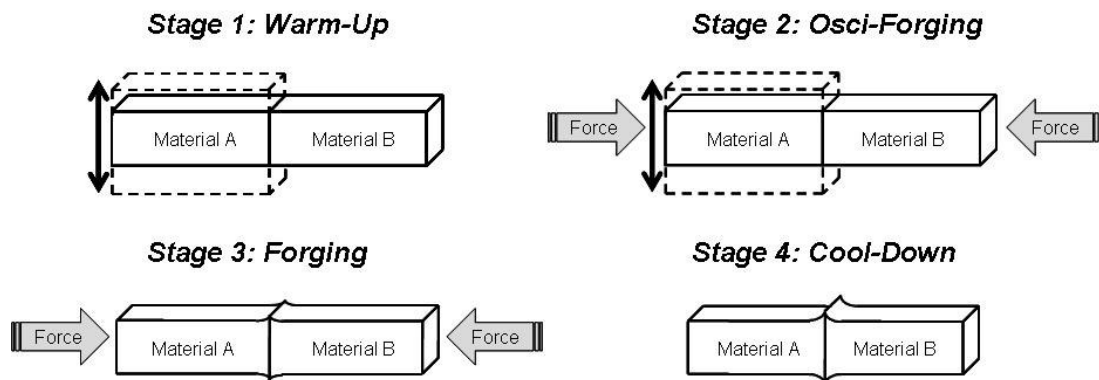


Figure 6.6 Schematic illustration of the stages of the linear friction welding process.

A particularly challenging part from the viewpoint of simulation is the oscillation-heat generation process. It requires coupled dynamic thermal and mechanical analysis, and the short time scales involved lead to very steep temperature and strain gradients. The analysis therefore requires very small increments, as well as element removal or large deformation simulation to represent the creation of flash and etc.

Instead of attempting to simulate the entire process, a novel approach was developed and will be presented here. In the Warm-Up and Osci-Forging stages, the

heat generation via mechanical work was quantified and replaced by heat flux inflow without the reciprocal motion being modelled explicitly. In other words, the view was taken to consider oscillation solely as a means of creating the heat flux. A brief description of the approximations involved in this representation of the process is given below.

Let us assume that the reciprocal motion of the component is harmonic, i.e. the displacement-time dependence is sinusoidal (see Figure 6.1). The shear stress exerted at the interface is

$$\tau = \mu P_N, \quad (6.4)$$

where μ is the friction coefficient and P_N is the pressure. The heat generation rate depends on the mechanical work transformation rate q that equals the product of the shear force and the rubbing velocity v , $q = \tau v$. The average heat generation rate then can be obtained through integration of the instant rate over a cycle, divided by the cycle time. The result can be expressed as:

$$\begin{aligned} q_0 &= \frac{1}{T} \int_0^T q dt = \frac{4}{T} \int_0^{T/4} q dt = \frac{4}{T} \int_0^{T/4} \mu P_N v dt \\ &= \frac{4}{T} \int_0^{T/4} \mu P_N \alpha \omega \cos(\omega t) dt = \frac{2}{\pi} \mu P_N \alpha \omega \end{aligned}, \quad (6.5)$$

where α is the oscillation amplitude and ω is the oscillation frequency [92]. The values adopted were as follows. The friction coefficient $\mu=0.5$ according to the approximation provided by the company technical data sheet. The contact pressure P_N was taken to be the average force over the first 1.5s divided by the contact area, giving the value of 81.2MPa. The oscillation amplitude α was 2mm, and ω was

50Hz in the setup used (cycle period $T=0.02s$). The knowledge of these parameters allowed the heat flux to be calculated.

In the simulation, the displacement was taken as the controlling parameter at each step of the process. The process was considered to be quasi-static, i.e. mechanical equilibrium was attained at each stage of the simulation procedure.

Figure 6.7 shows the residual Von Mises stress distribution at the end of the process (after cool down).

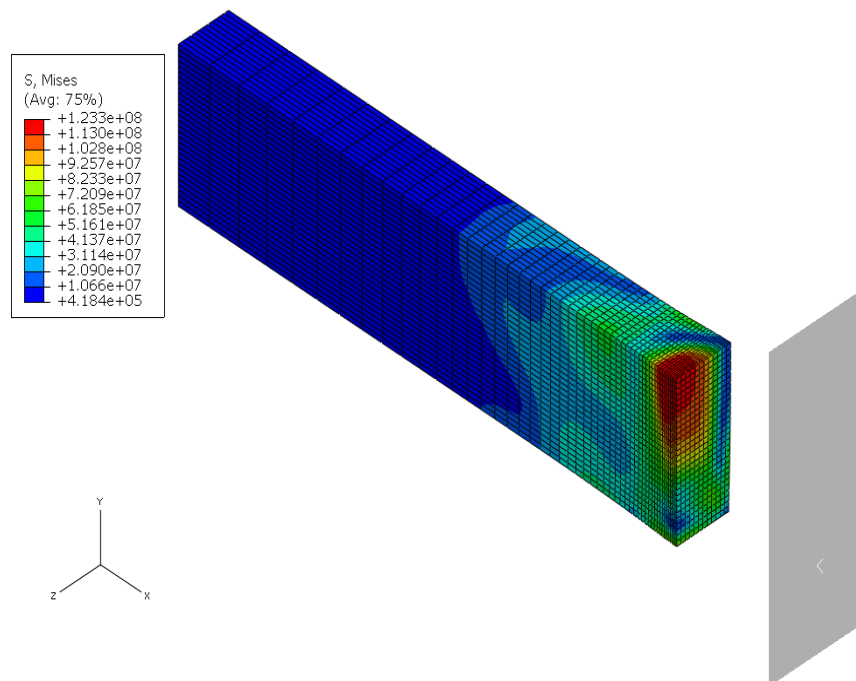


Figure 6.7 The 3D set-up for the LFW process simulation and its resulting RS profile at the end of the process (note that 1/8th of the work-piece is shown).

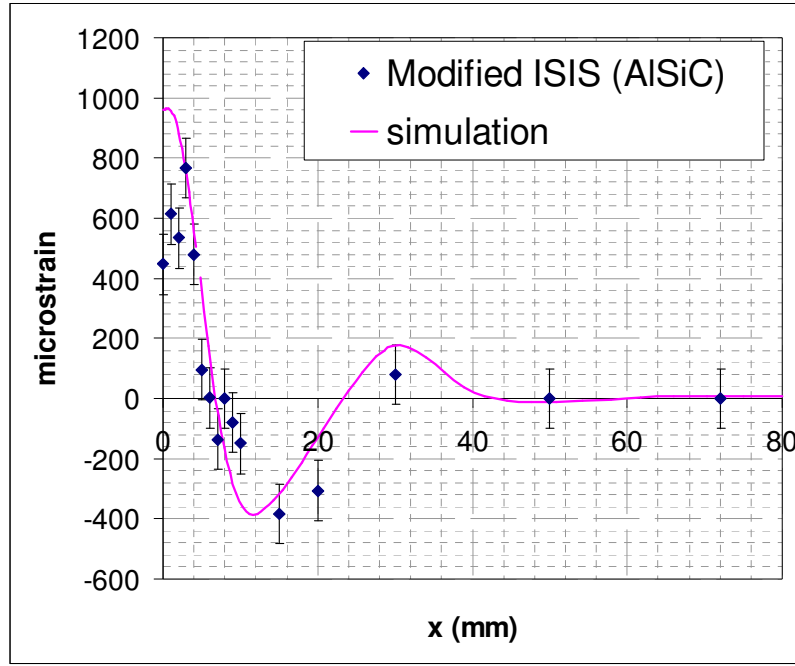


Figure 6.8 Residual elastic y-strain distributions obtained in the experiment and via the process modelling simulation.

For the end of the Cool-Down stage, the residual y-strain profile along the x -axis was extracted. In order to compare with the experimental neutron diffraction data, the diffraction gauge volume used in the neutron set-up ($2 \times 2 \times 10 \text{ mm}$) was taken into consideration in post-processing the simulation results. In the simulation the gauge volume averaging was realized by extracting the data for 9 parallel paths along the x -direction. The simulation result (Figure 6.8) clearly captures the trend and the magnitude of the residual strain profile within the experimental tolerance. The minor discrepancy arises at the very bond line region, where the FE prediction slightly overshoots. It may be caused by the severe shear plastic flow within the region due to the reverse yielding of the kinematic plasticity. The reaction force simulation result was also in good accordance with the experiment.

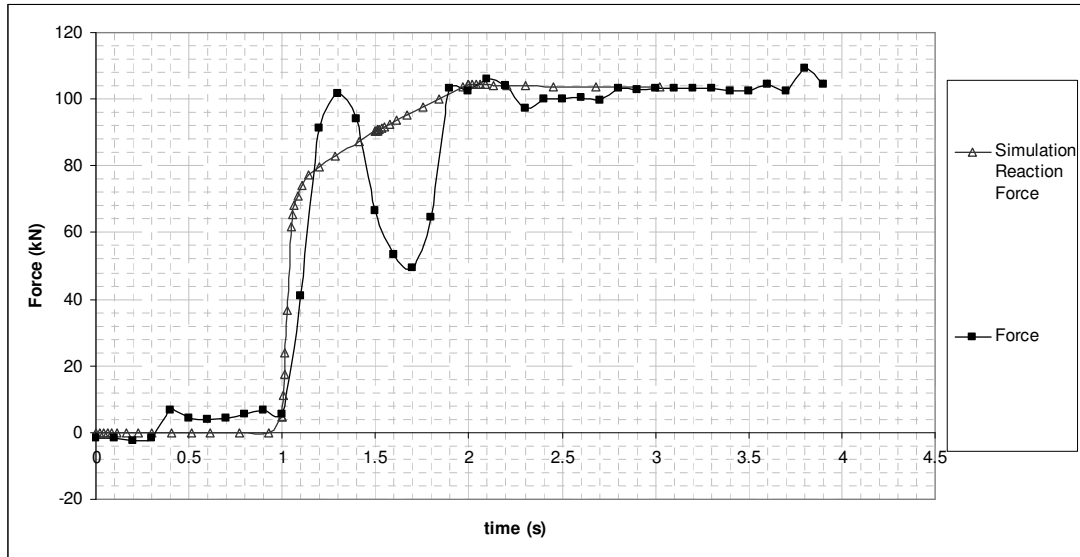


Figure 6.9 X-Axis reaction force evolution in the experiment and the process modelling simulation.

Figure 6.9 shows that in terms of the time dependence and the magnitude, the model clearly captured well the data at 1s and 2s, but somehow missed the “dip” in between. This is mainly due to the neglect of the dynamic effects, i.e. the acceleration and deceleration of the component in x -axis, when more and less force is needed within those short periods, respectively. Another way of describing this effect is to say that the “dip” was associated with the finite compliance and finite speed of the welding machine. In contrast, under the assumptions made in the present process simulation, the plot of reaction force is expected to consist of a sequence of linear ramps.

A 1-D inverse eigenstrain analysis was also carried out using the algorithm described in Chapter 4, in order to reconstruct the residual stress variation in the longitudinal direction. Figure 6.10 shows that the elastic strains from the eigenstrain reconstruction capture the trend and magnitude of the neutron diffraction measurement residual strain profile to within the experimental tolerance. It also shows good agreement with the results of the process modelling (Figure 6.10).

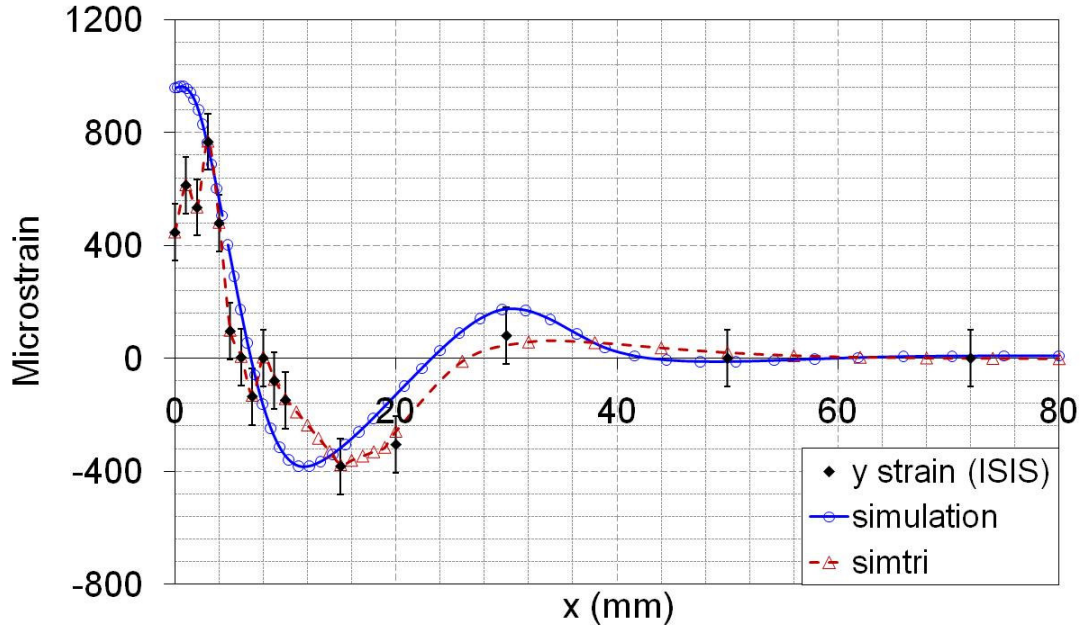


Figure 6.10 Residual elastic y-strain distributions from neutron diffraction experiments, process modelling and eigenstrain reconstruction

In order to understand the nature and extent of the residual stress profile, a parametric study was carried out to quantify the characteristic length scale of the process. A general equation was proposed to take into consideration all independent problem parameters that may affect the residual stress profile. The list of the relevant problem parameters is as follows:

$$\sigma_y, \partial\sigma_y/\partial T, \Delta T, k, h, t, w,$$

where σ_y denotes the yield stress and $\partial\sigma_y/\partial T$ the rate of change of the yield stress with temperature. ΔT denotes the total temperature drop in the process, and k, h are the thermal conductivity and the heat transfer coefficient, respectively. Finally, t, w are the sample thickness and width, respectively.

Using Buckingham's π -theorem, the characteristic length of the residual stress distribution can be expressed as follows:

$$\frac{L}{t} = F \left(\frac{\sigma_y / \Delta T}{\partial \sigma_y / \partial T} \frac{kw}{h} \right). \quad (6.5)$$

A brief investigation of the dependence of the characteristic length L on the problem parameters was carried out. The residual stress distribution was found to change with the variation of sample thickness t (the plane strain-plane stress transition) and sample width w , as illustrated in Figure 6.11. The component geometry is in fact one of the greatest factors that influence the LFW residual stress distribution. In Figure 6.12, the influence of the conductivity, heat flux, yield stress and plasticity is illustrated. It is shown that, among the parameters identified, the magnitude of the yield stress makes the biggest impact on the magnitude of the residual stress distribution after the LFW process. At the same time, the characteristic length scale of the distribution does not appear to be greatly affected by these changes.

6.4 Conclusion

A novel LFW process modelling approach was proposed in this Chapter to capture the residual stress distribution in the linear friction weldments of AMCs. A parametric study on the influence of the material properties on residual stress was also carried out. Neutron diffraction measurements and inverse eigenstrain reconstruction methods were used to validate the model. Adequate agreement was obtained between different techniques, suggesting that the chosen approach to the analysis was justified.

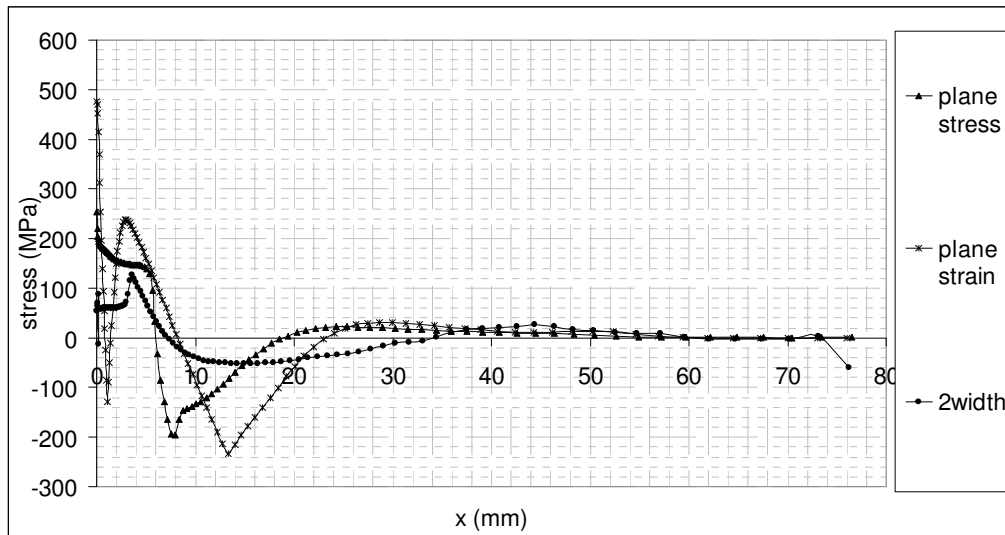


Figure 6.11 The variation of the yy stress component along the x-direction obtained in the process modelling simulation using different component geometries.

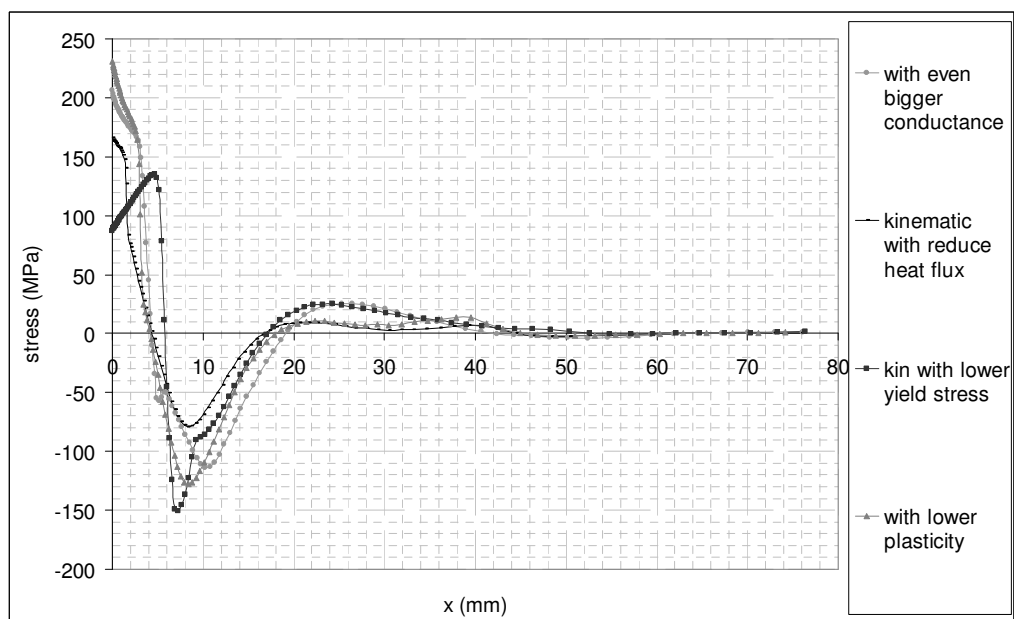


Figure 6.12 The variation of the yy stress component along the x-direction obtained from process modelling simulations for different material property parameters.

Chapter 7 3-D meso-scale analysis of elastic-plastic deformation in HCP polycrystals: crystal plasticity and strain gradient crystal plasticity modelling with synchrotron XRD measurement

7.1 Introduction

Most engineering alloys used in structural applications are polycrystalline. The majority of the material volume is occupied by grains (rather than grain boundary material), unless the grain size is very small (sub-micrometer). With each grain being a small crystallite, its properties depend on orientation, creating mismatch between neighbouring grains. Therefore, the deformation of most polycrystalline metallic alloys is strongly inhomogeneous. This has significant implications for the collective behaviour of the grain ensemble, manifested in the macroscopic deformation response of the material. To advance the understanding of these phenomena, we focus our attention on the plastic deformation within each grain. At low homologous temperatures, this is dominated by the crystal slip across grains. In the present study we describe the application of a grain-level crystal plasticity formulation and a strain gradient crystal plasticity formulation to the analysis of inelastic deformation in polycrystalline aggregates with HCP crystal structure. We concentrate on some issues of general concern, namely: (i) the use of three-dimensional (3-D) formulations, as opposed to previously reported two-dimensional (plane stress/plane strain) formulations [65]; (ii) the use of a ‘static’ regular mesh, as opposed to a grain-based mesh specific for a particular microstructure; and (iii) the procedure for model calibration by comparison with experimental measurements by high energy X-ray diffraction, which provides a means of assessing mesoscale average values of grain-

level elastic strains; (ix) the adoption of a strain gradient crystal plasticity algorithm to construct the diffraction peaks based on the information about the grain-level elastic strains.

7.2 Crystal plasticity modelling of near- α phase Ti-6Al-4V and synchrotron XRD measurement of grain group elastic strains

7.2.1 Rate-independent crystal plasticity model: formulation

The details of the crystal plasticity model formulation have been presented in Chapter 2. Therefore, only a brief summary of relevant points will be given here.

The stress rate at a point within a grain during elastic-plastic deformation is given by

$$\dot{\boldsymbol{\sigma}} = \mathbf{C} : \mathbf{D} - \boldsymbol{\sigma} \text{tr}(\mathbf{D}) - \boldsymbol{\Omega} \boldsymbol{\sigma} + \boldsymbol{\sigma} \boldsymbol{\Omega} - \sum_{\alpha=1}^n (\mathbf{C} : \mathbf{P}^{\alpha} + \boldsymbol{\beta}^{\alpha}) \dot{\gamma}^{\alpha}, \quad (7.1)$$

where $\boldsymbol{\beta}^{\alpha} = \mathbf{W}^{\alpha} \boldsymbol{\sigma} - \boldsymbol{\sigma} \mathbf{W}^{\alpha}$. Here $\mathbf{D}$ is denotes the deformation rate and $\boldsymbol{\Omega}$ is the spin tensor. The summation over α represents the contributions to the plastic strain rate from all active slip systems. Thus, in order to obtain the Cauchy stress rate, it is necessary to determine the shearing rate $\dot{\gamma}^{\alpha}$ on the α^{th} active slip system. The conditions under which a slip system is active or inactive are based on the yield and loading–unloading criteria. The magnitude of $\dot{\gamma}^{\alpha}$ can be determined using the constitutive equation for plastic slip on each slip system,

$$\sum_{\alpha=1}^n \mathbf{h}_{\alpha\beta} \dot{\gamma}^{\beta} = \mathbf{P}^{\alpha} : \left(\mathbf{C} : \mathbf{D} - \mathbf{C} : \sum_{\alpha=1}^n \mathbf{P}^{\alpha} \dot{\gamma}^{\alpha} - \boldsymbol{\sigma} \text{tr}(\mathbf{D}) \right) + \boldsymbol{\beta}^{\alpha} : \left(\mathbf{D} - \sum_{\alpha=1}^n \mathbf{P}^{\alpha} \dot{\gamma}^{\alpha} \right). \quad (7.2)$$

The above equation can be rewritten in the form

$$\sum_{\alpha=1}^n \mathbf{A}^{\alpha\beta} \dot{\gamma}^{\beta} = \dot{b}^{\alpha} . \quad (7.3)$$

Since the matrix appearing in Equation 7.3 may become singular, the problem is most efficiently solved by using singular-value decomposition to obtain the pseudo-inverse of the matrix.

7.2.2 Finite element implementation

Heterogeneous materials generally exhibit a random distribution of phases according to specific statistical distributions, so that one single computation may not be enough. Instead, a sufficient number of realizations of the microstructure will be necessary to estimate both the wanted property and its dispersion. In particular, the question of the size of the RVE for a given geometrical physical property must be addressed.

Microstructural mechanics analysis proceeds in three main steps: representation of the microstructure in a realistic manner, the identification of suitable constitutive equations for the constituents, and the choice of the numerical techniques to solve the boundary value problem. We first deal with the representation of microstructure in three-dimensional problems.

7.2.3 Sub-modelling and microstructure representation

The need to describe polycrystalline aggregate deformation at different scales has already been discussed in the introduction, and the various levels of refinement necessary were justified there. Here we focus on the modelling at the mesoscopic level, with the dimensions between 0.1 μm and 1mm. At such scales, the proposed mechanical model is implemented in the Finite Element framework after introducing

the concept of Representative Volume Element (RVE). Some considerations about the boundary value problems to be solved when using the sub-modelling techniques will be also briefly discussed here.

The polycrystalline RVE is a material element that must include a “sufficient” number of grains, in terms of crystallographic orientation, shape and size, in order to reflect the overall material response. The size of the RVE will depend of course on the typical length scales of the microstructure, and on the statistical distribution of the properties. In the micro- to macro- transition, the information passed on to the coarser level of description usually consists only of specific average strain and strain tensors representing the material state within an RVE. However, having access to the information about the variation of strain and stress fields within an RVE can nevertheless be very useful, particularly for the purpose of understanding the inhomogeneity of deformation and the crack initiation processes. The improved insight into intra-granular deformation can be achieved by means of Finite Element (FE) computations, provided the morphology (grain boundary geometry and orientation) and the material behaviour are correctly represented.

The latter two points give rise to rather stringent requirements to the model. First, a detailed grain-based mesh may have a very large number of degrees of freedom. On the other hand, although one has to assume that the material behaviour within the grain is known, it may in fact differ from the behaviour of a larger amount of the same material (such as a large single crystal or polycrystal). The consideration of an intermediate scale may be helpful here, whereby the FE computation is post-processed to provide some selective averages across the grain ensemble. In that case, constitutive equations are satisfied for each grain, while certain other criteria are only verified “in average”. Note that the influence of the neighbourhood on the results is

still present, as the response of any individual grain is modified due to the presence of the surrounding grains constraining it. This is distinct from self-consistent formulations, where e.g. all grains having similar properties or orientation are considered as a “phase” regardless of their geometrical location in the aggregate.

For the computations of RVEs, homogeneous boundary conditions in strain or stress, periodic boundary conditions or mixed boundary conditions can be applied. Finite Elements require the use of a mesh representing the microstructure. A systematic way for meshing of interfaces is possible in particular in the case of Voronoï polyhedra using standard 2D and 3D free meshing techniques. Examples of 2D and 3D polyhedra generation are shown in Figure 7.1.

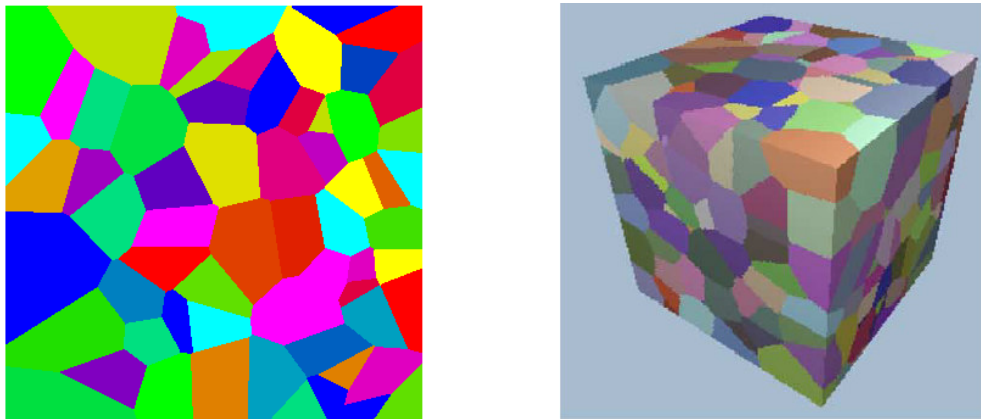


Figure 7.1 Simulation of Voronoï polyhedra: 3D distribution (right); section of cube made of Voronoï polyhedra with a periodicity constraint at the boundary (left).

The method can be compared with morphogenetic process of nucleation and growth from random seeds. It is quite relevant to the present study, and gives rise to planar grain boundaries. For a given nuclei distribution, Voronoï polyhedra are the influence zone assigned to each nucleus. Under the assumption of isotropic and steady state growth, boundaries between different solid volumes are described by the polyhedra.

In the current implementation the polyhedra are specified at a given resolution, defined by the size of the three-dimensional domain (cubic RVE). A particular set of

seeds, each corresponding to the centre of the grain, is distributed within the domain. Each Gauss point within the 3D domain is associated with the properties of its closest seed. The simplest way to distribute centres of polyhedra is to use a Poisson process. In this case, all points are independently distributed with a uniform spatial density of probability. A repulsion distance can also be introduced in an iterative process in order to control distance between points.

7.2.4 Representation of the RVE: meshing and Gauss point properties specification

The polycrystalline volume is discretised as a regular cubic mesh and the material properties are distributed at each Gauss point. The main advantage of this technique is that flexible descriptions of the polycrystalline structures can be generated automatically, allowing large numbers of microstructure *implementations* to be produced, and statistical variation of the results to be considered. In this approach the mesh itself is best chosen to regular and ‘static’, with grain orientation prescribed at integration points. This may lead to elements possessing points belonging to two or more different grains, so that grain boundaries are smeared out. This means that the grain boundaries are not as sharply defined as they would be using grain-based meshing of the boundary polyhedra. In this study we compare the two approaches, and show that the former, less computationally expensive ‘static’ mesh does not present a problem when computing average values within the grains, and only constitutes a limitation for the computation of the localisation of deformations at grain boundaries.

The relationship between the number of elements used for the finite element discretisation and the number of grains within an RVE presents an interesting

question. Barbe et al. and Diard et al. [96-98], looking at FCC and HCP crystals respectively, established some guidelines for the number of Gauss points needed to achieve good results at different levels of refinement. In particular, Diard et al.[98] conclude their work with some practical recommendations on the necessary number of elements per grain for providing good predictions and descriptions of macroscopic responses, average values in each grain, and the local stress and strain fields inside the grains. Average stress–strain curves over the whole aggregate can be provided with a good accuracy with only one 20-noded element per grain. This means 27 integration points per grain (small strain computations). It should be emphasized that the type of element used is significant, and higher order elements are preferred. Statistical distributions and grain-by-grain values of mean stress and strain in each grain can be captured with an $18 \times 18 \times 18$ mesh or slightly less. The lower bound of around 350 integration points per grain is proposed for obtaining average values for each grain with an error lower than 1%. Local results and intragranular heterogeneities are more sensitive to the mesh density, with discrepancies localized near grain boundaries.

Since material properties are prescribed at each Gauss point, for the formulation described in section 2.1 the definition of grain orientations is needed with respect to a global coordinate system. This enables the determination of slip system orientation of every single grain within the RVE, and the use of appropriate rotation matrix for the computation of the local elastic stiffness associated with each grain.

Three Euler angles (ϕ, ψ, θ) are needed to represent the spatial orientation of the single crystal with respect to the laboratory coordinate system. In order to assign the Euler angles to every single crystal present in the RVE, a ship analogy can be used (Figure 7.2).

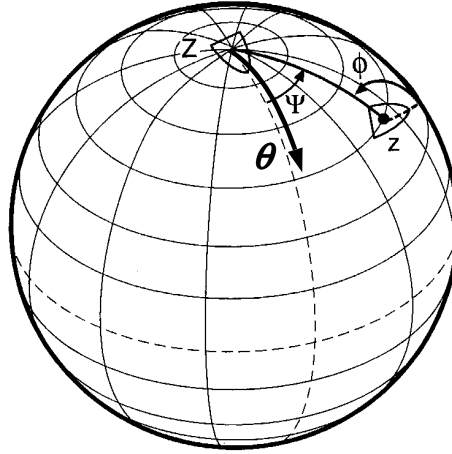


Figure 7.2 Ship analogy for the definition of the single crystal orientation in respect to the specimen global coordinate system.

The single crystal orientation is described by the position and heading of a boat with respect to the globe (the global system of the RVE). *Longitude* (ψ or p) and *latitude* (θ or t) describe the position of the boat; third angle describes the *heading* (ϕ or f) of the boat relative to the line of longitude that connects the boat to the North Pole.

7.2.5 Polycrystal finite element implementation

In the present study we consider the deformation behaviour of a pure HCP polycrystalline alloy, and validate the modelling predictions against some experimental measurements of elastic strains by high energy X-ray diffraction on the near- α titanium alloy Ti-6Al-4V.

An HCP crystal structure may have a total of 30 slip systems: 3 basal $\langle a \rangle$, 3 prismatic $\langle a \rangle$, 6 pyramidal $\langle a \rangle$, 12 1st-order pyramidal $\langle c+a \rangle$, and 6 2nd order pyramidal $\langle c+a \rangle$, which are illustrated in Figure 7.3.

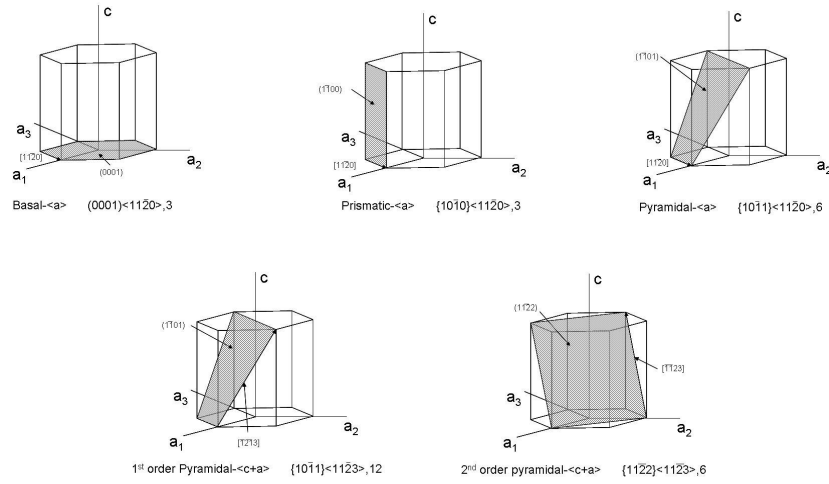


Figure 7.3 Illustration of 30 HCP Ti-6-4 slip systems.

The crystal plasticity constitutive model requires setting the initial critical resolved shear stress for each slip system τ_c^α , and the hardening moduli matrix $\mathbf{h}_{\alpha\beta}$. There are many forms suggested for the hardening modulus matrix. Here we have taken one of the simple forms suggested by Peirce et al.[99]:

$$\mathbf{h}_{\alpha\beta} = \left[q + (1-q)\delta_{\alpha\beta} \right] h, \quad (7.4)$$

with h denoting the self-hardening rate and the parameter q , with values in the range $1 < q < 1.4$, representing a latent-hardening parameter. The latent-hardening parameter q is not necessarily a constant, and may of course be history-dependent, in the same way as the self-hardening parameter h . This simple form for $\mathbf{h}_{\alpha\beta}$ yields an acceptable description of the physical phenomenon of latent hardening.

In order to optimise the model, three plasticity parameters need to be determined: the initial critical resolved shear stress, τ_c^α , the self-hardening rate h and the latent-hardening ratio q . In addition, the knowledge of (anisotropic) elastic moduli is required.

The monotonic and cyclic stress-strain experimental data for Ti-6-4 alloy were used to calibrate the plasticity parameters required. Preliminary results and

considerations about the efficiency of the model in describing classical results from the literature and the implementation of elastic anisotropy within the finite element framework will be discussed in the next section.

The crystal plasticity constitutive equations were implemented into a user-defined material subroutine within the ABAQUS nonlinear finite-element solver. Random crystallographic orientations for each grain were generated. All Gauss points falling within a grain were therefore allocated the crystallographic orientation corresponding to that grain.

The type of geometrical aggregates shown in Figure 7.1 can be used to investigate grain average stress-strain and displacement fields, but also to contribute to a better knowledge of the state of stress and strain in a current point of a polycrystal, and in more critical areas like the vicinity of the surface or at the grain boundaries. However, to be significant for these critical areas, the calculation must involve a reasonable number of grains and a reasonable number of elements in each grain. Here we are only interested in a model which would allow the computation of the average values at a “mesoscopic” level (across grains), capable of analyzing multiple ‘realizations’ of microstructure with the same statistical parameters (texture, grain size distribution) and allowing statistical variation of properties to be studied. At the same time we want to avoid very bulky computations that will take too much CPU time to run.

The best compromise has been achieved by iterative analyses of the RVE using different elements, number of elements employed for the regular mesh and number of grains (or “phases”) allocated within the RVE. Good results in terms of average macroscopic response of the material, together with the average values of the properties within the grains have been achieved using an $8 \times 8 \times 8$ ‘static’ regular

rectangular mesh, and 600 grains. This allows for a relatively quick computation of LCF cycles (5 full cycles at 1% deformation require 20 hours on a single processor workstation).

Multiphase polycrystals were generated by assigning to a random distribution of seeds different sets of crystal orientations. A random set of orientations is obtained by distributing the Euler angles uniformly within the domain (using Bunge's notation, Figure 7.2):

$$\begin{aligned} 0 < \psi < 2\pi \\ 0 < \phi < 2\pi \\ -1 < \cos(\theta) < 1 \end{aligned} \tag{7.5}$$

By varying the angular distributions it is possible to prescribe different textures. Grain size distribution can also be controlled by prescribing seed locations and anisotropic distance measures.

In all the analyses presented here the RVE was subjected to uniaxial controlled displacement cycling. Different boundary conditions have been applied to the RVE. The initial configuration is depicted in Figure 7.4.

The front face of the cubic RVE was subjected to normal displacements, while the back face was fixed from displacing in the same direction. Symmetric boundary conditions were prescribed on the two pairs of side faces. Alternatively, side faces could be either left free to displace in any direction, or periodically linked. Periodic boundary conditions also require the use of a periodic microstructure; this could be generated using a separate algorithm implemented in a FORTRAN subroutine outside the main UMAT, as illustrated but the result in Figure 7.5, where the contour map shows different orientations of grains within the RVE. It is apparent that grain

3D visualization of a cube element (8 elements) with nodes and displacement vectors. The cube is shown in a 3D coordinate system with axes 1, 2, and 3. The nodes are marked with blue and orange arrows indicating displacement vectors. The text at the bottom indicates the step and time: Step: Step=1, Increment: 21, Step Time = 100.0, Deformed From: U, Deformation Scale Factor: +1.000e+00.

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stress, strains and local displacements within a single grain varied noticeably both due to the change of microstructural realisation (from random to “random periodic”) and side conditions, the stiffest configuration resulting from symmetric boundaries.

7.2.6 Calibration and validation of the model

One of the requirements for the implementation of adequate crystal constitutive model is the use of the appropriate elastic stiffness matrix. While in some single crystals elastic response is close to isotropic (e.g. aluminium), in most HCP metals elastic anisotropy must be taken into account.

A general procedure for the implementation of elastic anisotropy and the transformation of the elastic stiffness matrix from the local (crystal) to global (laboratory) system has been developed, and comparison between predictions obtained using elastically isotropic and anisotropic models has been made here.

Elasticity requires tensorial description. Linear elastic coefficients appearing in the relations between strain, $\boldsymbol{\varepsilon}$, and stress, $\boldsymbol{\sigma}$, may be assembled either into a compliance tensor, written $\mathbf{S}$, or into a stiffness tensor, written $\mathbf{C}$. It is written, in the vector-tensor notation using double dot “:” to signify the inner product (i.e. summation of products over two common indices), as:

$$\begin{aligned}\boldsymbol{\sigma} &= \mathbf{C} : \boldsymbol{\varepsilon} \\ \boldsymbol{\varepsilon} &= \mathbf{S} : \boldsymbol{\sigma}\end{aligned}\tag{7.6}$$

In *component* form:

$$\begin{aligned}\sigma_{ij} &= C_{ijkl} \varepsilon_{kl} \\ \varepsilon_{ij} &= S_{ijkl} \sigma_{kl}\end{aligned}\tag{7.7}$$

Now the elastic moduli (stiffnesses or compliances) of the single crystal in the laboratory coordinates must be described. A 6×6 *matrix* (or Voigt) notation is

adopted for convenience. If the stress and strain tensors are written in the *6-vector* notation, then the elastic tensors are reduced to *6×6 matrices*. The stress and strain become:

$$\begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{pmatrix} \longleftrightarrow \begin{pmatrix} \sigma_1 & \sigma_6 & \sigma_5 \\ \sigma_6 & \sigma_2 & \sigma_4 \\ \sigma_5 & \sigma_4 & \sigma_3 \end{pmatrix} \longleftrightarrow (\sigma_1, \sigma_2, \sigma_3, \sigma_4, \sigma_5, \sigma_6) \quad (7.8)$$

$$\begin{pmatrix} \epsilon_{11} & \epsilon_{12} & \epsilon_{13} \\ \epsilon_{21} & \epsilon_{22} & \epsilon_{23} \\ \epsilon_{31} & \epsilon_{32} & \epsilon_{33} \end{pmatrix} \longleftrightarrow \begin{pmatrix} \epsilon_1 & 1/2\epsilon_6 & 1/2\epsilon_5 \\ 1/2\epsilon_6 & \epsilon_2 & 1/2\epsilon_4 \\ 1/2\epsilon_5 & 1/2\epsilon_4 & \epsilon_3 \end{pmatrix} \longleftrightarrow (\epsilon_1, \epsilon_2, \epsilon_3, \epsilon_4, \epsilon_5, \epsilon_6)$$

Pairs of indices are substituted with single indices, so that *matrix* $C_{11} = \text{tensor}C_{1111}$, according to the following table

Tensor	11	22	33	23	32	13	31	12	21
Matrix	1	2	3	4	4	5	5	6	6

If the material is anisotropic, the stiffness matrix is affected by the change of coordinate system from local (crystal) to global (laboratory). Rotation of the stiffness matrix is obtained using the transformation rule that involves a rotation matrix for stiffness, $[\mathbf{M}]$:

$$[\mathbf{C}_G] = [\mathbf{M}][\mathbf{C}_L][\mathbf{M}]^T \quad (7.9)$$

where subscripts G and L refer to the global and local coordinate systems, respectively. Matrix $[\mathbf{M}]$ can be explicitly derived as a *6×6 matrix* with terms that are trigonometric functions of the three Euler angles defined previously.

Once the rotation has been implemented into the UMAT, comparisons between the material responses induced by different elastic matrix (but having the same plastic properties) could be performed.

Note that the same macroscopic Young's modulus E can arise from various combinations of independent elastic single crystal constants. The stiffness matrix in the local (crystal) axes has the form:

$$\mathbf{C}_L = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{13} & 0 & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{bmatrix}, \quad (7.10)$$

and contains 6 independent stiffness terms.

A comparison was made between the predictions of elastically isotropic and anisotropic models that were implemented in the code so that the same macroscopic Young's moduli were recovered. The comparison of the macroscopic response of the material under uniaxial load is plotted in Figure 7.6. It should be noted that the onset of plasticity and the plastic behaviour are both affected by the choice of isotropic or anisotropic elasticity of the material.

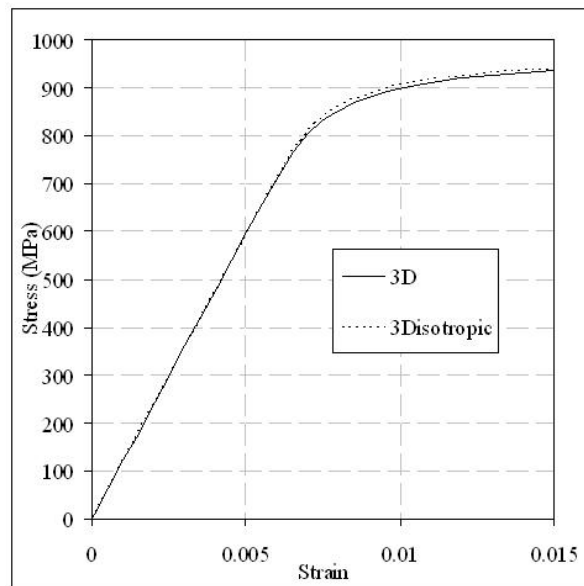


Figure 7.6 Influence of anisotropic and isotropic moduli.

The monotonic stress-strain data for Ti-6Al-4V were collected at 20°C, and

used in this work for two purposes:

1. To calibrate the elastic stiffness
2. To compare different realizations, and determine suitable element size/number of grains to use for routine calculations to match the LCF macroscopic response.

The anisotropic elastic stiffness matrix which leads to the best match of the experimental monotonic results was (in the Voigt notation): $C_{11}=160\text{GPa}$, $C_{33}=181\text{GPa}$, $C_{44}=465\text{GPa}$, $C_{66}=465\text{GPa}$, $C_{12}=900\text{GPa}$, $C_{13}=660\text{GPa}$. The plastic parameters used were: no hardening ($h=0$) and critical resolved shear stress $\tau_c^a=353$ MPa (basal $\langle a \rangle$), 397 MPa (prismatic $\langle a \rangle$), and 441 MPa (pyramidal $\langle a \rangle$), and 503 MPa (1st and 2nd order pyramidal $\langle c+a \rangle$). In order to identify the most suitable material model, various RVEs (all unit cubes) were considered with different resolutions in terms of the mesh size and number of grains. These were subjected to the same strain-controlled monotonic loading. Figure 7.7 shows the result for one of these numerical computations which gives the best approximation to the experimental tensile test result. The FE model plot is from an $8 \times 8 \times 8$ mesh and the number of grains was equal to 600. This is also the discretisation of the RVE that was adopted for the characterisation of the LCF behaviour of the HCP Ti-6Al-4V alloy.

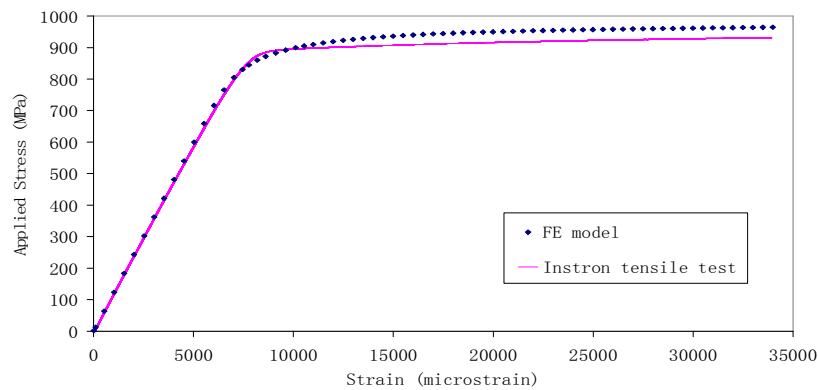


Figure 7.7 Comparison of stress-strain response between FE model prediction and Instron tensile test.

In the previous section the concept of using the RVE was introduced in order to represent polycrystalline aggregate mechanical model at the scale of between 0.1 μm and 1 mm. However, attempts are often reported in the literature of using two-dimensional simplifications (e.g. plane strain or plane stress models) as a means of reducing the computational cost. In the 2D case, the RVE may take the form of a unit square. However, such plane models of the 3D phenomenon of crystal slip require careful reduction from the real three-dimensional geometry.

In the present study, we used an ensemble of 64 grains represented by a ‘static’ square 8×8 mesh using eight-noded plane strain or plane stress elements was employed, and comparison against the 3D model made (Figure 7.8).

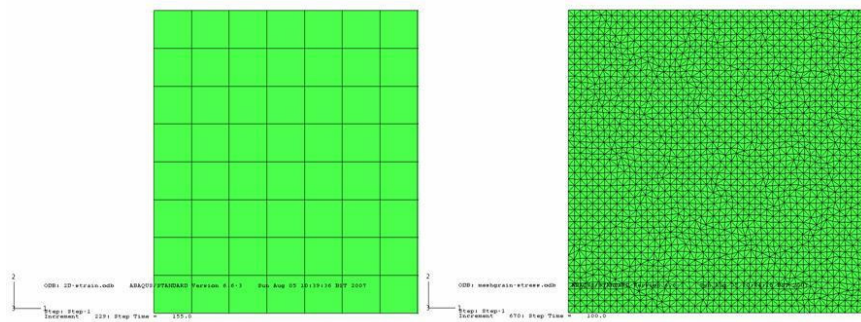


Figure 7.8 2D model set-up with RVE square mesh (left) and grain mesh (right)

The 4×4 plane strain and 3×3 plane stress stiffness matrices had to be computed specially within the UMAT in order to satisfy the element type requirements, and the number of stress components updated at each increment of the computation had to be modified accordingly.

The use of plane-strain elements to simulate uniaxial loading in the case of isotropic material means that the plane-strain-compensated elastic modulus $E(1-\nu^2)$ must be used in the calculations, when comparisons were made with plane stress or 3D experimental results. In the case of anisotropic material this meant that the stiffness matrix had to be scaled by the factor $(1-\nu^2)$, where ν is the macroscopic

Poisson's ratio. Although this allows achieving a reasonable match with the 3D and plane stress simulations, this arrangement is clearly somewhat unsatisfactory.

Strain-controlled uniaxial tests at the strain amplitude of 1.5% were carried out on the 2D RVE, and the resulting macroscopic stress calculated, at any moment in the simulation, by summing up the nodal reaction forces on the displaced edge, and dividing the resultant force by the current cross-sectional area. The 3D model stress-strain loop is also shown in Figure 7.9 as comparison.

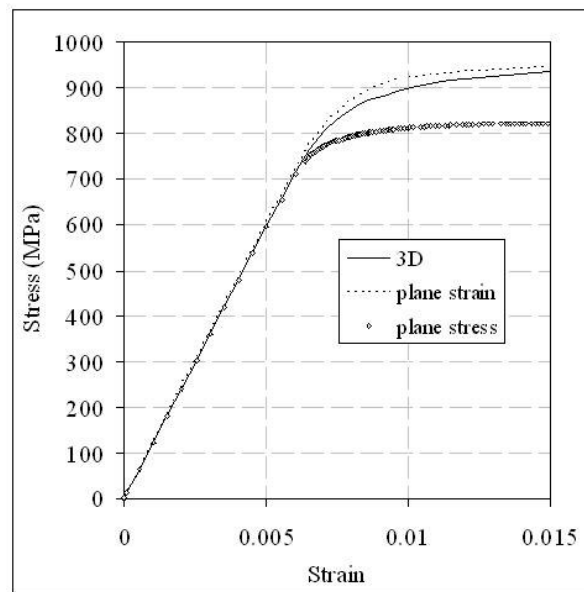


Figure 7.9 Stress-Strain curve comparison between plane stress, plane strain and 3D models.

Although the three models considered (3D, plane strain and plane stress) have approximately similar yield strengths, they clearly behave differently in the plastic regime. While the 3D matches tensile test results reasonably well, plane strain and plane stress models do not deliver the same quality of agreement. More importantly, the assumptions required in order to obtain 2D simplifications ($\sigma_{13} = \sigma_{23} = \sigma_{33} = 0$ or $\epsilon_{13} = \epsilon_{23} = \epsilon_{33} = 0$) impose restrictions on crystal slip in the 3rd direction, causing the stress concentration in certain areas that are in fact not physical, but represent merely artefacts of the model. This phenomenon is especially common at grain boundaries,

since they correspond to locations where different slip systems interact. Figure 7.10 shows local stress concentrations in plane stress (on the left) and plane strain (on the right) simulations under 1.5% strain-controlled extension.

Stress concentration influences stress distributions within elements that contain Gauss points belonging to more than one grain. To avoid the loss of microscopic fidelity caused by this phenomenon, grain-based meshing may be employed, so that the orientation and initial mechanical properties of each Gauss point within an element are identical. Figure 7.8 shows the layout of such a grain mesh. Figure 7.9 shows stress-strain curve comparison between a ‘static’ square mesh, and a grain-based mesh results.

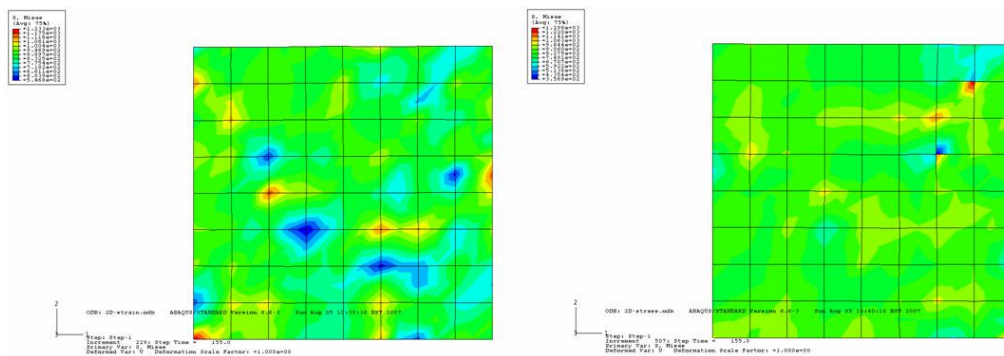


Figure 7.10 Stress concentration map for plane strain (left) and plane stress (right) model

Although grain meshing delivers an improvement in the macroscopic stress-strain curve agreement with 3D results (especially for plain strain analysis) and stress concentration within grains is no longer a problem, the grain-mesh method requires much greater numbers of nodes than the square-mesh method. Our 2D grain-mesh model contained 2601 nodal points, comparing with 2673 in the 3D ‘static’ mesh model. It is clear that grain meshing is relatively costly and is an unlikely choice for a simplified model aimed at reducing CPU time.

Numerical results obtained from the FE model need to be process in order to extract the information that can be compared with experimental measurements, be it

tensile test data or diffraction patterns. Post-processing enables one to obtain average strain values within grain families. “Grain family” here refers to the subset of grains which contribute to a particular diffraction reflection along a certain scattering direction. For instance, considering the loading direction only, the hkl grain family comprises all grains in which an hkl plane normal lies within the solid angle of a few degrees from the tensile axis.

Our mesoscopic approach to the FE implementation has the advantage that material properties and orientations are assigned to Gauss points. Hence, it is straightforward to predict which of the grains would eventually contribute to a hypothetical diffraction experiment carried out on it. Once the grain groups have been identified, the lattice strains computed at each time increment can be extracted from the state variables computed in the UMAT. A post-processor then automatically generates average elastic strain within each grain family. This allows the evolution of the average strain during loading of the RVE to be compared with experimental results.

Tensile test specimens were made from the Ti-6Al-4V alloy in the form of dog-bones with the cross section of $3 \times 3 \text{ mm}^2$. The sample was mounted in the Instron universal testing machine on the high energy X-ray scattering beam line (ID15) at European Synchrotron Radiation Facility (ESRF) in Grenoble, France. The *in situ* loading experiment was performed in the white beam energy dispersive mode, allowing multiple Bragg peaks to be measured simultaneously. The gauge volume was defined using 0.2 mm slits in both the incident and diffracted beam paths, and 2θ scattering angle of 5° . The irradiated volume in the sample was a parallelepiped of $0.2 \times 0.2 \text{ mm}^2$ cross section and 2.3 mm in length. The sample was loaded incrementally in 500N steps and held at the prescribed load level while diffraction

data were collected. The data acquisition time was 120 seconds. The loading axis was perpendicular to the incident beam and the twin-detector setup allowed simultaneous measurements of strains parallel to the loading direction and in the other direction perpendicular to both the beam and the loading direction.

The principle of elastic lattice strain measurement by diffraction relies on the fact that when a crystal is deformed elastically, the inter-planar spacing within it changes. In a polycrystal this phenomenon leads to observable shifts of multiple diffraction peaks. From each peak, elastic lattice strains can be obtained for crystallites oriented such that the particular hkl plane normal is parallel to the scattering vector. The diffraction spectra were analyzed by single peak fitting of individual hkl reflections and by Pawley refinement of the whole spectrum using General Structure Analysis System (GSAS).

Data for the longitudinal and transverse strains predicted from the FE model is plotted in Figure 7.11 and Figure 7.12, respectively.

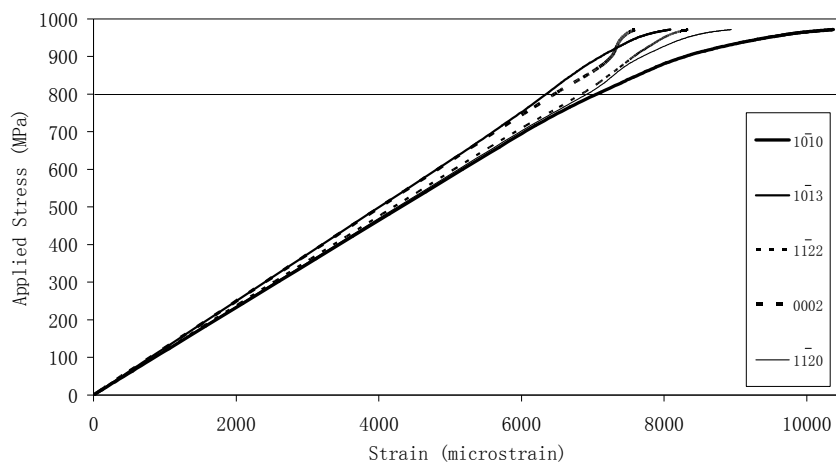


Figure 7.11 hkl longitudinal stress-strain response of Ti64 from the FE model prediction, with plane normal parallel and perpendicular to the applied load.

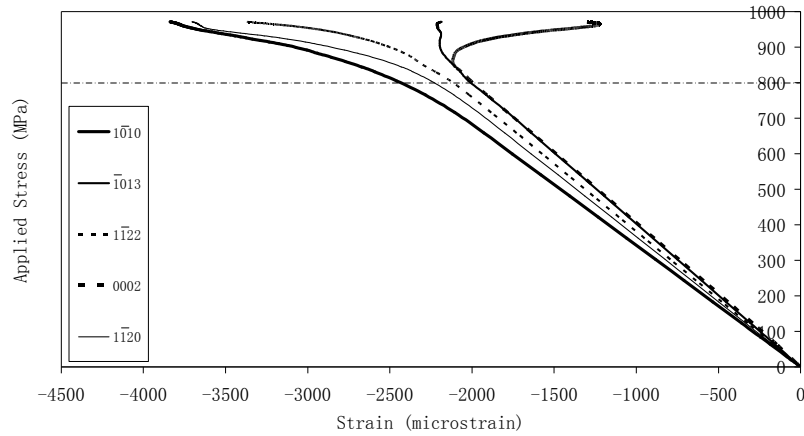


Figure 7.12 hkl transverse stress-strain response of Ti64 from the FE model prediction, with plane normal parallel and perpendicular to the applied load.

The responses of individual planes show linear behaviour (but different slopes) until reaching their own elastic limits. The individual tensile stiffness for each lattice plane varies from 107.7GPa for (100) plane to 132 GPa for (103) plane (Figure 7.11), with an average macroscopic Young's Modulus of 115GPa. The low symmetry of the HCP structure causes the highly anisotropic behaviour. The stress-strain curves from different lattice planes become even more divergent from the onset of plasticity. Some of the grain groups even show sign of strain relaxation (i.e. (002) plane) in transverse direction (Figure 7.12).

Figure 7.13 shows the comparison between FE model predictions and measurements from diffraction experiments for the $10\bar{1}0$ and $10\bar{1}2$ grains. Smooth curves without markers illustrate FE predictions, while the curves with markers correspond to the data obtained from diffraction experiments.

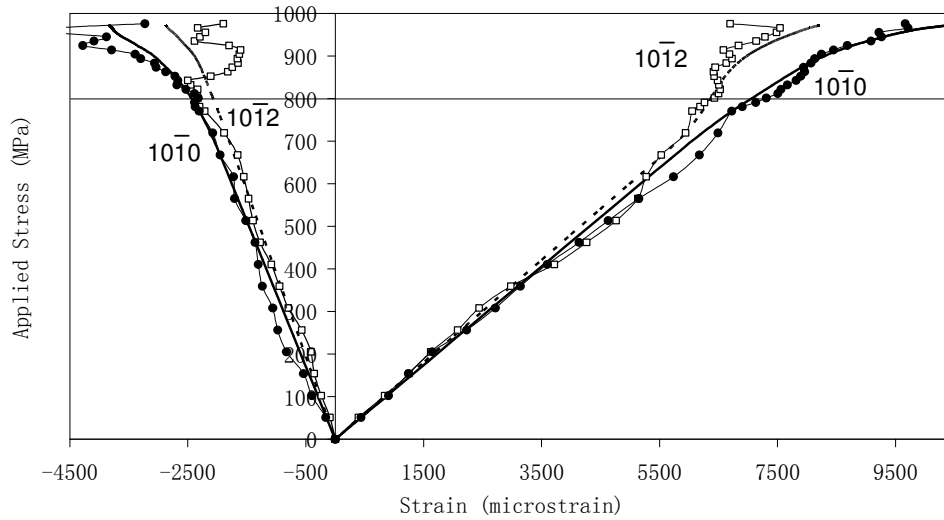


Figure 7.13 Comparison of FE simulation of Ti64 alloy to experimental data.

It is apparent from Figure 7.13 that the calibrated FE polycrystal elasto-plastic model predicts trends that are in good agreement with the experiment. Although the nominal errors of single diffraction peak fitting are very low (of the order of marker sizes in the Figure), these only reflect the accuracy of determination of the peak centre positions for grains that contribute to diffraction within the gauge volume. In practice this is further affected by other experimental uncertainties. The trends of the evolution of hkl elastic lattice strains with external loading (represented by the macroscopic applied stress plotted on the vertical axis) appear to be captured well.

It is reasonable to argue that, provided both the total macroscopic strain *and* the individual meso-average hkl elastic lattice strains are computed correctly, the meso-level plastic strains are also likely to be correct. This assertion is difficult to verify directly, but the current results go some way towards that direction.

7.3 Strain Gradient Crystal plasticity modelling of near- α phase Ti-6Al-4V and forward construction of diffraction peaks

As demonstrated in last section, the crystal plasticity model can capture the grain group average elastic strain reasonably well. In the diffraction experiment point

of view, it is the correct correspondence in terms of diffraction peak center positions. However, the diffraction patterns contain large amounts of further information that also needs to be understood, e.g. the relationship between the peak width and plastic deformation within the grain group. This analysis could provide a wealth of information about the material character, deformation history and dislocation activities.

The view taken in the present study is that a dislocation-based crystal plasticity theory must be adopted in order to obtain the correct interpretation of diffraction peak shapes in deformed metallic polycrystals. Below a time-dependent strain gradient crystal plasticity (SGCP) implementation is presented that incorporates the description of dislocation structure evolution, enabling the forward prediction of diffraction patterns on the basis of simulation results. This not only gives a means of gaining prior knowledge of the expected XRD results, but also provides a direct verification of the numerical model not relying on reverse interpretation of experiment data. It reveals the capability of the SGCP model to simulate the material microscopic deformation, which is further exploited in Chapter 8.

7.3.1 Configuration of the Representative Volume Element (RVE) and Microstructure Representation

In the current study a $0.2\text{mm} \times 0.2\text{mm} \times 0.2\text{mm}$ cube-shaped RVE was employed that consists of 600 grains, the same as the previous setup used for crystal plasticity modelling. The size of the RVE coincides with the XRD gauge volume, and the average grain size of the material under investigation is also matched. Grain orientations are randomly generated via the selection of rotations described by the Euler angles by a pre-processor that also prescribes the positions of grain “seeds”

(centres). The grains are “grown” isotropically from the “seeds” to form the 3D Voronoi tessellation morphology.

It is well established that for 3D Poisson-Voronoi tessellation, given enough number of grains, the distribution of the grain size follows a lognormal distribution[100]. In the current setup, the distribution gives an average grain size of 23.71 μm and standard deviation of 0.49. These parameters are later used for diffraction peak shape analysis.

In the previous section the deformation of the near- α titanium alloy Ti-6Al-4V with the total of 30 slip systems was simulated. However, it was found out that it is computationally redundant to simulate 30 slip systems simultaneously, as in reality the 1st and 2nd order pyramidal $\langle c+a \rangle$ are significantly more resistant to slip than the other 12 $\langle a \rangle$ slip systems. In order to reduce the computational effort, the slip in the HCP crystal structure in the present model was reduced to 12 slip systems: 3 basal systems $\langle a \rangle$, 3 prismatic systems $\langle a \rangle$ and 6 pyramidal systems $\langle a \rangle$. (Fig. 14) The microstructure was implemented into the RVE with regular hexahedral $10 \times 10 \times 10$ mesh (C3D20R element type) and crystal lattice orientation assigned at each integration point (IP).

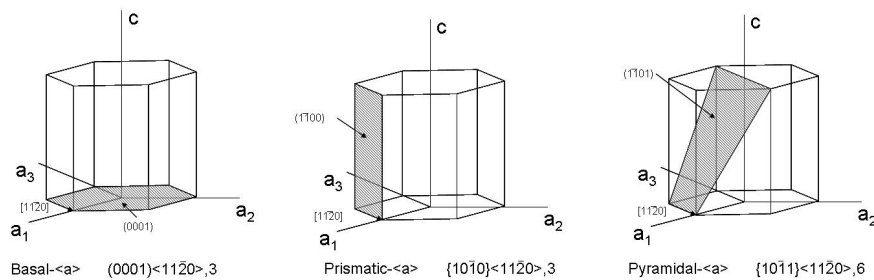


Figure 7.14 Twelve independent slip systems in the Ti-6Al-4V α phase HCP crystal.

7.3.2 A physically-based rate-dependent strain gradient crystal plasticity model: formulation

The present model has been implemented by the authors on the basis of the length-scale-dependent, rate-dependent formulation presented by Cheong and Busso [69]. Details of the formulation have been presented in Chapter 2. Only a very brief summary of the formulation is given here.

The formulation is built on the expression for the shear strain rate $\dot{\gamma}$ on a particular slip system α . This shearing rate is thermally dependent via a Boltzmann type exponential thermal activation expression, and also contains a dependence on the system-specific critical resolved shear stress and slip resistance (Eq. 7.11):

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \exp \left[- \frac{F_0}{k \theta} \left\{ 1 - \left(\frac{|\tau^{\alpha}| - S^{\alpha} \mu / \mu_0}{\hat{\tau}_0 \mu / \mu_0} \right)^p \right\}^q \right] \text{sgn}(\tau^{\alpha}) \quad (7.11)$$

The central element of the present dislocation-based deformation modelling approach is the system of evolution laws for the densities of edge and screw types of Statistically Stored Dislocations (SSD) and three types of Geometrically Necessary Dislocations (GND) (Eq. 7.12), and their contribution to the slip resistances on the corresponding planes (Eq. 7.13).

$$\rho_T^{\alpha} = \rho_S^{\alpha} + \rho_G^{\alpha} = (\rho_{S_e}^{\alpha} + \rho_{S_{sw}}^{\alpha}) + (\rho_{G_{sw}}^{\alpha} + \rho_{G_{et}}^{\alpha} + \rho_{G_{en}}^{\alpha}) \quad (7.12)$$

$$S^{\alpha} = [(S_S^{\alpha})^2 + (S_G^{\alpha})^2]^{\frac{1}{2}} = \lambda_s \mu b_s^{\alpha} \sqrt{\sum_{\beta=1}^N [h_s^{\alpha\beta} \rho_s^{\beta} + h_G^{\alpha\beta} \rho_G^{\beta}]} \quad (7.13)$$

The physical description of the SSD evolution captures both dislocation generation and annihilation mechanisms. The generation of dislocation loops is assumed to be related to the expansion of existing Frank–Read sources, and the annihilation is dominated by parallel dislocations of the same character (but opposite sign) reaching a critical distance. It is also taken into account that screw dislocations readily cross-slip (Eq. 7.14a), while edge dislocations do not (Eq. 7.14b):

$$\dot{\rho}_{S_e}^\alpha = \frac{C_e}{b_S^\alpha} [K_e \sqrt{\sum_{\beta=1}^N \rho_T^\beta} - 2d_e \rho_{S_e}^\alpha] |\dot{\gamma}^\alpha| \quad (7.14a)$$

$$\dot{\rho}_{S_{sw}}^\alpha = \frac{C_{sw}}{b_S^\alpha} [K_{sw} \sqrt{\sum_{\beta=1}^N \rho_T^\beta} - \rho_{S_{sw}}^\alpha \{K_{sw} \pi d_{sw}^2 \sqrt{\sum_{\beta=1}^N \rho_T^\beta} + 2d_{sw}\}] |\dot{\gamma}^\alpha| \quad (7.14b)$$

The GND contribution is closely linked to the emergence of plastic strain gradient, and thus causes size and scale dependent effects. This is described in Eq. 7.15:

$$b_G^\alpha (\dot{\rho}_{G_{sw}}^\alpha \mathbf{m}^\alpha + \dot{\rho}_{G_{et}}^\alpha \mathbf{t}^\alpha + \dot{\rho}_{G_{en}}^\alpha \mathbf{n}^\alpha) = \mathbf{curl}(\dot{\gamma}^\alpha \mathbf{n}^\alpha \mathbf{F}^p) \equiv \dot{\mathbf{\Lambda}} \quad (7.15)$$

It is important to note that in practice SSD and GND co-exist in deformed metallic (poly) crystals, so the separation of their contributions to overall deformation (hardening) behaviour is not a trivial task.

The FE implementation follows the framework outlined by Meissonier and Busso [55], further developed and simplified by Dunne [101]. The formulation is fully implicit and focuses on obtaining the spatial derivatives of the plastic deformation gradient by introducing a special shape function for internal Gauss points of the quadratic element.

7.3.3 Model parameter calibration against synchrotron X-Ray Diffraction experiment data

The data used for model calibration was collected from X-ray scattering experiments on the Ti-6Al-4V dog-bone sample loaded *in situ* with diffraction patterns collected simultaneously in the white beam mode with the beam size of 0.2×0.2mm [102].

The macroscopic tensile loading curve after instrument stiffness correction is presented in Figure. 7.15. The crystal elastic stiffness matrix for the dominant α -phase

obtained from the literature [103] was used to match the linear elastic part of the plot, while macroscopic nonlinear material behaviour is described by a set of five parameters in the flow rules: $(\dot{\gamma}_0, F_0, \tau_0, p, q)$. Two of these parameters are available from the literature [101]: $F_0 = 1.17 \times 10^{-19} (J)$ and $\tau_0 = 260 (MPa)$. The three remaining parameters were adjusted by fitting the macroscopic stress-strain curve. Since the range of these parameters is limited [69], this procedure readily yields the following values: $\dot{\gamma}_0 = 1 \times 10^{-6}$, $p = 0.05$, $q = 1.95$.

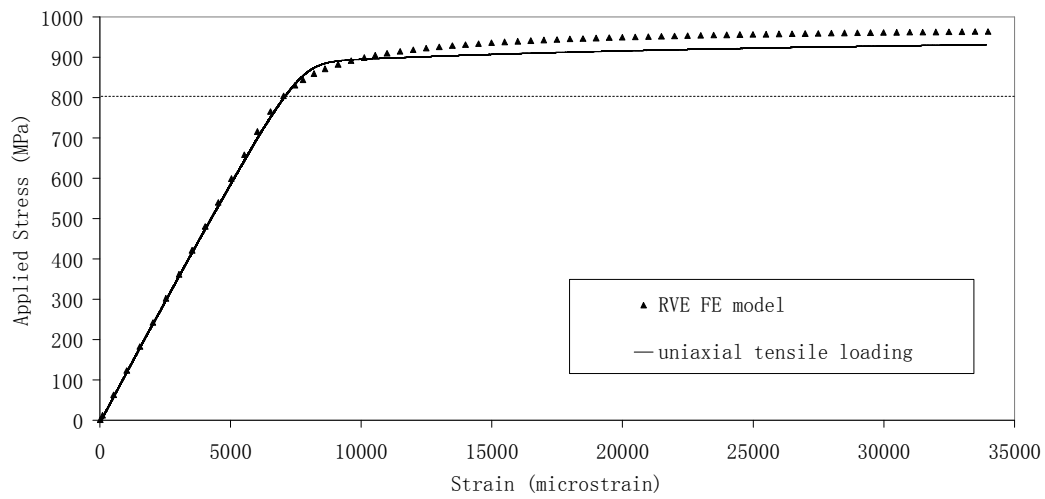


Figure 7.15 Comparison of macroscopic stress-strain curves between FE prediction and in situ tensile testing.

The remaining material parameters were then calibrated against the “grain family” stress-strain curves. “Grain family” here refers to the subset of grains which all contribute to the same particular reflection in a certain scattering direction. An *ad hoc* post-processor for the model was developed to identify the grains belonging to certain groups, allowing orientation-specific averages to be extracted. The remaining material parameters within the model, namely $(K_e, K_{sw}, d_e, d_{sw})$, were tuned against the measurement results from diffraction experiments for the $10\bar{1}0$ and $10\bar{1}2$ reflections in both elastic and plastic regions. (Figure. 16) The vertical axis represents the macroscopic stress applied to the sample/model and the horizontal axis is the hkl lattice (elastic) strain response. Smooth curves without markers illustrate FE

predictions, while the curves with markers correspond to the data obtained from diffraction experiments. Bearing in mind that diffraction peaks in Ti-6Al-4V α -phase pattern outnumber the unknown parameters in the model, the problem is over-determined and reliable values for the parameters could therefore be found. Parameter values found were close to those reported in the literature [69].

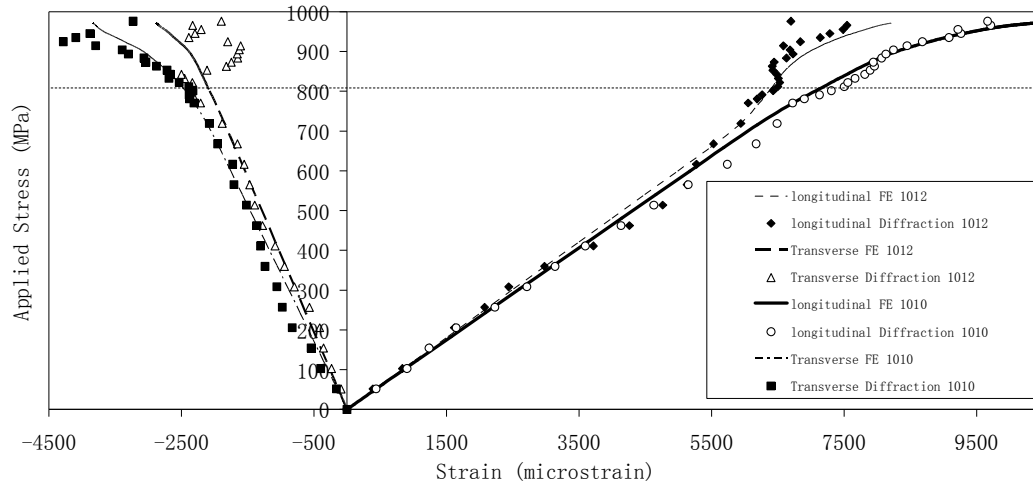


Figure 7.16 Post-processed FE simulation results with optimized parameters in comparison with the experimental diffraction data.

7.3.4 Diffraction peaks reconstruction

The post-processing procedure was developed further to allow the reconstruction of diffraction peaks. Peak centres could be readily calculated from the deviation of the average lattice parameter from its original (unstrained) value. To predict the peak shape, the framework introduced by Ribarik and Ungar [104] was employed. The formulation relies on the use of Fourier coefficients to reflect the broadening effects due to grain size distribution A^s , local lattice distortion A^D and instrumental broadening A^I , (Eq. 7.16)

$$A(L) = \frac{A^s(L)}{A^s(0)} A^D(L) A^I(L) \quad (7.16)$$

$$A^S(L) = \frac{m^3 \exp\left[\frac{1}{3}(9/4)(2^{\frac{1}{2}}\sigma)^2\right]}{3} \operatorname{erfc}\left[\frac{\log(|L|/m)}{2^{\frac{1}{2}}\sigma} - \frac{3}{2}2^{\frac{1}{2}}\sigma\right] - \frac{m^2 \exp(2^{\frac{1}{2}}\sigma)^2}{2} |L| \operatorname{erfc}\left[\frac{\log(|L|/m)}{2^{\frac{1}{2}}\sigma} - 2^{\frac{1}{2}}\sigma\right] + \frac{|L|^3}{6} \operatorname{erfc}\left[\frac{\log(|L|/m)}{2^{\frac{1}{2}}\sigma}\right] \quad (7.17)$$

$$A^S(0) = \frac{2m^3 \exp\left[\frac{1}{3}(9/4)(2^{\frac{1}{2}}\sigma)^2\right]}{3} \quad (7.18)$$

$$A^D(L) = \exp(-2\pi^2 g^2 L^2 \langle \varepsilon_L^2 \rangle) \quad (7.19)$$

$$\langle \varepsilon_L^2 \rangle \cong (b/2\pi)^2 \pi \rho C \ln\left(\frac{R_e}{L}\right) \quad (7.20)$$

The instrumental broadening was quantified by considering Si powder diffraction patterns used as calibration, due to the stress-free nature of the powder and the fact that particles exceeded several microns in size. The impact of the average grain size m and its standard deviation σ on peak shape is given explicitly by Eq. 7.17 and Eq. 7.18. In Eq. 7.19, given g is the absolute value of the scattering vector, the only unknown parameter is the mean square strain $\langle \varepsilon_L^2 \rangle$, which depends on the displacement of the atoms relative to their ideal positions. It can be expressed (Eq. 7.20) in terms of ρ , the dislocation density; C , the contrast factor for the dislocation; and R_e , the effective outer cut-off radius of dislocations. Given that the average (grain group level) dislocation density can be obtained from the model, we can further implement the functions above in to the post-processor with cosine Fourier transform function Eq. 7.21 to generate the entire diffraction pattern.

$$F(s) = 2 \int_0^{\infty} A(L) \cos(2\pi Ls) dL \quad (7.21)$$

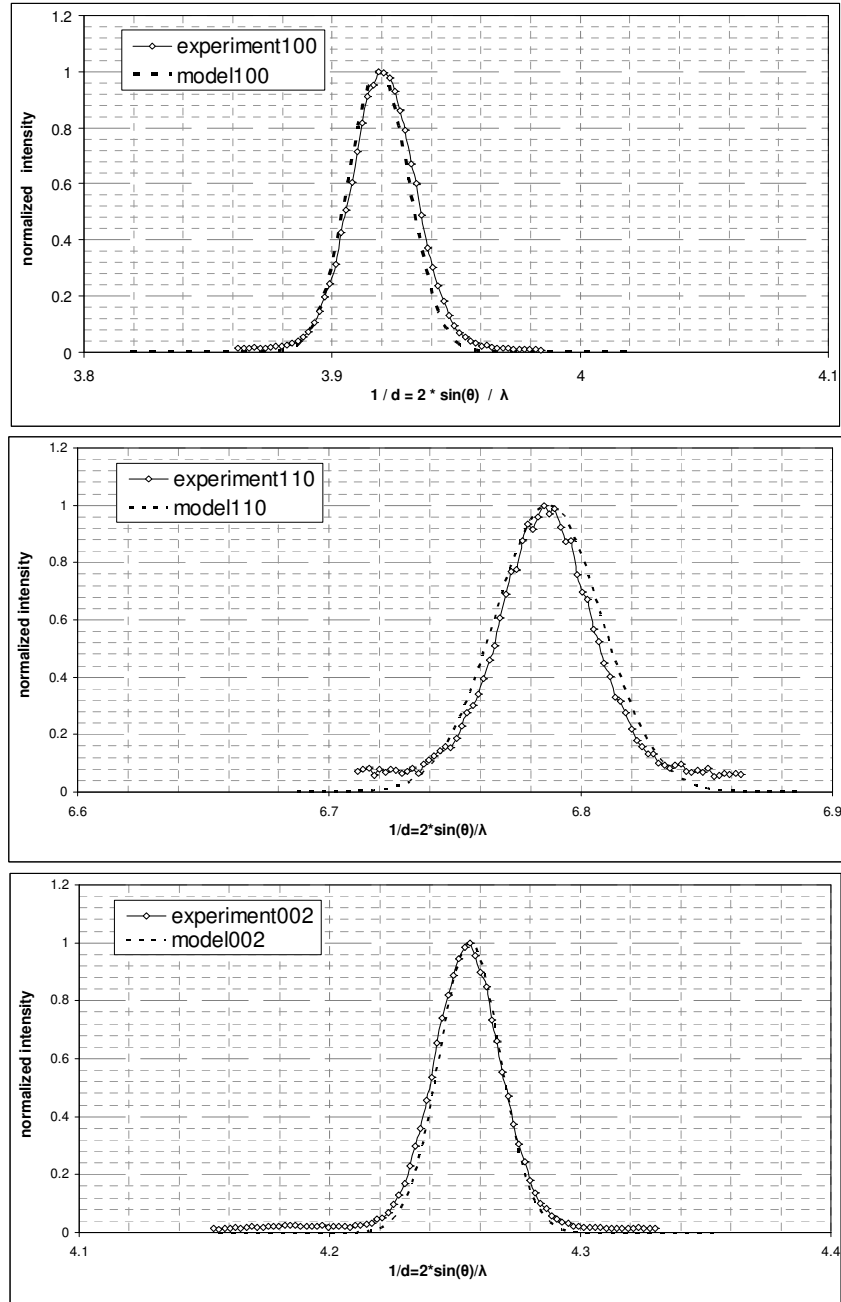


Figure 7.17 Comparison of peak predictions by the post-processor with diffraction data for different orientations.

Fig. 7.17 demonstrates the prediction capability of the post-processor. It is worth noting that all peaks are constructed simultaneously rather than individually. We conclude that the post-processor provides a good prediction of the diffraction

peaks, both in terms of their positions and widths (as measured e.g. by the Full Width at Half Maximum, FWHM).

7.4 Conclusion

It is apparent from Figures 7.11, 7.12 and 7.13 that the calibrated FE polycrystal plasticity model predicts the grain group average elastic strains that are in good agreement with the experiment. Based on this setup, a well-established strain gradient crystal plasticity algorithm was adopted to help reconstructing the entire diffraction pattern. Fig. 7.17 shows that the model successfully captures the distinctive features of individual peaks, i.e. the peak centre positions and peak widths. Thus, a unique tool for probing material deformation at the meso- to microscale has been developed. Combining it with other advanced diffraction techniques, it should be possible to obtain more insight into the microscopic lattice arrangement information, i.e. intra-granular elastic strain, local lattice rotation and misorientation, etc.

Chapter 8 3-D Microscopic Analysis of Elasto-Plastic Deformation in FCC Polycrystals

Strain Gradient Crystal Plasticity Modelling and Micro-beam Laue Diffraction of Polycrystalline Ni Foil

8.1 Introduction

The deformation behaviour of polycrystalline materials used to manufacture engineering components is crucial to the performance in service. Deformation does not occur uniformly in constituent grains, but shows strong inter- and intra-granular variations. They are caused by lattice misorientation, anisotropic elastic-plastic properties and different damage behaviour. Conventional continuum mechanics models in Chapters 4~6 do not capture the effects of complex grain shape, intra-granular strain variation and mesoscopic neighbourhood on the deformation of a particular grain. Hence, crystal plasticity theory [34, 65] was employed in last chapter to capture the mesoscopic inhomogeneity. Furthermore, length-scale effects in plasticity [38, 39, 52] must also be accounted for. This length-scale-dependent strengthening effect is due to the presence of plastic strain gradients, which leads to the development of geometrically necessary dislocations (GNDs) [45, 52, 71]. An explicit and succinct relationship between the two was found by Ashby [45] and generalized by Busso [55].

To obtain the information about the local variations of elastic strains and stresses experimentally, a technique with sufficient spatial resolution must be used. Micro-beam Laue diffraction is ideal for the purpose. By using the focusing mirrors or pinholes, sharp (sub)micron-sized white X-ray beams can be produced at synchrotron

sources. This creates a tool that can probe the deformation and crystal structure (including orientation) at the micron and sub-micron level [105, 106]. By analyzing Laue diffraction spots shapes, it is possible to obtain crystallographic information for the illuminated area, namely, the local lattice rotation and misorientation, deviatoric strain, lattice curvature, etc. This in turn can be related to the underlying dislocation structure and the presence of GNDs [79, 107-110]. It is also possible to pose the problem about the inverse analysis of the observed Laue spots, that is, about deducing from two-dimensional Laue spots the statistics of the underlying dislocation distribution. A less challenging and more straight-forward analysis step is to predict the Laue spot shapes from a known dislocation distribution - the so-called forward analysis. The output from the simulation-based predictions can be compared with the experimentally recorded Laue patterns. Judging from the results reported in the literature so far, the comparison between Laue diffraction results and the FE model simulation has been limited to the inverse analysis [111]. No forward prediction from strain gradient crystal plasticity FE models has been reported yet.

In this Chapter, we use the strain gradient crystal plasticity algorithm presented in the previous chapter, together with a newly developed model post-processor, to link the simulation of large grain pure Ni sample deformation to the prediction of the corresponding Laue diffraction patterns.

8.2 Rate and Gradient-Dependent Crystal Plasticity Modelling

8.2.1 Model configuration

In order to capture the inter- and intra-granular deformation, a realistic representation of the material's microstructure must be achieved. For this purpose we use a detailed "replica" model of the area characterised by micro-beam Laue

diffraction in our synchrotron experiments. The grain orientations were found from the analysis of Laue patterns using XMAS software [112], and the entire microstructure was then implemented in detail in a grain-based FE mesh (Figure 8.1). The scan area in the experiment was 4×2mm with the beam size of 50µm (square) and scan step size of 50µm. A pixellated the map of 80×40 pixels was collected. In the FE model, the material volume corresponding to each pixel (scan point) was represented by eight C3D20R elements (with 2 elements in each direction x, y and z), giving a total 64 IPs (Integration Points) per scan point (pixel), or 4 IPs in each direction. This choice was based on the reported studies of the sufficiency of FE discretisation to capture the intragranular deformation and local lattice misorientation [55]. The sample studied in the experiment was made from commercially pure Ni with FCC crystal structure having a total 12 {111} <110> slip systems.

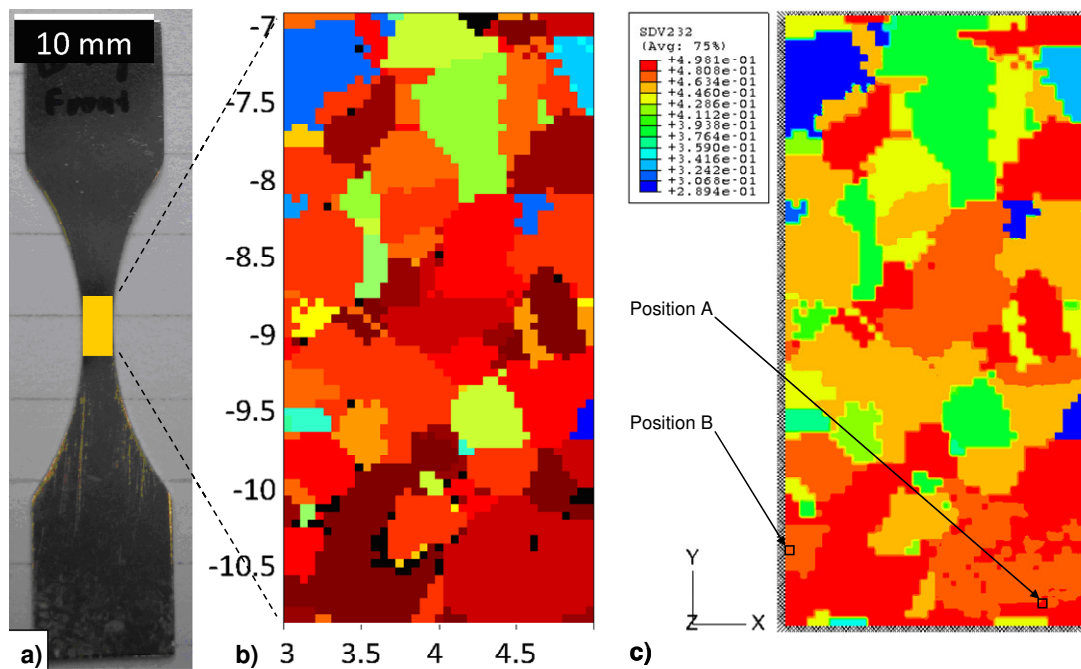


Figure 8.1 (a) Ni sample prior to deformation (b) Schmid factor map of the scan area analyzed by XMAS (c) Schmid factor map in FE model with two selected positions A and B

In order to visualize the grain morphology and orientation, the colour map used in Figure 8.1 corresponded to the Schmid factor with respect to tensile loading of the

sample along the y-axis. Figures 8.1(b) and (c) show the Schmid factor maps of the sample in the experiment and in the FE model, respectively.

8.2.2 Strain Gradient Crystal Plasticity (SGCP) model and parameter calibration

The FE simulation framework was adopted from that by Cheong and Busso [69] that was further developed by Dunne [101]. The incremental simulation algorithm have already been described in detail in Chapter 2, and employed in Chapter 7 to simulate the deformation of Ti-6Al-4V alloy. Here, the algorithm was modified to incorporate the material properties of large grained polycrystalline commercially pure Ni, and to simulate its intra-granular deformation. The majority of the model parameters were obtained from literature, while the remaining ones were calibrated using the monotonic stress-strain curve. The macroscopic tensile loading curve after the instrument stiffness correction is presented in Figure. 8.2. The elastic stiffness matrix was initially obtained from [113] with minor correction to match the linear elastic part of the current plot. The macroscopic nonlinear material behaviour was controlled by the flow rule parameters. Two of them were calculated on the data from the literature [113]: $F_0 = 1.8425 \times 10^{-19} (J)$ and $\tau_0 = 38.43 (MPa)$. The other three, whose ranges are limited [69], were adjusted by fitting the macroscopic stress-strain curve, giving $\dot{\gamma}_0 = 1 \times 10^{-6}$, $p = 0.2$, $q = 1.2$.

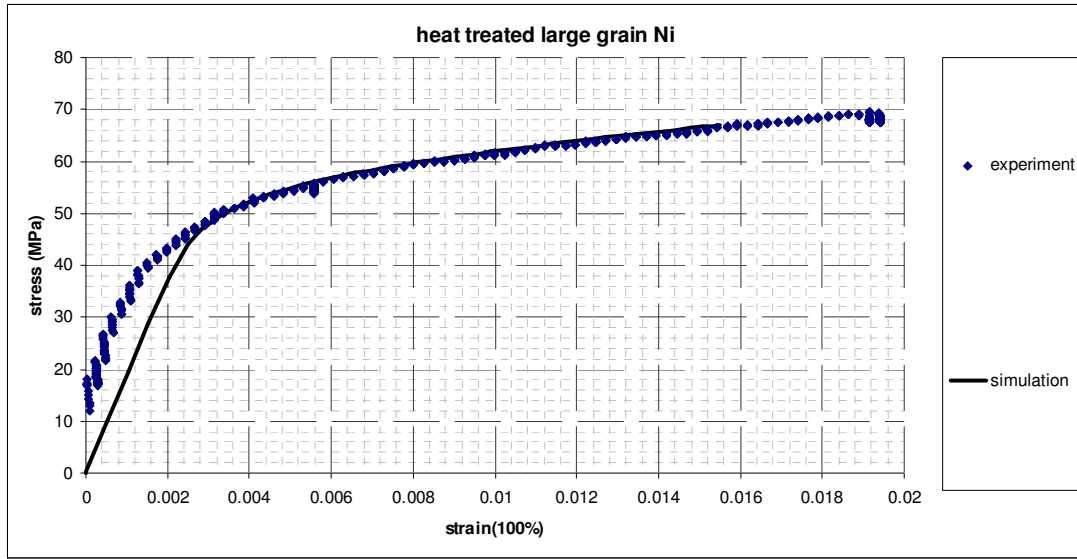


Figure 8.2 Comparison of the macroscopic stress-strain curves between FE model and experiment

The remaining set of parameters ($\lambda_{SSD}, \lambda_{GND}, C_e, C_s, K_e, K_{sw}, d_e, d_{sw}$), control dislocation motion and dislocation hardening. Assuming the same slip contributions from both dislocation types (edge and screw), C_e and C_s were set to be 0.5. Statistical hardening coefficients λ_{SSD} and λ_{GND} were assigned the same value of 0.3 based on the work of Kulmann-Wilsdorf [114] and Basinski [115]. The hardening-recovery parameters (K_e, K_{sw}, d_e, d_{sw}) were chosen to be the same as [116].

8.3 Micro-beam Laue Diffraction Experiments

Diffraction measurements were carried out on beamline B16, Diamond, UK. The incident beam with a beamsize of 50 μm and the energy range 5-25keV was used. The 90° reflection Laue setup for this instrument was developed and reported by Hofmann et al. [117]. It is illustrated in Figure 8.3. A brief description of the setup is given below.

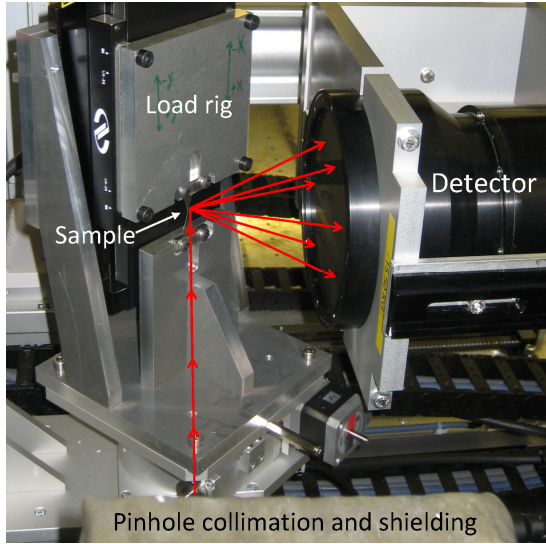


Figure 8.3 90° reflection Laue setup at beamline B16, Diamond Light Source[117]

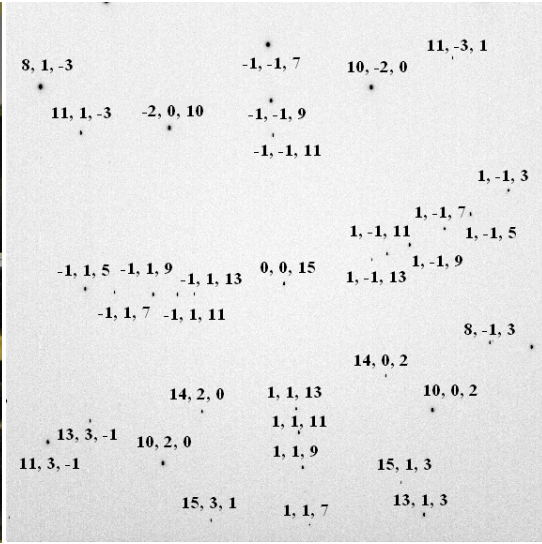


Figure 8.4 XMAS indexation of a Laue pattern from single-grained Si wafer

The sample was placed at 45° to the incoming beam in the reflection position with the loading direction perpendicular to the diffraction plane. A CCD detector with an active area of 94×94mm was set to collect the Laue pattern images at the nominal scattering angle 2θ of 90° with the sample-to-detector distance of about 100mm. The geometric parameters of the setup were then accurately determined through calibration shots collected from a Si wafer sample before the Ni sample was mounted. The precise determination of the sample-to-detector distance was accomplished by triangulation. The Ni sample was a 300μm-thick waisted dog-bone that was heat-treated beforehand to promote grain growth. The average grain size after heat treatment was around 350μm, which not only ensured the presence of a single grain through-thickness, but also allowed the use of the Laue technique to probe individual grains within the polycrystal (grain size > beam size). The sample was in-situ loaded to allow the Laue patterns to be collected at different loading stages. These patterns were subjected to automatic indexation using XMAS software. Details of the indexation procedure can be found in Chapter 3. The grain orientations (in the form of the rotation matrices) and deviatoric strain information can be obtained from the

procedure [118]. Fig. 8.4 shows a Laue pattern with XMAS indexation from single-grained Si wafer calibration shots.

8.4 Post-Processing and Results

A post-processor was developed to simulate the Laue diffraction patterns based on the FE simulation results. The 90° reflection Laue experimental setup is schematically illustrated in Figure 8.5. The Laue spot positions on the detector can be calculated from trigonometry [119]. Due to the complexity of the 3d configuration, a succinct vector space expression was used to derive the relationships. In Figure 8.5, the Cartesian coordinate system used here is based on the sample (x-y-z) system. The rotation matrices based on the incoming beam coordinate system from XMAS have to be converted to the sample system. Following a vector calculation, the spot positions need to be found in the detector coordinate system (d1-d2-d3). In the illustration, the normalized incident beam vector is labelled $\mathbf{S}_0$; $\mathbf{D}$ is the position vector of the detector; and $\mathbf{S}$ is the normalized diffracted beam vector. $\mathbf{S}$ can be calculated from Eq. 8.1a and 8.1b, where $\mathbf{q}$ is the scattering vector and $\mathbf{n}_q$ is the normalized unit vector of $\mathbf{q}$. $\mathbf{n}_q$ can be further determined by Eq. 8.1c, where $\mathbf{R}$ is the orientation matrix that rotates the grain orientation from the local (grain) system to global (sample) coordinate system. $\mathbf{H}_{hkl}$ is the index of the reflection corresponding to lattice planes in the FCC crystal, and $\mathbf{b}$ is the reciprocal space primitive lattice matrix.

$$\begin{aligned} \mathbf{S} - \mathbf{S}_0 &= \mathbf{q} & \mathbf{q} &= -2(\mathbf{S}_0 \cdot \mathbf{n}_q)\mathbf{n}_q & \mathbf{n}_q &= \mathbf{R}(\mathbf{bH}_{hkl}) \end{aligned} \quad \begin{array}{l} (8.1a, 8.1b \text{ and} \\ 8.1c) \end{array}$$

Once $\mathbf{S}$ is obtained, the Laue spot position vector $\mathbf{P}$ on the detector can be readily calculated from Eq. 8.2 (where $\mathbf{n}_D$ is the normalized detector vector):

$$\mathbf{P} = \frac{|\mathbf{D}|}{(\mathbf{S} \cdot \mathbf{n}_D)} (\mathbf{S} - (\mathbf{S} \cdot \mathbf{n}_D) \mathbf{n}_D) \quad (8.2)$$

Hence the Laue spot position coordinates in the detector coordinate system are given by

$$x = (\mathbf{P} \cdot \mathbf{d}_1), y = (\mathbf{P} \cdot \mathbf{d}_2) . \quad (8.3)$$

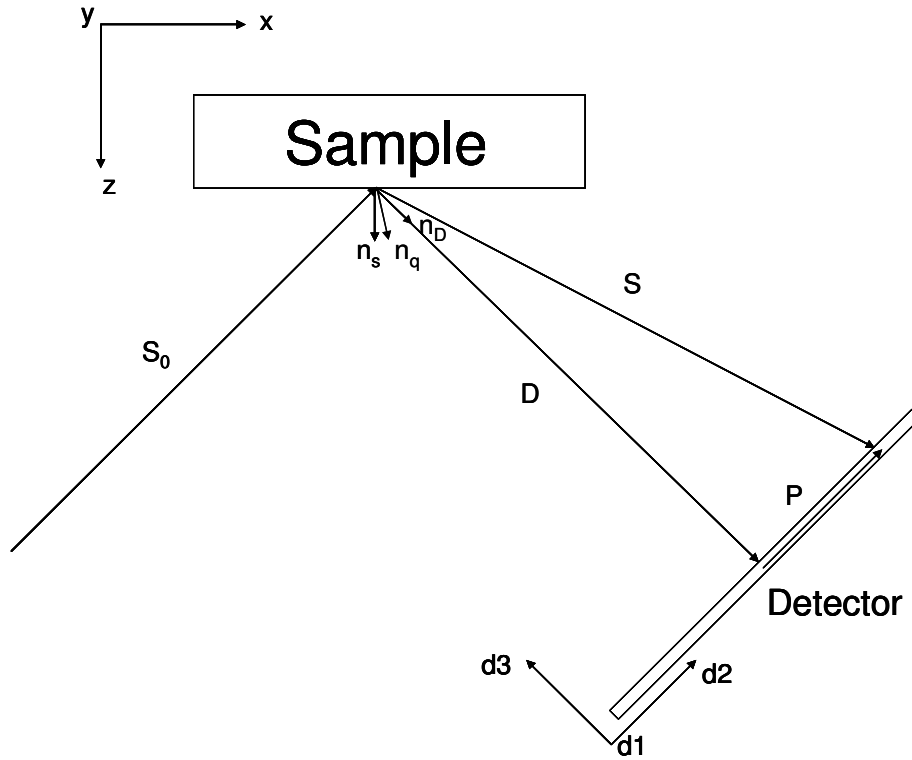


Figure 8.5 Illustration of the setup for 90° reflection Laue experiment

Based on the algorithm described above, the post-processor extracts the rotation matrix from each IP within the model, for the finite elements that correspond to the X-ray gauge volume, and calculates the Laue spot positions on the detector. The resulting spot is obtained by superposition of the reflections from each IP. Figure 8.6 illustrates the experimental Laue pattern from position A in the undeformed Ni sample. Figure 8.7 is the simulation result at the same point. It is apparent that

accurate match was achieved between the prediction and the experimental observation.

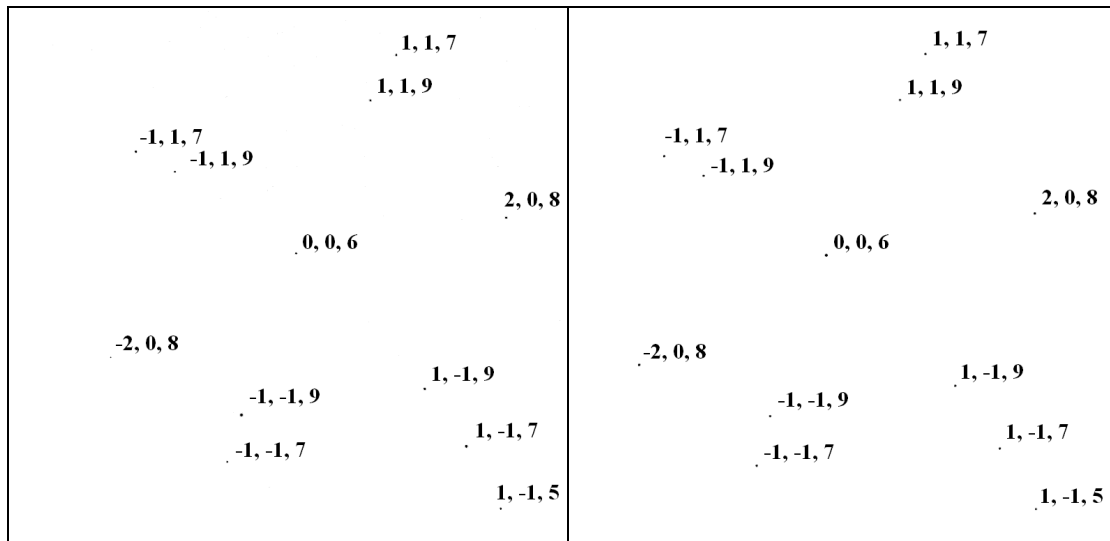


Figure 8.6 Laue diffraction pattern from undeformed Ni at position A (enhanced contrast)

Figure 8.7 Laue pattern from post-processing the SGCP model (position A).

In the situation corresponding to Figure 8.6 and Figure 8.7, the Laue patterns are collected from undeformed (annealed) individual grain within the polycrystal. Therefore, the lattice arrangement in the gauge volume is deemed to be uniform within a single grain, making the Laue spots very sharp (2D Gaussian spots with narrow width). In order to make the spots visible without changing their widths, the contrast was enhanced in Figure 8.6. It is worth noting, in passing, that it is important to preserve this aspect of the Laue peaks, since the peak width is a distinctive feature that is related to the total dislocation density. The widths of the simulated spots from each IP point were manually adjusted to provide good agreement with the experimental observation for undeformed material. Figures 8.6 & 8.7 demonstrate that the model can correctly represent the 90° Laue geometry, linking the local lattice orientation information with the Laue patterns on the detector. It is therefore a suitable tool to probe the local lattice orientation changes due to deformation.

Load was applied to the Ni specimen to reach 2% macroscopic plastic deformation. Laue patterns for the entire scan area were collected. Figure 8.8a shows an experimental Laue pattern from the sample position A. The SGCP model was used to simulate the application of the same tensile strain, and post-processed to generate the simulated diffraction pattern shown in Figure 8.8b. It is apparent that Figure 8.8a differs from undeformed Laue pattern in Figure 8.6 in at least two aspects: the spot positions and the spot shapes. It is generally believed [79, 107-110] that the change in Laue spot positions is due to the combined effect of lattice rigid body rotation and deviatoric strain; the change of Laue spot shape is due to the local lattice curvature [117]. Notably, the “streaking” (elongation) phenomenon of the Laue spots is due to the presence of GNDs [107, 108], a special type of dislocation related to plasticity-induced local lattice misorientation.

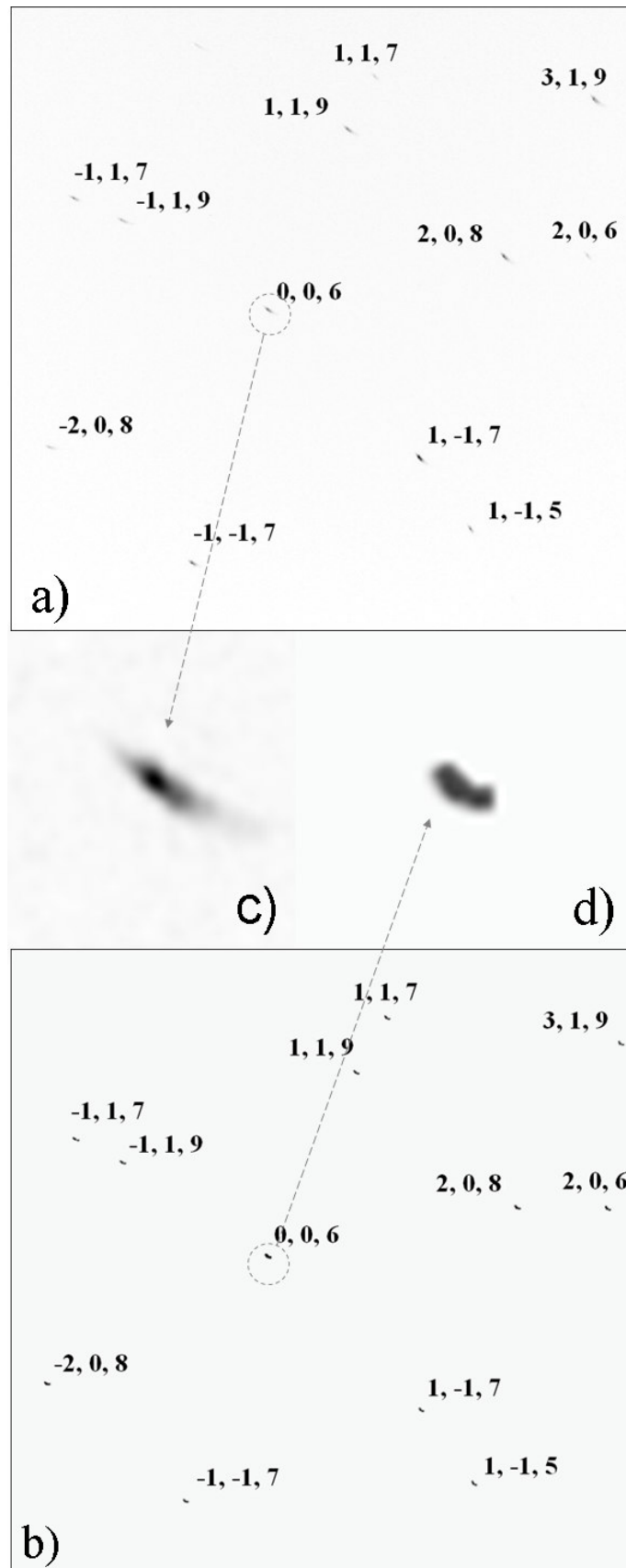


Figure 8.8 a. Experimental Laue diffraction pattern from 2% plastically deformed Ni at position A; b. Simulated Laue pattern from SGCP model; c. “Streaking” of the Laue spot (006) in the experiment; d. “Streaking” of the Laue spot (006) in the simulation

Figures 8.8a and 8.8b show reasonable agreement in terms of the spot positions, indicating that the model captures correctly some features of the elastoplastic deformation, particularly the rigid body rotation and deviatoric strain. In order to take a closer look at the spot shapes, reflection 006 was magnified by the same factor for comparison from the simulation and experiment (Figure 8.8d & 8.8c). Reasonable agreement is once again obtained, particularly in terms of the directionality of “streaking”.

The simulated spot in Figure 8.8d was constructed as follows. For each IP in the model gauge volume the lattice orientation matrix was stored. After post-processing, each IP produced a 2D Gaussian reflection spot on the detector. Collecting (superposing) these detector spots from all the IPs in the gauge volume, the final Laue spot shape was obtained.

The satisfactory agreement between the simulated Laue spot in Figure 8.8d and its experimental counterpart in Figure 8.8c in terms of streaking direction and length requires some discussion and interpretation. The agreement suggests that correct prediction has been obtained of mixed GND types of dislocation [107, 120]. It is worth repeating that in the simulation three types of GNDs were assumed to be present: $\rho_{G_{sw}}^\alpha$ denoted the density of screw type dislocations whose direction was parallel to the slip direction, $\rho_{G_{en}}^\alpha$ denoted the density of edge type dislocations with lines parallel to the slip normal, and $\rho_{G_{et}}^\alpha$ denoted the density of edge dislocations with lines parallel to $t^\alpha = m^\alpha \times n^\alpha$. (The details of the model formulation were given in Chapter 2). We interpret the satisfactory prediction of the Laue peak shape as partial confirmation that the GND evolution in the SGCP model reflected correctly the deformation and dislocation patterning that occurred in the experiment involving plastic stretching of the large grain Ni sample.

In order to validate the model further, a second point on the sample (position B) was selected (Figure 8.1c), located in a different grain in the sample with a different orientation. In position B, the Laue patterns from experiment (Figure 8.9a) and simulation (Figure 8.9b) were generated. A reasonable match between Figure 8.9a and 8.9b was also found. This provided additional argument for claiming that the current strain gradient crystal plasticity model demonstrated predictive capabilities in terms of dislocation structure evolution.

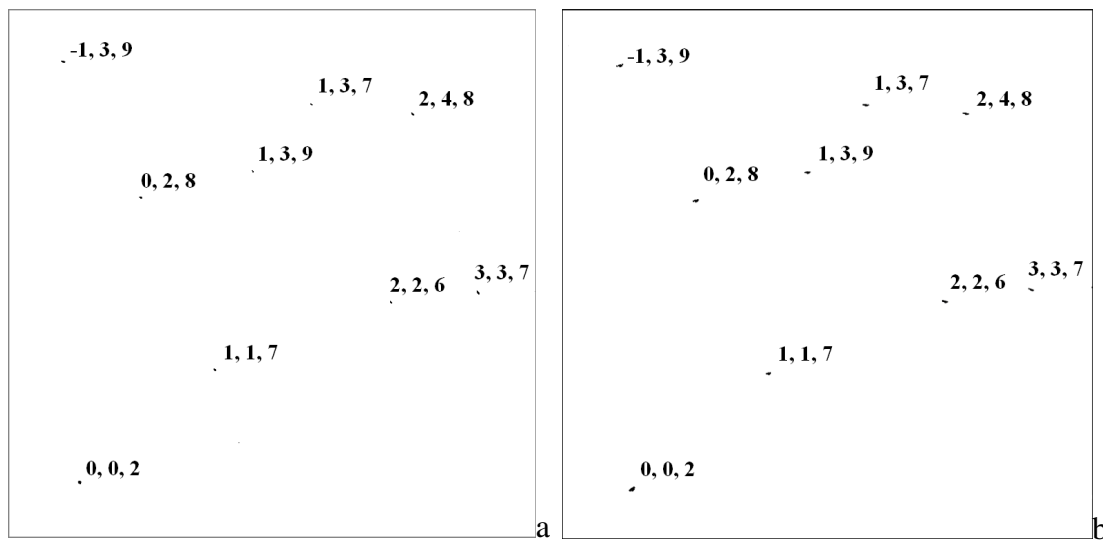


Figure 8.9 a. Laue diffraction pattern from 2% plastically deformed Ni at position B; b. Simulated Laue pattern from SGCP model at position B; c. Pattern indexation at position B;

8.5 Conclusion

In this chapter, forward prediction of Laue patterns from different grains in a polycrystalline Ni sample was carried out. It captured successfully the characteristic features of diffraction patterns, namely, Laue spot positions and the amount of “streaking” that was observed, revealing the local lattice arrangement information related to the rigid body rotation, deviatoric strain and local misorientation of the crystal lattice. This kind of correspondence was found for multiple points in the sample area studied. Based on these results it is argued that the dislocation-based

SGCP model captures the evolution of the dislocation in the large grain Ni sample reasonably well, providing unique insight into the inhomogeneity of polycrystal deformation at the intra-granular level.

Chapter 9 Conclusions and suggestions for future research

9.1 Conclusions

The primary aim of this research was to improve the understanding of deformation and residual stresses at different scale levels using Finite Element simulation and X-Ray diffraction characterisation techniques. A range of studies carried out in the course of work on this project and reported in this dissertation investigated the mechanisms of deformation and the descriptive models appropriate at different scales, and identified the sources of residual stresses. Based on the results obtained in these studies, the principal conclusions are drawn below.

9.1.1 Simulation and measurement techniques

In Chapter 2, the general basics of the Finite Element method were introduced. The methodology for the development of advanced ABAQUSTM material deformation models using subroutines UMAT, UEL and UEXPAN were discussed. Next, it was demonstrated how this methodology should be applied to the simulation of deformation at different levels, and the reconstruction of residual stress states using eigenstrain modelling. Chapter 2 thus introduced the complete modelling toolkit used throughout the study as a means of understanding and predicting the deformation response of materials across the scales, and also for the validation of the model predictions against experimental observations.

An important topic not covered in Chapter 2 concerns the pre-processing and post-processing developments undertaken in the current study. Since these developments are specific to particular studies and experimental configurations, their

discussion was left to specific Chapters devoted to those studies. It is important to note, however, that pre- and post-processor developments constitute an important step essential for (a) introducing the information about the material microstructure into FE models, and (b) obtaining predictions of the diffraction patterns from the simulations to allow direct comparison with the experimental data.

Chapter 3 provided an overview of the principles and applications of diffraction. Different diffraction modes (monochromatic and white beam) were described, with particular emphasis on the white beam mode that was used extensively in the present study. Two configurations of special interest to the current research were discussed in detail: the white beam polycrystal diffraction (including energy dispersive synchrotron X-Ray diffraction and time-of-flight neutron diffraction) and single crystal micro-focused white beam Laue diffraction (microbeam Laue). Details of the setup geometries used at different facilities were presented. The interpretation methods appropriate for each of the above techniques were next described. Two software packages used for data interpretation were introduced: GSAS (General Structure Analysis System) for energy dispersive polycrystal diffraction, and XMAS (X-ray Micro-diffraction Analysis Software) for microbeam Laue. The algorithms implemented in these software packages were explained briefly, and the approaches used for the interpretation of experimental results were explained. These methods were used to obtain the local parameters describing the material states, such as lattice spacings and grain orientations. The specific results obtained using these methodologies in each particular case are reported in subsequent chapters.

9.1.2 Macroscopic 1-D residual stress state analysis of Al/SiCp bent bars

Chapter 4 was dedicated to the development of the 1-D variation eigenstrain

technique. Example was set to be the evaluation of the residual stresses in a bar of a metal matrix composite (MMC) consisting of an aluminium alloy 2124-T1 matrix reinforced with 25vol% particulate silicon carbide (SiC_p). The residual strain distribution was introduced into the test piece by plastic deformation in a 4-point bending configuration. X-ray diffraction and EDM (electric discharge machining) incremental slitting with 3D profilometry (curvature measurement using CMM) were used to characterise its residual strain state. Both the X-ray diffraction and incremental slitting strain measurement results were then analysed using direct and inverse pseudo-thermal eigenstrain methods. Residual stress plots obtained by different experimental and numerical methods showed good agreement with each other. Thus, the capability of the 1-D eigenstrain method for residual stress reconstruction was demonstrated, providing the motivation and foundation for further eigenstrain studies [121-123].

9.1.3 Macroscopic 2-D inverse eigenstrain residual stress state analysis of a worn railhead

Chapter 5 introduced a new algorithm for 2-D variation residual stress reconstruction in engineering components using piecewise linear 2-D eigenstrain representation. The sample considered was a worn railhead sample. The residual elastic strain distribution was obtained by neutron diffraction measurement in STRESS-SPEC, FRM-II (TU München, Germany) and used as the input for eigenstrain reconstruction. A piecewise linear discrete eigenstrain base function – “tent function” - was introduced to represent the fully two-dimensional variation of eigenstrain. An automated “tent function” generation scheme was programmed as an ABAQUSTM pre-processor. The pre-processor also loaded the experimental data,

while a post-processor was used to carry out the inverse problem analysis (match optimization) to obtain the unknown coefficients of the eigenstrain basis functions (“tents”). The reconstructed eigenstrain field reproduced the residual stress distribution in the railhead with good fidelity, i.e. showed good agreement with the experimental data. This 2-D inverse eigenstrain method shared common ground with its 1-D counterpart, since both use the piecewise linear discrete representation of the eigenstrain field in the form of a sum of individual base functions, with the magnitudes (coefficients) obtained by optimization (inverse problem analysis). However, the 2-D method algorithm has certain novel features, not only because the interpolation was required from the experimental data grid to the FE mesh grid, but also since the introduction of another discrete basis for eigenstrain representation (the “tent grid”) was required. Further, it is necessary to note the coupling effect that exists between the two in-plane strain components. Furthermore, the scale of the 2-D implementation required the integration of individual tent function generation steps into one sequential run. An additional streamlining step taken was the inclusion of the inverse problem solution in the post-processing run. This allowed the automation of the complete process, so that the generation of the 2-D eigenstrain distribution solution consisting of a few hundred base functions becomes practically feasible and efficient. The newly developed 2-D eigenstrain method has the potential to become a useful tool for the development of the discrete inverse eigenstrain method, but the issue of computational efficiency has to be further addressed to make the program practical for industry application.

9.1.4 Macroscopic 3-D residual stress state and process modelling: linear friction welds in Al-SiCp composite

In Chapter 6, the process modelling of an aluminium alloy-based metal matrix composite (MMC) linear friction weldment was carried out to advance the understanding of deformation and its effect on residual stresses on macroscopic level. Linear friction welding (LFW) is a solid state joining process in which the bonding of two components is completed by their relative reciprocating motion under axial (compressive) forces. Four major stages of the process (Stage 1: Warm-Up; Stage 2: Osci-Forging; Stage 3: Forging; Stage 4: Cool-Down) were identified. A fully coupled thermo-mechanical process model was proposed to simulate the temperature field and residual strain distribution. A novel approach was developed to simulate the effect of oscillatory motion. Heat generation by oscillation-induced friction was replaced in the model by the heat flux at the interface without the reciprocal motion. A parametric study of the material property influence on the residual stresses was carried out. The influence of the model dimensionality on residual stresses was also taken into consideration. It is shown that the material temperature-dependent yield stress plays a significant role in the residual stress magnitude near the bond line. To better capture the permanent deformation distribution, an eigenstrain model calibrated by the neutron diffraction results was also employed. Reasonable agreement between the process modelling, eigenstrain reconstruction and the experimental measurement was found, linking eigenstrain method and process modelling together. However, due to the complexity of the interaction between thermal and mechanical effects during the process, further investigation of the LFW process is required.

9.1.5 3-D meso-scale analysis of elastic-plastic deformation in HCP polycrystals:
crystal plasticity and strain gradient crystal plasticity modelling validated
against synchrotron XRD measurement

In the first half of this chapter, a 3D, elastically anisotropic crystal-plasticity constitutive model was used to describe the deformation and hardening behaviour of the polycrystalline HCP titanium alloy Ti-6Al-4V. A diffraction post-processor was developed to allow validation of the model predictions against XRD data. Model results were expressed in the form of the relationship between applied macroscopic tensile stress and elastic strains (average or grain group specific). These results were compared with high energy synchrotron X-ray diffraction data. Good accordance was found between the two. The significance of elastic anisotropy and three-dimensionality of the model were discussed.

The second half of this chapter was devoted to the analysis of a different aspect of the prediction obtainable from the similar modelling approach that was extended to incorporate strain gradient effects. The problem posed concerned the possibility of constructing high energy synchrotron X-ray diffraction patterns, including peak position *and* peak shape. The extended strain gradient crystal plasticity algorithm took account of the generation and annihilation of two types of dislocations: statistically stored dislocations (SSDs) and geometrically necessary dislocations (GNDs). This framework was employed to simulate the polycrystalline plastic deformation in the HCP Ti-6Al-4V alloy². The macroscopic stress-strain plots and meso-scale elastic strain data were used to calibrate the model and to check that correct diffraction peak positions were obtained. The dislocation densities were extracted from the model using the specially written post-processor. The diffraction peak shapes were then constructed. It was established that it were, indeed, the local dislocation densities that controlled the peak widths. The model parameters were then adjusted to provide the best simultaneous match to multiple peaks in terms of

² The presence of the minority β -phase was ignored in this approximation.

intensity, position and shape. Good agreement was obtained between the forward prediction of diffraction peaks and the experimental results. The framework provides a considerably improved means of validating polycrystal plasticity finite element models, since the match is obtained not only for the macroscopic (global) deformation parameters, but also for the grain orientation specific response and statistics. The study represents an example of the parallel development of modelling and experimental tools that is useful for the study of SSDs and GNDs effects on the deformation behaviour of (poly) crystals at meso- to microscopic level.

9.1.6 3-D microscopic analysis of elasto-plastic deformation in FCC polycrystals: strain gradient crystal plasticity modelling and micro-beam Laue diffraction of polycrystalline Ni foil

The physically-based, rate and length-scale dependent strain gradient crystal plasticity framework from Chapter 7 was employed again in this Chapter to further our understanding of deformation at microscopic level. The model was used to simulate the polycrystalline plastic deformation in a large-grained, commercially pure Ni sample. A real sample was first characterised in terms of the grain morphology and orientation (in the bulk) by using the programme XMAS to interpret microbeam Laue diffraction experiments carried out on beamline B16 at Diamond Light Source. The corresponding FE model was developed by creating a grain-based mesh with appropriate grain orientation assignment. Sample stretching to 2% plastic strain was simulated, and a post-processor was developed to extract the information about the local lattice misorientation (curvature). Extracting this information from the model allowed the simulation of the micro-beam Laue diffraction patterns to be developed. The “streaking” phenomenon of the Laue spots (anisotropic broadening of two-

dimensional diffraction peaks observed on the 2-D detector) was correctly captured by the simulation, as confirmed by direct superposition of reflections from different IPs within the diffraction gauge volume. Excellent agreement was found between the images collected from the experiment and simulation patterns at various positions in the sample.

9.2 Suggestions for future work

The research results reported in this thesis make a significant contribution to the current capabilities for the modelling and evaluation of residual stresses and deformation. Further work is required aimed at applying the current methods to more cases of material deformation and residual stress generation for the purposes of model verification and optimization. The fundamental conclusion emerging from the body of work conducted in this project is as follows. Gaining a better understanding of the complex and intricate processes that control material deformation and residual stresses across the scales is only possible using a tight integration between simulation and experimental characterisation. Some success has been evident in improving the fidelity of current models using this principle. However, further studies are required, in particular in the directions identified below.

In the area of eigenstrain reconstruction for residual stress analysis, the 1-D eigenstrain reconstruction technique has now been extensively studied and exploited [121-123]. The focus of further development should be placed on improving forward predictions. This could be achieved by incorporating further, more advanced regularisation and smoothing techniques. With the capability of efficient and fast simulation of experimental procedures, e.g. such as incremental hole-drilling, this method then become mature for wider industrial applications.

The newly invented discrete 2-D eigenstrain reconstruction method has great potential for simulating 2-D variations of residual stresses. More examples are needed to establish the method on a firmer footing, and optimisation needs to be carried out to reduce the total run-time for “tent” base function generation and analysis.

The 3-D eigenstrain reconstruction capability at this stage remains limited to the use of continuous functions to represent the eigenstrain distribution. A discrete reconstruction approach similar to the “tent” base function in 2-D needs to be developed. The 3-D base function can not be visualized for the 3-D case as easily as for the 2-D, but the principle remains the same; namely, a variable (normally the eigenstrain value) is set to unity at one grid node, and to zero everywhere else. Then the influence coefficient matrix can be generated that is required for optimisation. Based on this principle, the 3-D eigenstrain reconstruction algorithm can be developed. The computational efficiency is the principal issue that must be addressed in order to prove the feasibility of this approach.

For the process modelling of LFW (Linear Friction Welding), a better understanding of the material’s thermo-elastic-plastic properties is needed to capture the post-weld residual stress distribution. Better detailed knowledge of the thermal boundary conditions is required. This can be achieved by installing multiple thermocouples within the parts being joined and recording temperatures in-situ while the welding process is under way.

The 3-D mesoscale simulation and energy-dispersive XRD measurement of elastic-plastic deformation in HCP polycrystals has afforded good forward prediction of diffraction peak positions and shapes. If there is any improvement that can be made, it should seek to provide the correct prediction of peak intensities, so that the pattern in its entirety is matched well to the experimental data.

The 3-D microscale simulation and Laue diffraction analysis of elasto-plastic deformation in pure Ni polycrystals is the first of its kind. It predicts the Laue spots positions and 2-D shapes on the detector, matching the experimental observations at different locations in different grains within one polycrystalline Ni sample. The natural next step will be to consider a line scan or 2D map of the grain boundary regions to compare the predicted and collected Laue patterns. Different amount of “streaking” is expected at different locations within one grain due to the GND pile-up at the grain boundaries. Capturing these effects correctly would not only demonstrate the forward prediction capability of the model, but also provide further insight into the physics of plastic deformation at the microscopic scale. Further attempts should be made for the extraction of dislocation distribution densities from combined analysis of the model predictions and the experimental Laue spot shapes. Image analysis techniques (i.e. DIC-Digital Image Correlation) can be used to study the relationship between the predicted and experimental Laue spots. Matching calculations can be used to extract the information about crystal lattice distortion (lattice rotation and misorientation). Ultimately, the densities of dislocation of different types should be quantified. This work offers a very interesting but challenging direction to pursue.

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APPENDIX

Journal Publication:

1. **Song, X.**, Hofmann, F., Korsunsky, A.M., “Strain Gradient Crystal Plasticity Modelling and Micro-beam Laue Diffraction of Polycrystalline Ni Foil”, *Philosophical Magazine*, Accepted
2. **Song, X.**, Jun, T.-S., Korsunsky, A.M., “Fully Two-Dimensional Discrete Inverse Eigenstrain Analysis of Residual Stresses in a Rail Head”, *Journal of Applied Mechanics- Transactions of the ASME*, under review
3. **Song, X.**, Zhang, S.Y., Korsunsky, A.M., “Strain Gradient polycrystal Plasticity analysis: FE Modelling and Synchrotron X-ray Diffraction”, *International Journal of Modern Physics B* 24 (1-2), pp. 10-17.
4. **Song, X.**, Zhang, S.Y., Dini, D., Korsunsky, A.M., “Finite element modelling and diffraction measurement of elastic strains during tensile deformation of HCP polycrystals”, *Computational Materials Science* 44 (1), pp. 131-137
5. **Song, X.**, Chardonnet, S., Savini, G., Shu, Y.Z., Vorster, W.J.J., Korsunsky, A.M., “Experimental/modelling study of residual stress in Al/SiCp bent bars by synchrotron XRD and slitting eigenstrain methods”, *Materials Science Forum* 571-572, pp. 277-282
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Conference Contribution:

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