

# Influence of Magnetic Fields on Structural Martensitic Transitions.

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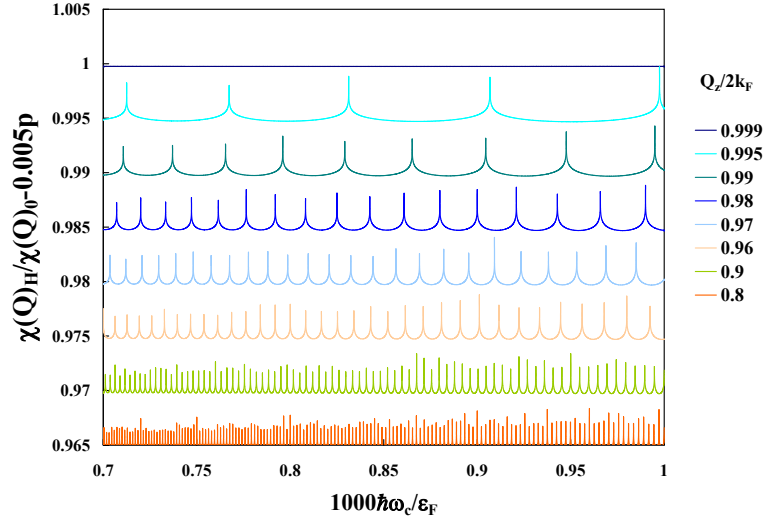
## Abstract.

We propose a model which suggests that structural martensitic transitions are related to significant changes in the electronic structure, and are effected by high-magnetic fields. The magnetic field dependence is considered unusual as many influential investigations of martensitic transitions have emphasized that the structural transitions are primarily lattice dynamical and are driven by the entropy due to the phonons. We provide a theoretical framework which can be used to describe the effect of high magnetic field on the transition and lattice dynamics in which the field dependence originates from the dielectric constant. The model is compared with some recent experimental results.

## 1. Introduction

Martensitic transitions are often defined as diffusionless structural transitions that lower the symmetry, and in which the order parameter has a discontinuity. This definition is generic and is compatible with a group theoretical analysis performed by Anderson and Blount[1] which showed that the transition is usually first-order and could only be second-order with probability zero. Anderson and Blount then proceeded to argue that the apparently second-order martensitic transition in  $V_3Si$  was an example of a ferroelectric transition. Recently, Lashley *et al.* performed inelastic neutron scattering measurements on the Hume-Rothery alloy AuZn [2] which showed that although the transition was strongly first-order in the non-stoichiometric compounds, the hysteresis was greatly reduced and the order parameter extracted from the satellite intensity was a continuous function of temperature for stoichiometric AuZn.

We shall, in this note, consider AuZn in which the lattice dynamics and structural transition is strongly affected by an applied magnetic field, although the transition temperature is at most only weakly field dependent. The field dependence is considered unusual as many influential investigations of martensitic transitions have emphasized that the structural transitions are primarily lattice dynamical and are driven by the entropy due to the phonons[3, 4]. We shall provide a theoretical framework which can be used to describe the effect of the field on the lattice dynamics in which the field dependence originates from the dielectric constant. The weak field



**Figure 1.** The oscillations of the normalized Lindhard function  $\chi_H(Q_z)/\chi_0(Q_z)$  with the magnetic field directed parallel to  $\underline{Q}$ . For clarity, the response is normalized to the  $H = 0$  value and then is lowered by 0.005 for successively lower values of  $Q_z/2k_F$ . The curves are limited by the resolution of the plotting program.

dependence of the martensitic transition temperature in AuZn is contrasted with the strong field dependence in  $V_3Si$  and the difference is related to the difference in the dimensionality of these two materials.

## 2. Theory

For a first-order martensitic transition where the phonons only partially soften[5, 6], the martensitic transition temperature  $T_M$  can be found by considering the balance between the difference in the structural energy[3, 4] of the two phases  $\Delta E_s$  and the difference in the phonon entropies  $\Delta S$

$$\Delta E_s = T_M \Delta S \quad (1)$$

A rough approximation for the structural energy  $E_s$  of a metal with a monoatomic basis is given[7] as a sum over reciprocal lattice vectors of the squared modulus of the structure factor  $S(\underline{Q})$  and the screened atomic pseudo-potential  $V_0(\underline{Q})$

$$E_s = \frac{1}{2} \frac{N^2}{V} \sum_{\underline{Q} \neq 0} |S(\underline{Q})|^2 |V_0(\underline{Q})|^2 \chi(\underline{Q}) \varepsilon(\underline{Q}) \quad (2)$$

in which  $\chi(\underline{Q})$  is the Lindhard function and  $\varepsilon(\underline{Q})$  is the dielectric constant. It is expected that the main field dependence of the transition temperature will be governed by the field-dependence of the Lindhard function at the reciprocal lattice vectors ( $Q < \text{or } \sim 2k_F$ ) which are appreciably different between the two structures.

The Lindhard function can be expressed as a sum over the occupied Landau levels  $n$

$$\chi(\underline{Q})_H = - \frac{1}{2\pi^2 \hbar \omega_c Q_z r_c^4} \sum_{n,m,\sigma} |F_{n,m}(Q_\perp)|^2 \ln \left| \frac{2m_e(n-m)\omega_c/\hbar - Q_z^2 - 2Q_z k_{F,n\sigma}}{2m_e(n-m)\omega_c/\hbar - Q_z^2 + 2Q_z k_{F,n\sigma}} \right| \quad (3)$$

where  $k_{F,n\sigma}$  is the Fermi wave vector of the  $n$ -th spin split occupied Landau level

$$k_{F,n\sigma} = \sqrt{\frac{2m_e}{\hbar^2} \left[ \epsilon_F - \left( n + \frac{1-\sigma}{2} \right) \hbar \omega_c \right]} \quad (4)$$

and the Larmour frequency is given by

$$\omega_c = \frac{|e| \hbar}{m_e c} H_z \quad (5)$$

The Fourier Transform of the matrix elements of the density operator between the various Landau levels is given by

$$F_{n,m}(Q_\perp) = \left( \frac{n!}{m!} \right)^{\frac{1}{2}} \left( \frac{r_c (i Q_x - Q_y)}{\sqrt{2}} \right)^{m-n} \exp \left[ -\frac{r_c^2 Q_\perp^2}{4} \right] L_n^{m-n} \left( \frac{r_c^2 Q_\perp^2}{2} \right) \quad (6)$$

for  $m > n$  and where the radii of the Landau orbits  $r_c$  is given by

$$r_c = \sqrt{\frac{\hbar c}{|e| H_z}} \quad (7)$$

and where  $L_m^n(x)$  represents the associated Laguerre functions. The  $k_y$  dependence of the matrix elements occurs in the form of a trivial phase factor, which we have omitted since it drops out of the Lindhard function. To obtain an estimate of the relative contributions to the field dependence from the Landau quantization and the spin splitting, we shall set  $Q_\perp = 0$ . Since  $F_{n,m}(0) = \delta_{n,m}$ , only one summation remains and the resulting expression

$$\chi(Q_z)_H = -\frac{1}{2\pi^2 \hbar \omega_c Q_z r_c^4} \sum_{n,\sigma} \ln \left| \frac{Q_z + 2k_{F,n\sigma}}{Q_z - 2k_{F,n\sigma}} \right| \quad (8)$$

The summation includes a term which is logarithmically divergent when  $Q = 2k_{F,n\sigma}$ . The Lindhard function is a periodic function of

$$\left[ 1 - \left( \frac{Q_z}{2k_F} \right)^2 \right] \left( \frac{\epsilon_F}{\hbar \omega_c} \right) \quad (9)$$

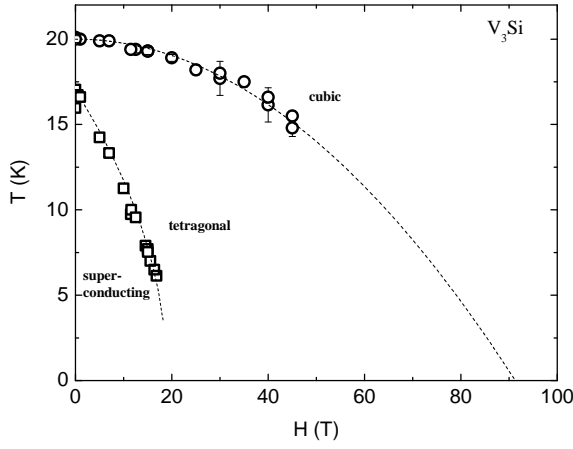
for  $1 > \frac{Q_z}{2k_F}$ . The oscillations in  $\chi_H(Q_z)$  are shown in Fig. 1 for various values of  $Q_z/2k_F$ . It is expected that disorder, temperature and many body effects will smear and diminish the amplitude of the oscillations due to Landau level quantization. However, it is expected that these effects will not alter the field-dependence originating from the spin split Fermi surfaces.

The change in  $T_M$  with field can be estimated by considering a spin splitting between the up spin and down spin Fermi surfaces. In the limit of low magnetic field, the spin splitting is expected to result in a change  $T_M$  given by

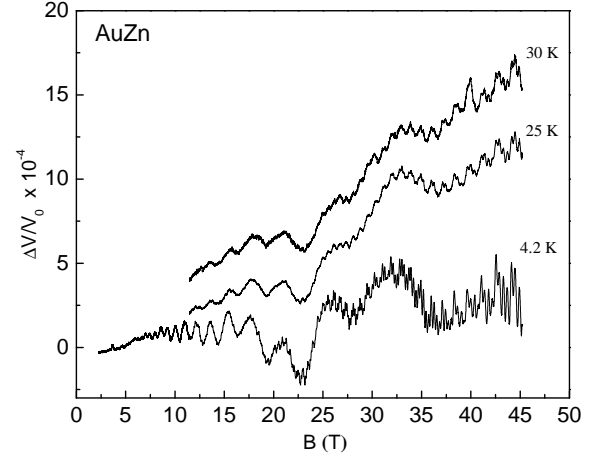
$$\frac{\Delta T_M(H)}{T_M(0)} \approx \frac{k_F^2}{2! \chi(Q)_0} \frac{\partial^2 \chi(Q)_0}{\partial k_F^2} \left( \frac{\mu_B H}{\epsilon_F} \right)^2 \quad (10)$$

Hence, one expects that the relative change in  $T_M$  will depend on the field through the factor  $(\frac{\mu_B H}{\epsilon_F})^2$ , but can be extremely large if  $Q$  is extremely close to  $2k_F$ . For an applied magnetic field of 9 T one expects a relative change in  $T_M$  only of the order of  $10^{-7}$ , since it is quite three-dimensional. By contrast, for the case of V<sub>3</sub>Si considered by Dieterich and Fulde, the Labbe-Friedel[13] model suggests that the Fermi-energy lies extremely close to the bottom of a quasi-one-dimensional density of states, so that  $\epsilon_F$  has the extremely small value of 22 K. Hence, for V<sub>3</sub>Si one expects a large depression of  $T_M$  with increasing field [15] as can be seen in the cubic to tetragonal martensitic transition phase diagram in Fig. 2.

Alternatively, one can also obtain a similar criterion by considering the softening of the phonon modes as was considered by Dieterich and Fulde[8]. Their analysis can be extended



**Figure 2.** The field-dependence of the martensitic (cubic to tetragonal) phase transition and superconducting temperatures in  $V_3Si$ . [After P. A. Goddard *et al.* (2009).]



**Figure 3.** The oscillations of the speed of sound of AuZn measured at several temperatures in the martensitic phase. [After J.C. Lashley *et al.* (2007).]

to the case of second order martensitic phase transitions[2] in which the softening occurs at a finite value of  $q$  as is the case for AuZn. In particular, the phonon frequencies  $\omega_\alpha(\underline{q})$  and the polarization vectors  $\underline{\epsilon}_\alpha(\underline{q})$  are determined from the eigenvalue equation[9]

$$M \omega_\alpha^2(\underline{q}) \underline{\epsilon}_\alpha(\underline{q}) = N \sum_{\underline{Q}} (\underline{q} + \underline{Q}) \Theta(\underline{q} + \underline{Q}) (\underline{q} + \underline{Q}) \cdot \underline{\epsilon}_\alpha(\underline{q}) - N \sum_{\underline{Q}} \underline{Q} \Theta(\underline{Q}) (\underline{Q} \cdot \underline{\epsilon}_\alpha(\underline{q})) \quad (11)$$

where the sum over  $\underline{Q}$  is a sum over reciprocal lattice vectors and where the Fourier Transform of the pair-potential  $\Theta(\underline{k})$  is approximated by the screened Coulomb interaction

$$\Theta(\underline{k}) = \frac{1}{V} \left( \frac{4 \pi Z^2 e^2}{k^2 \epsilon(\underline{k})} \right) \tilde{V}_0(k)^2 \quad (12)$$

and  $\tilde{V}_0(k)$  is a dimensionless oscillatory function of  $k$  that only depends on the core radius. Therefore, we argue that the field dependence of the phonon frequencies originates from the dielectric constant. Furthermore, one expects that the end result for  $\Delta T_M(H)$  would be a similar expression to that given previously in eqn(10), in which the field-dependence of  $T_M$  is related to the field-dependence of the density-density response function.

### 3. Discussion

Therefore, we argue that the field dependence of the phonon frequencies originates from the dielectric constant. This conclusion is consistent with the earlier observations of the oscillations of the sound velocity with increasing magnetic field at temperatures well below the martensitic transition[10]. The oscillatory field-dependence of the speed of sound is shown in Fig. 3.

Because the Fourier spectrum of the oscillations of the speed of sound shows peaks at the frequencies obtained from de Haas - van Alphen measurements[11, 12] and the amplitudes follow the Lifschitz-Kosevitch formula[10], it was concluded that these oscillations originate from Landau-level quantization as manifested by the dielectric constant at  $Q \rightarrow 0$ .

We have indicated that, irrespective of the order of the transition, that structural properties of AuZn are strongly affected by magnetic field. Furthermore, we have proposed a model of the structural properties in which the field-dependence originates through the dielectric constant. The proposed model forms a connection between phonon-entropy stabilization pictures with Jones's description[14] of Hume-Rothery's observations[16]. Jones's explanation was that the structural transitions are purely electronic and driven by the Fermi-surface nesting with the Brillouin Zone boundary. It is proposed that the model can provide a consistent explanation of the observed field-dependent anomalies found in AuZn and other materials, such as the InTi system [17, 18] which exhibit martensitic transitions.

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