FOURIER2D and FOURIER3D: programs to demonstrate Fourier synthesis in crystallography

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FOURIER2D and FOURIER3D are stand-alone computer programs that demonstrate for teaching purposes the summation of plain waves from lists of structure amplitudes and phases.

Introduction

It is important for students of crystallography to be able to understand the process of Fourier synthesis whereby electron density is built up from a summation of plane waves described by structure amplitudes together with their phases. It is particularly instructive for students to see how each wave can be superimposed to gradually build up a picture of the crystal structure. As an example, many years ago an ingenious device was constructed by von Eller(von Eller, 1965), the so-called “photosommateur”. This used a technique to superimpose on a photographic film a sequence of black-white fringes. The fringe intensity was proportional to the structure amplitude and this determined the length of exposure on the film. By shifting the origins of the waves, change of phase could be introduced and the orientation of the fringe pattern was made to coincide with (hkl) planes by rotating the film to specific angles determined by the reciprocal lattice. The result was an image closely resembling a photograph of the atomic arrangements. I was fortunate to use such a machine as a graduate student and have never forgotten the impression it made on me.

Of course, these days we have computers that enable us to carry out the same procedure. One of the earliest uses of computers to plot Fourier maps was published by Pepinsky (Pepinsky, 1947) using an oscillographic presentation. Later, the program FOURDEM (Welberry & Proffen, 1997)(Welberry & Owen, 1992) was written to demonstrate the features of the photosommateur. In 1999 a Fourier teaching and research Fourier synthesis program which ran on Silicon Graphics computers was published (Glykos, 1999). The website http://www.ysbl.york.ac.uk/~cowtan/sfapplet/sfintro.html also can be used to teach the principles of Fourier summation. Moreover, one can also find large software packages that contain Fourier plotting routines, a good example being Olex2 (Dolomanov et al., 2009).

Despite the availability on the internet of many software packages that can be used to demonstrate Fourier methods, for first time users, the request for input data is much easier with a dedicated application . The present two standalone programs provide simple teaching tools to demonstrate the way in which recognizable electron densities can be built up from summation of plane waves. The author has successfully used the programs to explain the concept of Fourier synthesis to beginning students of crystallography. The programs were written in Delphi to run in a Microsoft Windows environment, and have been tested on an Apple Mac computer with Windows emulation. FOURER2D is used to demonstrate Fourier projections, whereas FOURIER3D enables two-dimensional slices to be made of the Fourier maps. A complete help file and tutorial is included in the programs.

Use of the programs

There are three ways in which data can be entered into the program. First of all the menu item entitled Single Reflections enables the user to enter *h k l |F(hkl)|* and phase $\phi(hkl)$ one by one manually. This is particularly useful for teaching purposes since one can then show how each wave adds together gives reinforcement and cancellation of waves according to the values of *|F(hkl)|* and $\phi(hkl)$.

The second method is to use the example files selected from the main menu. These files are simple text files with the following entries:

Crystal structure name					
a	**b**	**c**	**α**	**β**	**γ**
h	**k**	**l**		**|F(hkl)|**	**ϕ(hkl)**
.	.	.		.	.
.	.	.		.	.

The lists of reflections in the example files are then read in automatically so that the user can see each wave being added one after another in real time i.e. an updated synthesis is shown for a short time before adding the next reflection. A facility is available to enable the reading process to be slowed down as required. The third method is to read in a CIF and let the program calculate the values of enter *h k l |F(hkl)|* and $\phi(hkl)$ internally.

Figure 1 shows the main window during the process of building up the Fourier map for the high-temperature quartz structure. On the left the most recent plane wave is presented; in this case this is the 0 -4 0 reflection with a value of |F| = 22.4 and ϕ = 0. On the right the effect of summation of plane waves can be seen. This window can be resized using the bottom right handle.

Figure 2 shows the Parameters dialog box in FOURIER2D. This enables the user to select a number of different views, including various ways of colouring or contouring the plots. Selection can be made to plot a normal Fourier or a Patterson map. In addition, one can select the use of random phases or random structure amplitudes to demonstrate to the student that the knowledge of phases is generally more important than relying on the amplitudes alone. The effect of resolution can also be demonstrated by setting a maximum Bragg angle, computed on the basis of a wavelength of 1.5418Å.

Figure 3 shows some examples of Fourier projections for a crystal of quartz in its high-temperature phase, space group $P6_422$ viewed on (001). Figure 4 shows a projected structure for hexamethyl benzene space group $P\bar{1}$ using pale colours. In addition, in FOURIER2D it is possible to create a video AVI file showing the build-up of density with time. An example AVI for quartz is available from the supplementary information.

In the FOURIER3D program one can let the program automatically scan through layers in the Fourier maps or select a particular layer on its own. Figure 5 shows examples for high-temperature quartz viewed down the c-axis and selected for z = 0.0 and 0.30.

Availability

The programs FOURIER2D and FOURIER3D are freely available to download from the website http://www.amg122.com/programs/fourier.html.

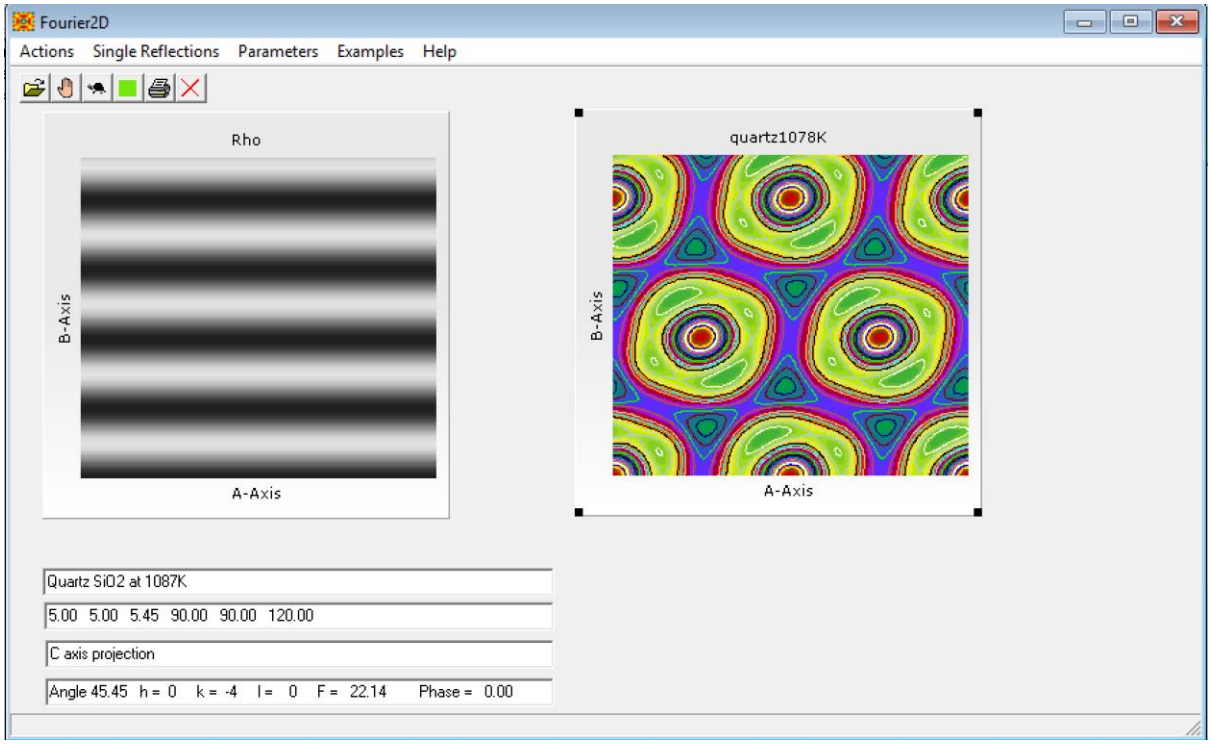


Figure 1. FOURIER2D: general view of main window.

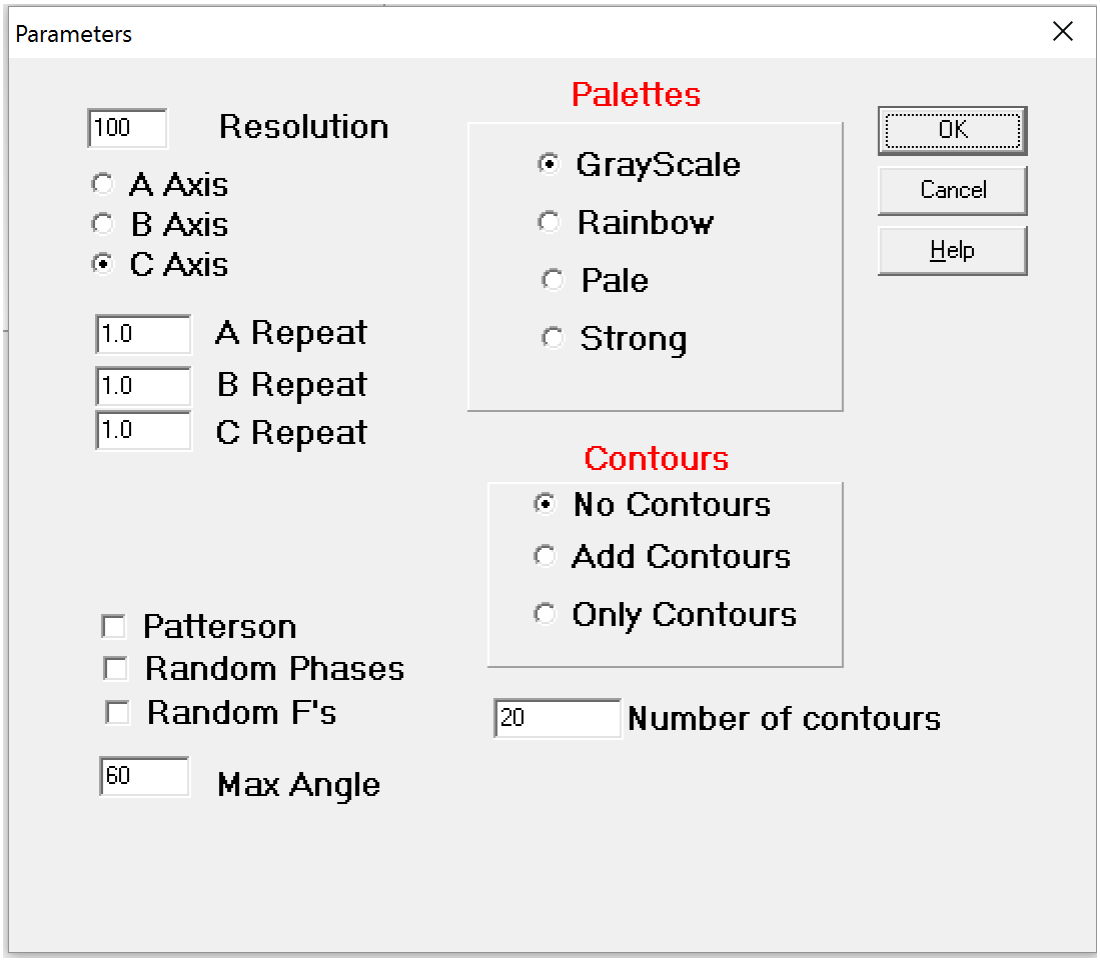


Figure 2. Parameters dialog box in FOURIER2D.

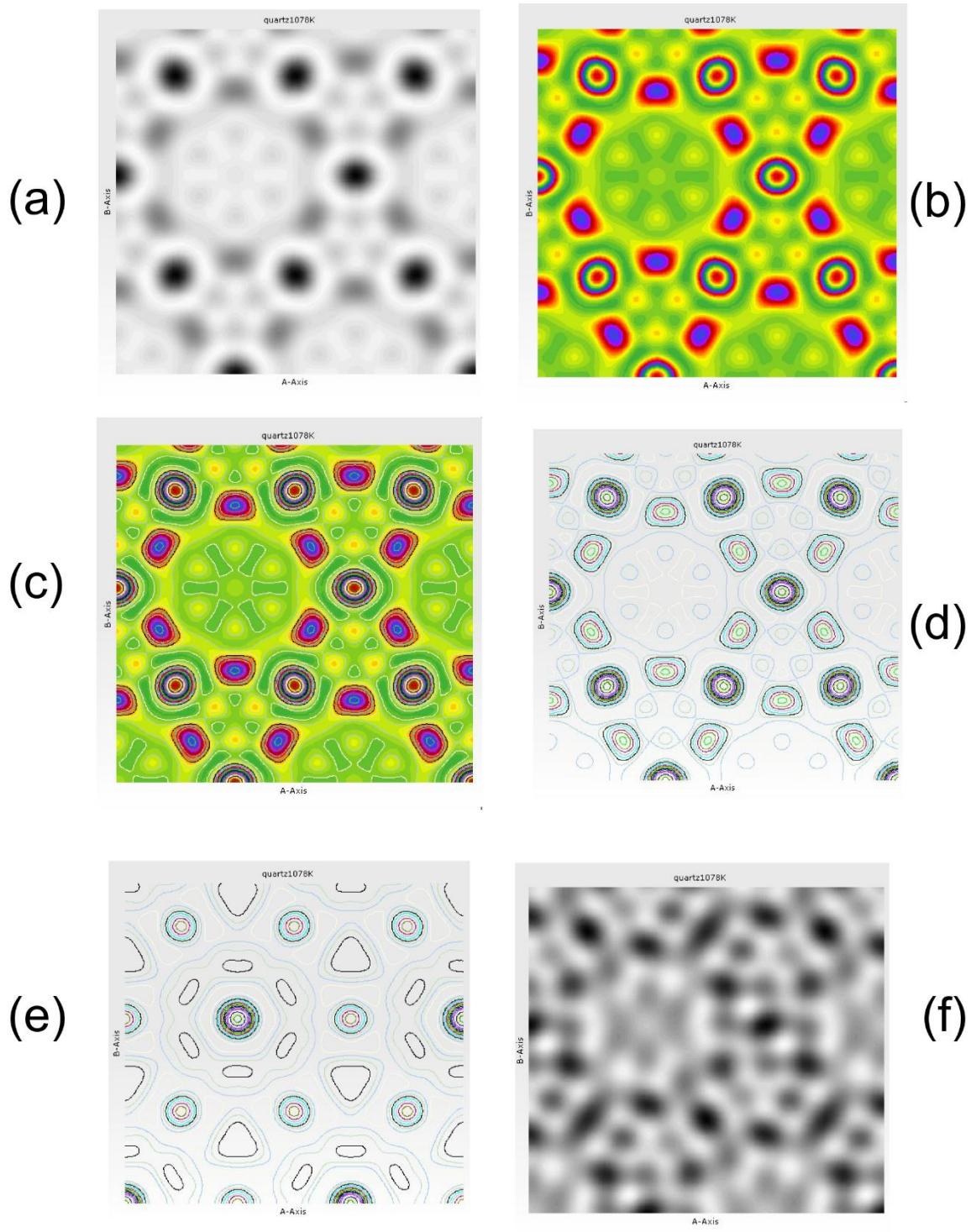


Figure 3. Fourier synthesis using FOURIER2D for high-temperature quartz structure on (001) (a) default grayscale (b) rainbow (c) contours added (d) contours only (e) Patterson projection (f) Random amplitudes, correct phases.

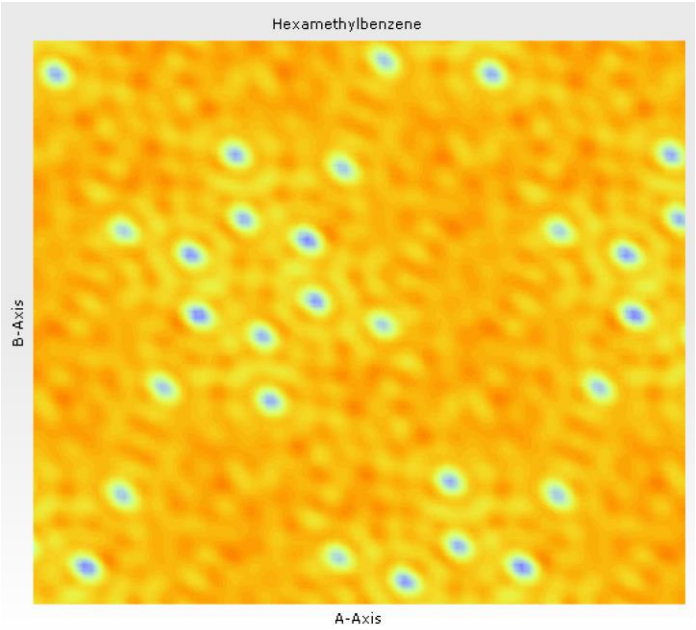
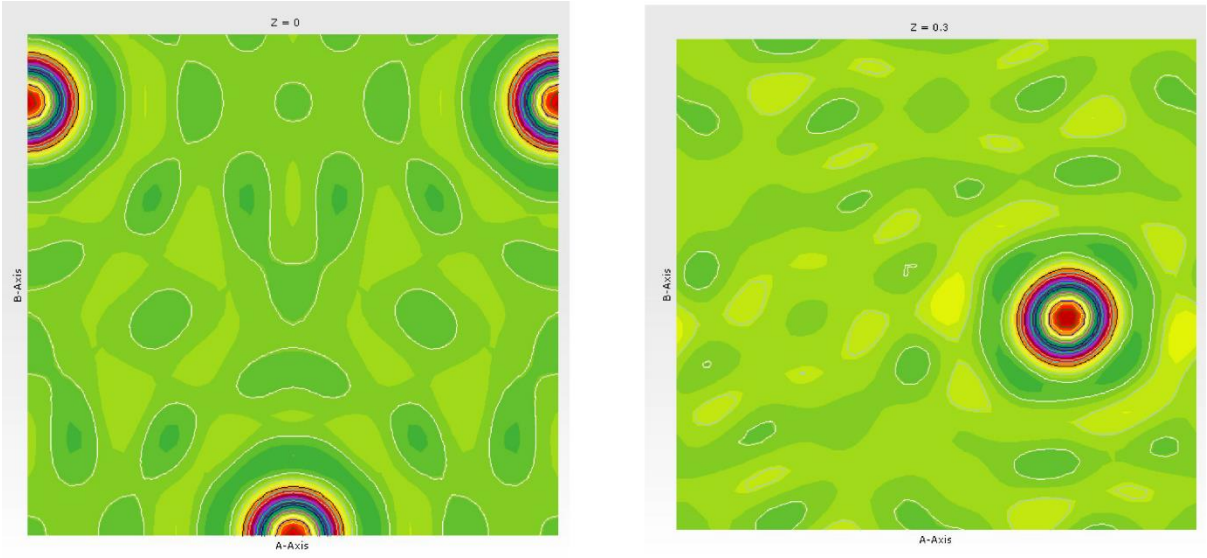


Figure 4. (001) projection of hexamethyl benzene using pale colours.



(a) (b)

Figure 5 FOURIER3D: sections viewed down the c-axis using rainbow colours + contours for high-temperature quartz (a) z = 0.0 (b) z = 0.30

References

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K., & Puschmann, H. (2009). *J. Appl. Crystallogr.* **42**, 339–341.

von Eller, G. (1965). *Acta Crystallogr.* **18**, 1000–1004.

Glykos, N. M. (1999). *J. Appl. Crystallogr.* **32**, 821–823.

Pepinsky, R. (1947). *J. Appl. Phys.* **18**, 601–604.

Welberry, T. R. & Owen, K. (1992). *J. Appl. Crystallogr.* **25**, 443–447.

Welberry, T. R. & Proffen, T. (1997). *J. Appl. Crystallogr.* **30**, 567.