

**s7.m3.o5 Teaching Diffraction Using Computer Simulations over the Internet.** Th. Proffen<sup>1</sup>, R.B. Neder<sup>2</sup>,

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Notes

Computer simulations are a versatile tool to enhance teaching diffraction physics and related crystallographic questions. We use these simulations to create various structures from single atoms to complex disordered crystals and to study the corresponding scattering intensity or even the amplitude and phase angle of the scattering amplitude which are otherwise not accessible. Students will rapidly acquire a rich experience on the relationship between real-space structure and the corresponding diffraction pattern. Previously we have presented a course<sup>1</sup> guiding students from the diffraction of a single atom to disordered crystal using the defect structure and diffuse scattering simulation program DISCUS<sup>2</sup>. Using DISCUS and subsequently plotting the results requires some familiarization. Although this is usually minimized by providing the students with DISCUS command files, in some cases (e.g. due to time constraints) learning how to use the programs might distract the attention of the students from the crystallography itself.

Here we present an extension of our diffraction course that uses a simple World Wide Web interface for DISCUS that allows the students to input the desired, essential simulations parameters, such as the number and type of atoms in a simple row, the monoclinic  $\beta$  angle etc., in a form in their WWW browser, click the RUN button and see the resulting structure and diffraction pattern plotted on the screen. Using this interface in the semester 1999/2000 for the first time, we indeed found that students focus much more on the science than on computational details such as how to use the programs, edit a file and so on. This allows the efficient use of these computer simulations in lectures where diffraction is only one of many topics. More complex simulations of disordered materials will still require to learn the command language of DISCUS to explore and use all its possibilities.

[1] R.B. Neder, R.B., Proffen, Th. "Teaching diffraction with the aid of computer simulations", (1996), *J. Appl. Cryst.*, **29**, 727-735

[2] Proffen, Th., Neder, R.B. "DISCUS a Program for Diffuse Scattering and Defect Structure Simulations" (1997), *J. Appl. Cryst.*, **30**, 171-175