

P.26.01.1*Acta Cryst.* (2005). A61, C491**Successfulness of a new Approach in Crystallographic Educator's Activity**Polina B. Kodess, Boris N. Kodess, *IPRAE, Crystals Metrology Dept., VNIIMS, Russia*. E-mail: bnkodess-vm@vniims.ru

A new approach for creation and application of interactive computer educator-oriented lectures in crystallographic teaching has been developed. Enhancement of efficiency is due to the more complete consideration of the characteristics of transfer and mastering of educational information, and creation of the more favorable medium of pedagogical interaction. The results of studying the content of educational environment has been shown that its influence the definition, extent and the content of life strategy of students. The characteristics of the personality of successful teacher have been examined within the framework of multidimensional model, including different levels of the complexity of the united complexes.

Examples of providing an educator with the lectures of three levels have been given. In the lectures of the first level the modern methods of computer graphics, presentation, are used. In the second level lectures the special software and series of animated slides are used, in which the lecturer can govern the parameters of the described phenomena, processes and installations. In the third level intended for the students of the first courses and senior student the interactivity elements have acquired basic meaning, providing the active cooperation of educator with the audience. High saturation of educational environment by the developing technologies, higher intellectual demands and intensity of intellectual activity give opportunity to students to form clearer life strategy and to realize long-term objectives. Due to value content of the interpersonal contact is connected with the intrinsic goals and social manifestations.

Keywords: teaching aids in crystallography, instructional software, pedagogis

P.26.01.2*Acta Cryst.* (2005). A61, C491**Three Crystallographic Aids for Teaching Early Science Classes. Start Them Young!**James H. Loehlin, Christina Woo, *Department of Chemistry, Wellesley College, Wellesley, MA 02481 USA*. E-mail: jloehlin@wellesley.edu

Crystallographers, like crystals, have to begin with a nucleating step. This presentation explains three separate exercises, designed to present some basic crystallographic principles to students before or at the beginning of their formal scientific education. Each of these aids will be explained and the results illustrated.

The first exercise builds on the startling beauty and symmetry of snowflakes, and illustrates how an almost limitless number of snowflake designs can arise from the same basic pattern using the crystallographic concepts of symmetry, unit cell, and lattice. It has been used successfully with those aged 8 and older. A template marked by each individual shows where to cut. Using a special punch and properly folded paper yields a beautiful, unique, paper snowflake for each participant.

The second exercise involves a model constructed of uniform spheres to illustrate closest packing in cubic and hexagonal crystals. Either ccp or hcp unit cells fit the model as the layer ordering is changed. This can also serve to illustrate the concepts of *lattice* and *motif*.

The third exercise uses laser diffraction from carefully designed slides. Several motif patterns are constructed on identical 2-D lattices, showing the unchanging diffraction geometry. A student calculates lattice constants from diffraction measurements and infers from intensities, the orientation and bond length of 'diatomic' scatterers.

Keywords: teaching aids, lattice, unit cell

P.26.04.1*Acta Cryst.* (2005). A61, C491**Writing Papers for Section C of Acta Crystallographica**Anthony Linden, *Institute of Organic Chemistry, University of Zurich, Switzerland*. E-mail: alinden@oci.unizh.ch

With the mandatory use of checkCIF (derived from PLATON check.def [1]) it is now rare for technically incorrect CIFs to be submitted to *Section C* of *Acta Crystallographica*. Why then were almost half of the submissions to the journal in 2004 not accepted? Principally, either the Comment section of the paper did not provide the required significant added value to the numerical data freely available in the CIF, or the Comment section was poorly crafted and difficult to understand. It is a requirement that the paper be written in clear and grammatically correct prose. The discussion of the presented crystal structures should go well beyond merely quoting some of the geometrical parameters of the molecules being studied, which any interested reader can readily obtain by downloading the deposited CIF. The discussion should include: concise details of why the presented crystal structures were determined, why the structures and the compounds themselves are novel and/or interesting, the chemical, natural or biological background and significance of the compounds, interesting features of the structures that are not directly derivable from the CIF data, how a knowledge of the structures helps the understanding of the chemical or physical properties of the compounds, and a comparison with the structures of related compounds. Comparisons should be more than superficial comments and should detail similarities and differences based on numerical analyses of the literature data. Over-analysis of the structures and throw-away statements of low, or no, scientific value should be avoided.

[1] Spek A.L., *J. Appl. Crystallogr.*, 2003, 36, 7.

Keywords: journal publication, publishing, technical writing

P.26.05.1*Acta Cryst.* (2005). A61, C491**Internet-Based X-ray Server**Sergey Stepanov, *Argonne National Laboratory, USA*. E-mail: sstepanov@anl.gov

X-ray Server is a public project for online analysis of X-ray diffraction and scattering data that recently passed the milestone of 100,000 calculations. The aim of this project is to explore novel opportunities given by Internet for sharing research results with wide scientific community, establishing collaborations, and refining scientific software. The Server provides Web-based access to a number of data analysis programs based on author's publications in the fields of X-ray optics and X-ray material science. The software operates directly on the Server available for use without downloading. This has proven to be the most efficient technology for having feedback from users and refining and extending the software. The advantages on users' side are also essential as confirmed by the Server success. Currently Server programs provide: (1) Interpolating X-ray dispersion corrections from discrete sets with an original algorithm; (2) Calculating X-ray rocking curves from strained crystals and multilayers for any Bragg-case diffraction including grazing incidence and/or exit and with scans around arbitrary axes; (3) Calculating X-ray specular reflection from multilayers with interface roughness using new recursive algorithm converging faster than the Parrat recursions; (4) Calculating X-ray resonant specular reflection from magnetic multilayers with magnetic interface roughness; (5) Calculating X-ray diffuse scattering from correlated interface roughness in multilayers; (6) Calculating multiple Bragg diffraction of X-rays with the help of new algorithm applicable to grazing incidence and/or exit. The report overviews the Server structure and the physical models beneath the server programs and demonstrates some applications.

Keywords: simulation X-ray diffraction, web internet techniques, X-ray diffraction theory