XVis: an educational open-source program for demonstration of reciprocal-space construction and diffraction principles
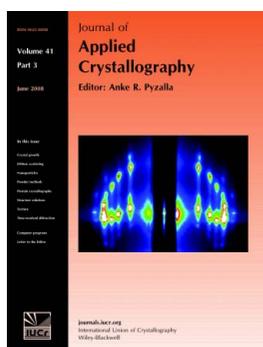
Oleksandr Yefanov, Vasyl Kladko, Mykola Slobodyan and Yulia Polischuk

Many research topics in condensed matter research, materials science and the life sciences make use of crystallographic methods to study crystalline and non-crystalline matter with neutrons, X-rays and electrons. Articles published in the *Journal of Applied Crystallography* focus on these methods and their use in identifying structural and diffusion-controlled phase transformations, structure–property relationships, structural changes of defects, interfaces and surfaces, *etc.* Developments of instrumentation and crystallographic apparatus, theory and interpretation, numerical analysis and other related subjects are also covered. The journal is the primary place where crystallographic computer program information is published.

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XVis: an educational open-source program for demonstration of reciprocal-space construction and diffraction principles

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The program *XVis* is designed for interactive demonstration of different diffraction issues, such as reciprocal-space construction, connection between real and reciprocal space *via* diffraction phenomena, different methods of reciprocal-space scanning, accessible reciprocal-space regions for coplanar and noncoplanar diffraction for both transmission and reflection geometries, *N*-beam diffraction phenomena, reciprocal space for two-layered systems and experimental examples. All demonstrations are calculated using real structure parameters. For better information representation, the program displays most demonstrations in real and reciprocal space simultaneously. The program is open source and can be downloaded from http://x-ray.net.ua/xvis.html.

1. Introduction

Any X-ray experimenter must have a good understanding of how reciprocal space is built and why the diffraction phenomena can be described in reciprocal space. These issues are addressed in many books, but invariably with a small amount of visual demonstration and in the form of static illustrations. Unfortunately, such description is usually not sufficient, so a good interactive demonstration is needed. The program *XVis* was created for this purpose.

The main advantage of the program is its ability to demonstrate different diffraction issues simultaneously in real and reciprocal spaces, thus showing how these spaces are interconnected. Most demonstrations are displayed as three-dimensional color pictures, while some are presented as animations, thus making the information easier to understand. All demonstrations in *XVis* are realistic and not schematic in the sense that real parameters of actual structures, like lattice constants and structure factors, are used and all pictures are calculated using the formulae of geometrical diffraction (Yefanov, 2008). Thus the program can also be applied to find suitable experimental geometry (§5).

XVis has many checkboxes and edit fields to set the demonstration parameters, and buttons for performing different actions (§2). Thus, setting up different demonstrations can take some time (the program has more then 70 controls). For this reason, *XVis* is equipped with a 'lecture mode' (§4) that allows a lecturer to prepare the lesson in advance and to show different topics by just clicking one button. All 'slides' of the lecture are described as simple text in the file `lecture.txt`, so no special programming skills are needed for lecture preparation. The program is distributed with a ready-to-use lecture that covers most of its abilities.

The program is free for noncommercial use and can be downloaded with sources from http://x-ray.net.ua/xvis.html (Yefanov, 2007). It was demonstrated for the first time at the summer school in V. Novgorod in May 2007.

Figure 1
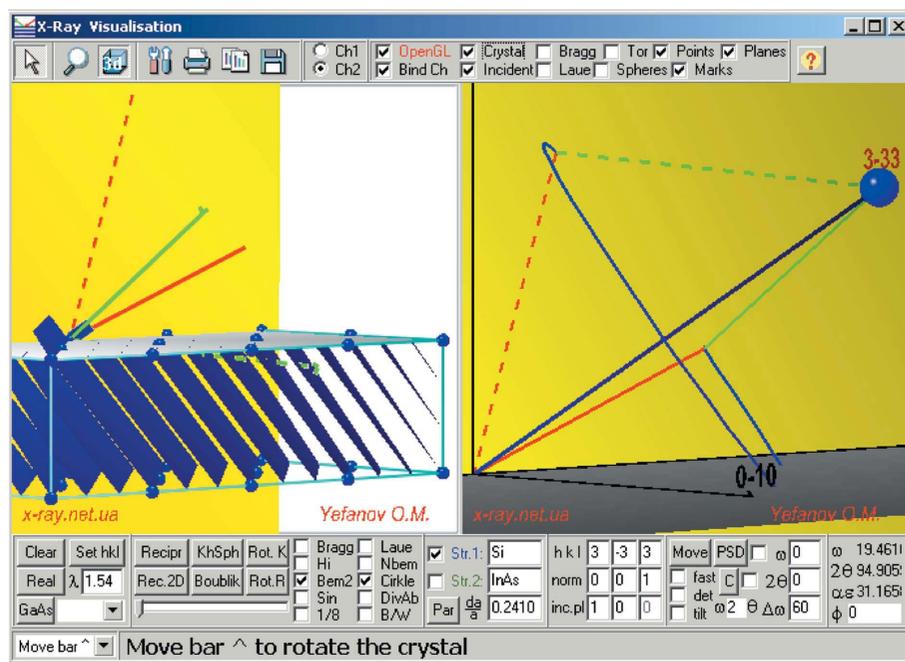The main screen of the program. Two possible ways to perform diffraction from the 3$\bar{3}$3 reflection are shown for the (0$\bar{1}$0) plane of incidence. Bragg case: solid lines; Laue case: dashed lines; incident beam: red; diffracted beam: green.

2. Interface and controls

The program includes many edit fields, checkboxes and buttons. All controls have

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hints with short descriptions of their function. The main window (Fig. 1) is divided into four panels. At the top, the visualization controls are placed. They include *TeeCommander* (SteemaSoftware, 2006) with radio-boxes for selecting which chart the commander is to use ('Ch1' = left, 'Ch2' = right) and checkboxes for turning on and off different visualization objects. At the bottom of the window, the main control buttons, checkboxes and edit fields are placed. A status bar below shows a description of the lecture 'slide'. In the bottom-left corner of the window, a drop-down list-box for navigation through the lecture is available. The main part of the window is occupied by two identical square *TeeChart* panels: the right panel shows reciprocal space, while the left panel shows real space or experimental examples.

To make the program present a demonstration, the user should first set all needed checkboxes and edit fields in the bottom panel and only then press the corresponding button. A slider in the bottom part of the window can be used to rotate the crystal around the surface normal. In chart panels, the left mouse button can be used to rotate the whole picture, while the right button moves it; the mouse wheel can be used to zoom the picture. To navigate through the lecture (see §4), the 'PageUp' and 'PageDown' keys can be pressed, or the drop-down list in the lower-left corner of the window can be selected.

For most demonstrations, OpenGL must be turned on (red checkbox at the top of the window). On computers that do not support OpenGL, some demonstrations cannot be shown. To store pictures, the user should set 'Ch1' or 'Ch2' and use one of the *TeeCommander* functions, like 'Save', 'Copy' or 'Print'. If the picture is needed in black and white, before starting visualization the 'B/W' checkbox should be checked. This mode does not remove all colors,

but makes some visualizations easier to understand when printed in black and white. For further picture editing (*e.g.* line width enhancement), the 'Edit' function of *TeeCommander* can be used. This launches a window with a huge number of drawing parameters.

The button 'Par' was designed to allow some additional control over the demonstrations. On pressing this button, an additional window appears, where lattice parameters and angles for both slabs, as well as some other visualization parameters, can be changed.

3. Functions of the program

For most demonstrations it is possible to set an arbitrary crystal surface normal orientation **N** (the default value is [001]) and plane of incidence by indicating a point belonging to this plane (default: 010). For most demonstrations, any wavelength λ can be considered. When polarizability is involved in calculations, λ should be in the range between 1.4 and 1.6 Å. To extend this range to 0.125–400 Å, the file f1f2.dat must be replaced with original one from the *XOP* program (ESRF & APS, 2004). The sample crystal structures are described in the subfolder Base; some combinations like In5Ga5As can also be
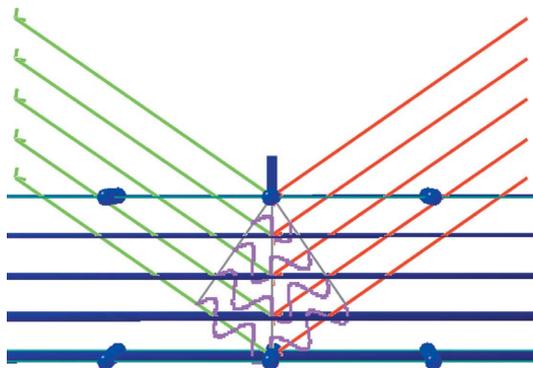

Figure 2
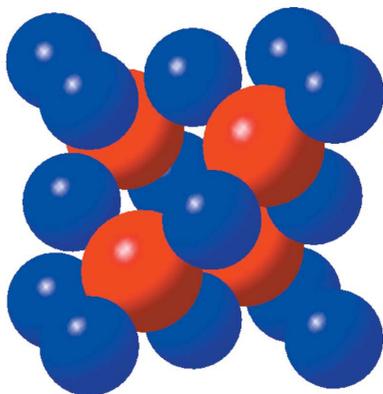Demonstration of Bragg's law in real space for (004) planes.
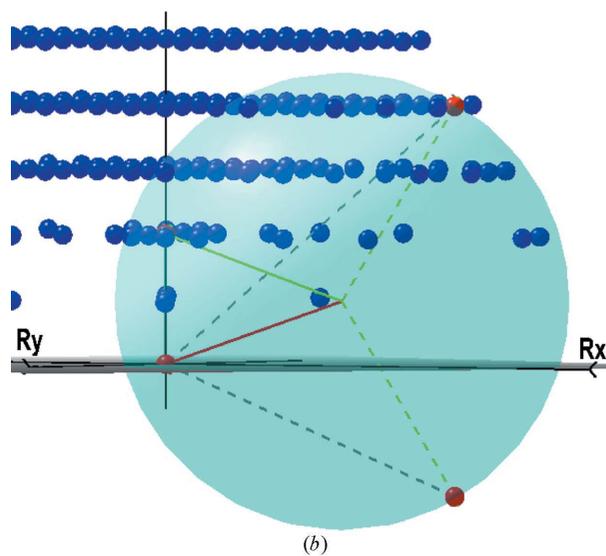

Figure 3
Zincblende unit cell.

(a)

(b)

Figure 4
Multiple-beam diffraction (λ = 1.54 Å): (a) real space; (b) reciprocal space.

considered. More crystals can easily be added because the format of the crystal structure file *.stf is quite simple. The name of each element in the structure must start with a capital letter, followed by a small letter (if necessary) and, optionally, a number specifying the composition, *e.g.* Si, Si3Ge7, Al0.5Ga0.5As, In1Ga1As.

The program is designed to illustrate the following issues concerning diffraction.

(i) Reciprocal-space construction for primitive cubic, tetragonal and triclinic crystals. On setting *hkl* and pressing the 'Real' button, the program shows in the right panel the reciprocal node *hkl* together with its reciprocal vector, and in the left panel the corresponding set of crystal planes with an indication of interplanar distance.

(ii) Drawing incident and diffracted beams for any reflection in reciprocal space and the corresponding crystal planes with the same

beams in real space ('Set hkl' button; Fig. 1). Both possible beam paths for a fixed plane of incidence can be shown (checkbox 'Bem2'; see Fig. 1). A circle formed by the beginning of the incident beam satisfying Bragg's law for the current crystal planes can also be drawn (button 'Rot.K' or checkbox 'Circle'; Fig. 1).

(iii) Illustration of Bragg's law in real space by plotting the phase of beams diffracted from parallel crystal planes (checkbox 'Sin' and 'Set hkl' button; Fig. 2). If the diffraction conditions are satisfied, the diffracted beam in reciprocal space points into the reciprocal-lattice node.

(iv) Plotting the unit cell of zincblende (if structure 1 is GaAs) or cubic diamond (for Si) crystals (button 'GaAs'; Fig. 3).

(v) Demonstrating the nature of forbidden and quasi-forbidden reflections (with checkbox 'Div' and 'Set hkl' button).

(vi) Showing multiple-beam diffraction (checkbox 'NBeam'; Fig. 4). Different reflections can be involved in diffraction when they belong to the Ewald sphere. This can be achieved by rotating the crystal around its surface normal using the slider at the bottom of the window. This mode can also be used to demonstrate why *N*-beam diffraction occurs more often with shorter wavelengths (Fig. 5).

Figure 5
N-beam diffraction with $\lambda = 0.4$ Å.

Figure 6
Accessible region for Bragg geometry with fixed plane of incidence and an Si [111] crystal.

Figure 7
(*a*) Different methods of reciprocal-space scanning ($\omega/2\theta$: red; ω: blue; 2θ: maroon; ω/θ: green). (*b*) Double-crystal scans in $\omega/2\theta$ (red) and ω (blue) modes.

(vii) In some demonstrations the size of the reciprocal node is proportional to the corresponding structure factor (polarizability); Fig. 6.

(viii) Experimental geometry calculation to achieve diffraction from a given reciprocal point: setting the azimuthal angle (plane of incidence) and calculating the incident and diffracted angles (shown in the bottom-right corner of the main window).

(ix) Plotting the coplanar accessible region for the current wavelength ('Rec.2D' button). For a better picture, the 'OpenGL' checkbox and '3D' button in *TeeComander* should be disabled.

(x) Drawing of the Ewald sphere for the current incident beam (button 'KhSph') and the fundamentally accessible region for a fixed plane of incidence (button 'Boublk'). The full three-dimensional accessible region for the current wavelength as well as the accessible regions in the Bragg (Fig. 6) and Laue geometries (Yefanov, 2008) can be plotted (button 'Recipr', with checked 'Tor', 'Bragg' or 'Laue'

checkboxes in the top panel, respectively). In addition, an incorrect accessible region can be plotted (Stangl *et al.*, 2004) (checkbox 'Spheres') with a demonstration of why it is wrong (by drawing inaccessible reflections inside this 'accessible' region).

(xi) Movable demonstrations of different reciprocal-space scans (ω, $\omega/2\theta$, 2θ, $\omega/N\theta$; Fig. 7a) with corresponding beam movement in real space with fixed crystal or fixed incident beam (button 'Move' with corresponding checkboxes; Fig. 8). In addition, it is possible to perform scans both in triple-crystal configuration and double-crystal configuration (checkbox 'det'; Fig. 7b).

(xii) Showing different ways to construct a reciprocal map by sequential combination of different scans (*e.g.* $\omega/2\theta$) and shifts (*e.g.* ω) (Fig. 9a).

(xiii) Demonstration of reciprocal-space measurement with a position-sensitive detector (PSD or CCD) (button 'PSD'; Fig. 9b). In addition, it is possible to show the geometry for grazing-incidence
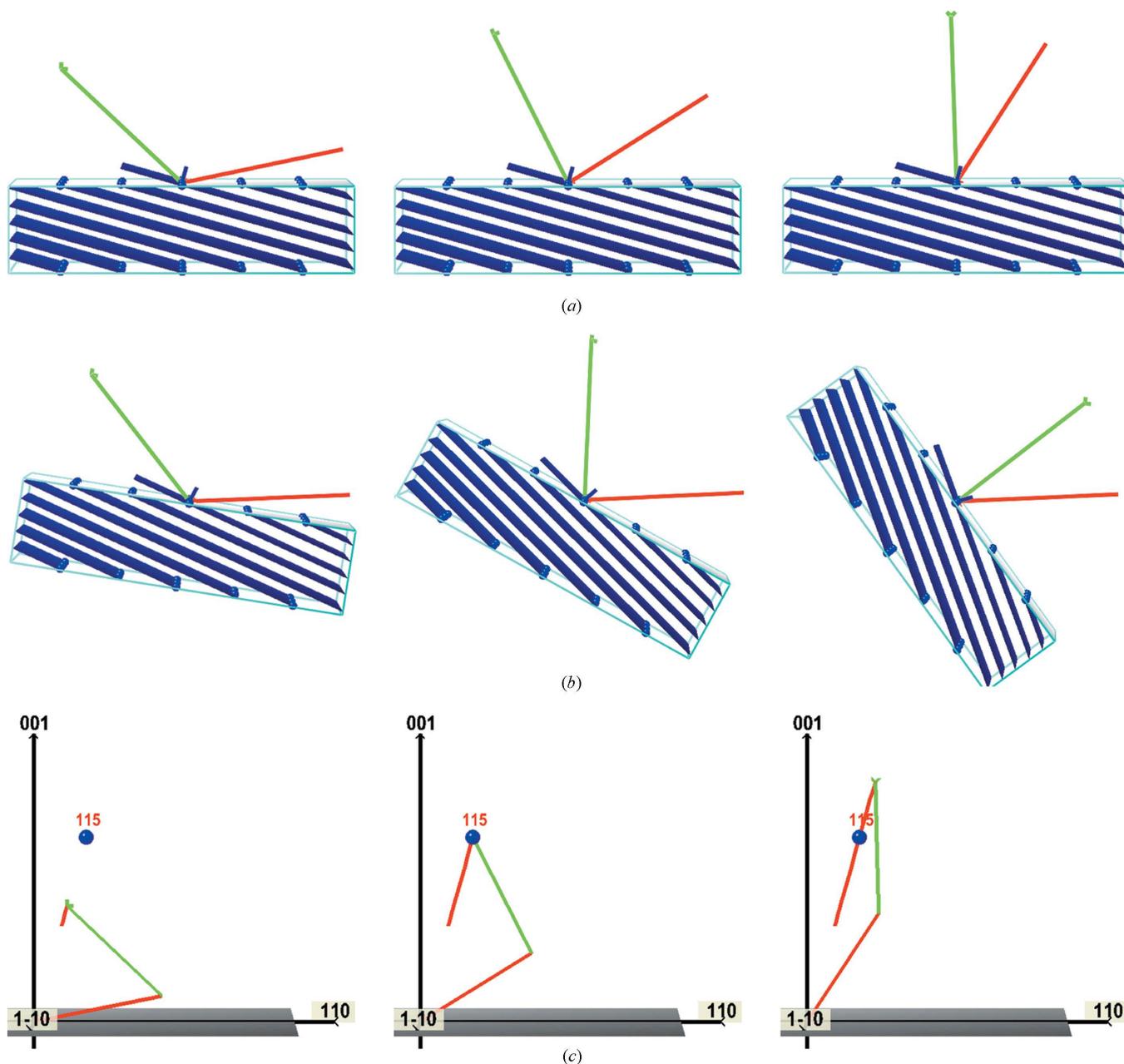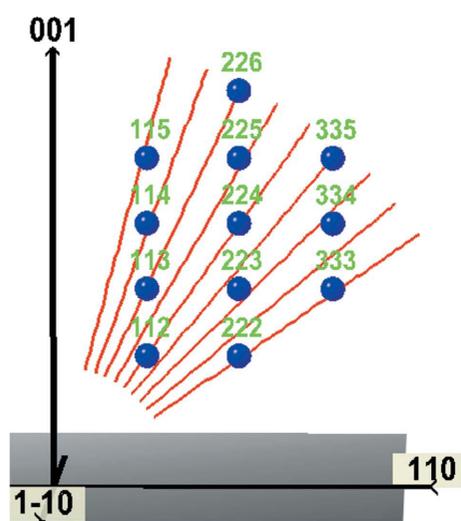

Figure 8
$\omega/2\theta$ scan: (a) real space with fixed sample; (b) real space with fixed incident beam; (c) reciprocal space.

(GISAX and GID) measurements, as well as the way to measure reciprocal space in three dimensions with the help of a PSD.

(xiv) Construction of reciprocal space for double-layer structures (substrate and one layer; Fig. 10). To use this mode, both checkboxes 'Str.1' and 'Str.2' must be checked. Different levels of strain in the upper layer can be considered: 'da/a' can be set to 'r' = relaxed, 'a' = fully strained, or some arbitrary strain level (number). By pressing 'Real', two layers are presented in real space (Fig. 10d), and by pressing 'Set hkl', a schematic view of both layers is drawn in real space (Figs. 10a and 10b) and the corresponding nodes are shown in reciprocal space (Fig. 10c). The latter mode of drawing in real space is not realistic, but it is more understandable because the angle between the crystal planes in both layers is shown more clearly.

(xv) Showing some experimental examples (drop-down list near the bottom-left corner).
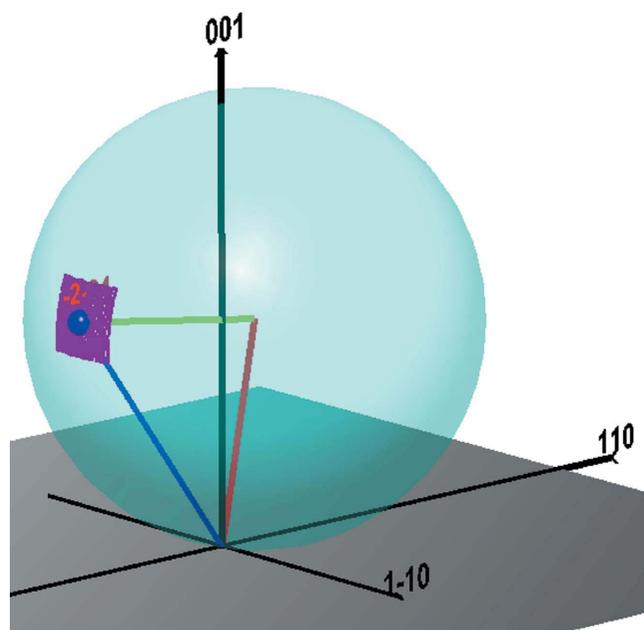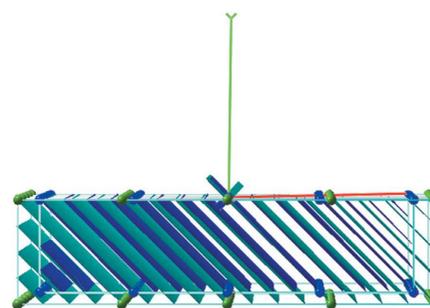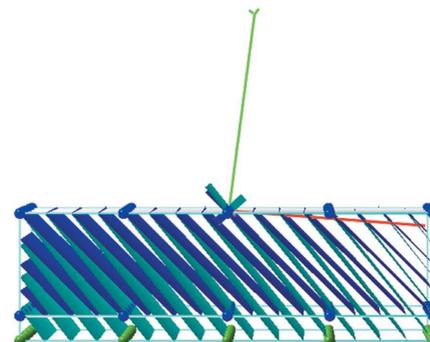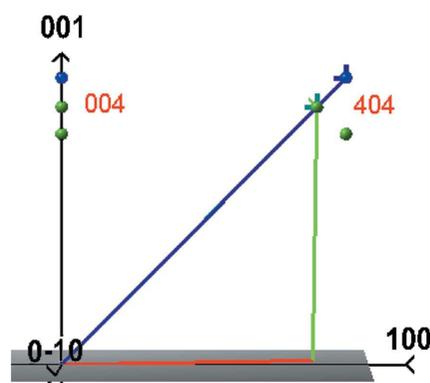

Figure 9
(a) Reciprocal map by combination of $\omega/2\theta$ scans with ω shifts. (b) Position-sensitive detector (maroon) with Ewald sphere.

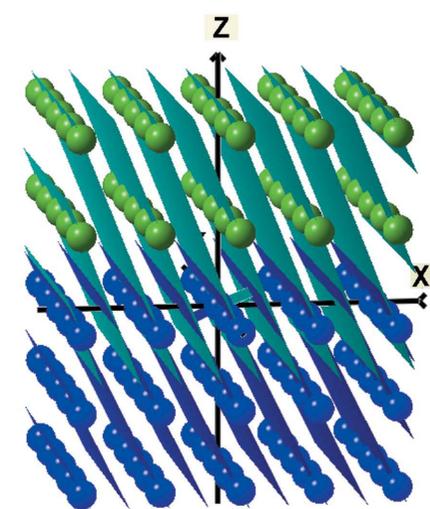**Figure 10**
Two-layered systems: (a) both layers relaxed; (b) one layer fully strained (green); (c) corresponding points for 004 and 404 reflections in reciprocal space; (d) demonstration of the structure under consideration (upper layer fully strained).

4. Lecture mode

As the program has many checkboxes and buttons, it could be quite difficult to use for demonstrations. For this reason there is a lecture mode, in which, when the user presses one button ('PageDown' = forward or 'PageUp' = backward), the program shows different topics with comments in the status bar at the bottom of the main window. The other way to navigate through the lecture is to use the drop-down list of topics in the bottom-left corner of the window. The lecture itself is described in the file lecture.txt as simple text. The format of this file is described at the beginning of the file. Each string is treated as a description of a separate 'slide' of the lecture. If the first character of any string is not a number (or minus sign), the whole string is considered to be a comment. The string can consist of edit-field values and checkbox flags (1 is usually checked); different groups of flags are separated by commas. After this, optional names of buttons to be pressed are listed; the button names are separated by commas and are listed in the order in which they would be pressed. If at the end of the buttons the word 'Next' is present, then the next string will be processed automatically; this is used for sequential 'slides'. At the end of the string, a tilde '~' (preceded by a comma) followed by a description should be present. If the 'slide' is selected manually from the drop-down list, it is better to start from the beginning of the subtopic (marked with '*****'), because some 'slides' are dependent on previous slides.

5. *XVis* for experiment preparation

Since the program calculates everything using real structure parameters and precise geometrical formulae, it can also be used for experiment planning. For example, to achieve diffraction from a reciprocal node under investigation, a user can set this node and find the appropriate plane of incidence with the corresponding incident and diffracted angles. In addition, it is easy to determine which reflections with valuable diffracted intensity could be analyzed for some plane of incidence and fixed wavelength. Such utilizations of the program are especially useful for unusual crystal-surface normal orientation (for example [117]).

Most diffractometers are equipped with some commercial software that can find the geometry for achieving diffraction from a given reflection, but usually this could be done in different ways, so if a user has any additional requirements for the experiment, the appropriate geometry will have to be found manually. In such cases, *XVis* can be very useful.

The other example of experiment planning is finding conditions for multiple-beam diffraction. This can be achieved by rotating the crystal around its normal and finding the plane of incidence when more than two reciprocal nodes lie on the Ewald sphere simultaneously.

6. Known limitations

Projection of the crystal surface normal on the z axis must be positive (last index of 'norm', $N_z > 0$), but owing to the symmetry of the indices, this limitation is very easy to overcome by changing the order of the indices.

In the current version, two-layered systems and strained lattices can be considered only when the surface normal is oriented along the [001] direction.

In lecture.txt, all indices hkl can be up to one digit, in the range from -9 to 9.

7. Structure of the program and sources

XVis is designed to run under Microsoft Windows from 98 to XP. The program is written using the C++ programming language in the free integrated development environment (IDE) *TurboC Explorer Edition* (Borland, 2006). The sources also include a project file for Borland Builder 6. For visualizations, the *TeeChart* component from SteemaSoftware (SteemaSoftware, 2006) is used (royalty free in compiled desktop applications). For the structure-factor (polarizability) calculation, the open source library *HiCalc* (Saveleva *et al.*, 2006) is used. This library uses atomic constants and $f1$, $f2$ corrections from the *XOP* program (ESRF & APS, 2004) and positions of atoms from Sergey Stepanov's site (Stepanov, 2007).

The program is open source and is distributed under the GPL license. It can be downloaded from http://x-ray.net.ua/xvis.html.

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