MATHEMATICA Software for Anisotropic Resonant Scattering

Viatcheslav A. Tchijikov[a], Stephen P. Collins[b], Vladimir E. Dmitrienko[a], [a]*Institute of Crystallography, Moscow, Russia.* [b]*Diamond Light Source Ltd, Rutherford Appleton Laboratory, Didcot, Oxon, UK*. E-mail: chizhikov@ns.crys.ras.ru

Forbidden reflections induced by atomic factor anisotropy appear in diffraction patterns of non-symmorphic crystals when the photon energy is tuned to an absorption edge resonance [1]. In order to simulate the properties of such reflections, the program package has been developed using Wolfram Research MATHEMATICA (version 4.0 and over). The package is now applicable for the crystals of cubic and hexagonal groups and it allows us to calculate the tensorial structure factor, hence the reflection intensity and polarization properties. Dipole-dipole, dipole-quadrupole and quadrupole-quadrupole contributions are included.

With this package the intensity azimuthal dependence was calculated for the 113 reflection in ZnO with wurtzite structure. This reflection forbidden by space group $P6_3mc$ was observed in [2]. The calculation results have shown to be in good accordance with synchrotron diffraction data.

The work was supported by INTAS grant 01-0822.

[1] Dmitrienko V.E., Ovchinnikova E.N., *Cryst. Rep.*, 2000, **48**, S59. [2] Collins S.P., Laundy D., Dmitrienko V.E., Mannix D., Thompson P., *Phys. Rev. B*, 2003, **68**, 064110.

Keywords: forbidden reflections, x-ray anisotropy, crystallographic software