

Hence we present MoProViewer: a molecular viewer designed as an interface to VMoPro, and thus especially dedicated to the field of charge density analysis. MoProViewer offers a wide range of features, among which:

- Compatibility with the MoPro molecular file format (including exportation), and with all the other formats allowed by the MoPro conversion program (CIF, shelxl RES, XD ...).
- Several molecule representation modes (lines, balls & sticks).
- All standard molecular viewer capabilities (configurable atoms labeling and atoms coloring scheme, images exportation).
- All "classical" crystal structure analysis tools (stereochemistry measurements, symmetry handling, thermal ellipsoids drawing).
- Representation and modification of multipolar model atomic axis systems and chemical equivalencies constraints.
- Setup and control of most of the VMoPro possible computations (electron densities, electrostatic potentials, $\rho(r)$ topology ...).
- Representation of the properties computed by VMoPro, or readable in XPLOR or Gaussian CUBE format, as 3D isosurfaces, 2D isocontours plots, 3D gradient lines or 2D slices of scalar fields.
- Possibility to color any isosurface on the basis of values of any other loaded scalar field.
- Drawing of critical points and bond paths obtained from an electron density topology analysis.
- A powerful atom selection tool, which allows for instance to easily perform computation focusing on any fragments or regions of a molecule.
- Computation of the electrostatic interaction energy between two molecules in the crystal, or between any selected fragments of the loaded crystal structure.
- Handling of transferable electron density parameters database.
- Specific tools for protein structures: hydrogen atoms and water molecules handling, sequence explorer.
- Specific tool for a fast and efficient model examination in the context of a MoPro structural or charge density refinement.

MoProViewer is written in C++ and is based on the Qt SDK and on the Armadillo [2] and OpenGL libraries. It will be released as free of charge and open-source software under the GNU-GPL license.

[1] C. Jelsch, B. Guillot, A. Lagoutte, C. Lecomte *J. Applied Cryst.* **2005**, *38*, 38-54. [2] C. Sanderson, "Armadillo: An Open Source C++ Linear Algebra Library for Fast Prototyping and Computationally Intensive Experiments" *NICTA Technical Report*, **2010**.

Keywords: charge density, molecular graphics

MS41.P15

Acta Cryst. (2011) **A67**, C512

Electron microscopy and x-ray diffraction study of the 1-D (NbSe₄)_{10/3}I system

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The linear chain compound (NbSe₄)_{10/3}I [1] shows nonlinear transport properties with a CDW transition at 285K [2]. Single crystals were examined with a four-circle x-ray diffractometer, with HREM and by measuring the temperature dependent electrical resistivity. Diffuse streaking perpendicular to the *c** direction was clearly detected

in electron and x-ray diffraction patterns, both above and below the CDW transition temperature. A reversible structural transformation was observed on cooling through the CDW transition at 285K.

The RT (NbSe₄)_{10/3}I structure (P4/mcc, *a* = 0.9464 nm, *c* = 3.1906 nm) is formed of NbSe₄ antiprisms, stacked along the *c* direction in a screw-like arrangement with 10 Nb-Se antiprisms per unit cell. Nb atoms are grouped into Nb₂ and Nb₃ segments and the Se-Se distances are correlated with the Nb chains. In accord with previous studies [3], the I atoms occupy two types of channels; those running along the [00*z*] direction contain four iodine atoms connected to four Se atoms, while the channels along the [11*z*] direction host two I atoms bonded to eight Se atoms in a square antiprismatic arrangement. Although the symmetry of the LT phase is reduced (at 100K: P2/c, *a* = 0.9442 nm, *b* = 0.9424 nm, *c* = 3.1883 nm and β = 92.35°) its structure is obtained from the RT one by a minor deformation.

The electron diffraction patterns show strong diffuse streaks perpendicular to the *c** directions, confined to the (*l* = ±10*n*) layers. Additional, short and very weak diffuse streaks appear on (*l* = ±2*n*) layers. Due to the needle-like crystal morphology, the planes perpendicular to *c** direction were examined by x-ray diffraction. Reconstruction of the reciprocal space (CrysAlis software) show that the diffuse scattering observed in electron diffraction patterns at (*h*,*k*,±10*n*) represent projections of concentric diffuse rings. A model for the disorder in the crystal structure, based on a mismatch between the infinite NbSe₄ chains with random shifts along the *c* direction is proposed. A computer simulation of the disordered structure was performed for the x-ray patterns with the DISCUS package [4,5], where in addition to the shifts of the infinite NbSe₄ chains correlated displacements within the thermal factors were applied to the I atoms. It is shown that the disorder of the NbSe₄ chains is responsible for the diffuse scattering on the (*h*,*k*,±10*n*) planes, whereas the disorder in I positions is responsible for the weak streaking at (*l* = ±2*n*). The proposed model is used to simulate the HREM images showing defects, attributed to a precursor effect to the phase transition.

[1] Z.Z. Wang, P. Monceau, M. Renard, P. Gressier, L. Guemas, A. Meerschaut, *Solid State Comm.* **1983**, *47*, 439-443, [2] C. Roucau, R. Ayrolesw, P. Gressier, A. Meerschaut, *J. Phys.* **1984**, *C17*, 2993- 2998, [3] A. Meerschaut, P. Gressier, L. Guemas, J. Rouxel, *J. Solid State Chem.* **1984**, *51*, 307-314, [4] Th. Proffen, R.B. Neder, *J. Appl. Cryst.* **1997**, *30*, 171-175, [5] R.B. Neder, Th. Proffen, *Diffuse Scattering and Defect Structure Simulation 2008*, Oxford University Press.

Keywords: 1D_structure, Disorder, Diffuse_scattering

MS41.P16

Acta Cryst. (2011) **A67**, C512-C513

Resonant X-ray diffraction from CB-type charge-orbital order in Nd_{1.5}Sr_{0.5}NiO₄

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Layered nickelate Nd_{2-x}Sr_xNiO₄ (NSNO) with K₂NiF₄-type structure is a rare example of a two-dimensional antiferromagnetic insulator-metal transition system, providing a contrastive counterpart to superconducting La_{2-x}Sr_xCuO₄ (LSCO) with the same crystal structure.