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Thermal expansion and atomic vibrations in $CaWO_4$ studied by neutron and synchrotron powder diffraction

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Alkaline-earth tungsten and molybdenum oxides with scheelite structure are applied as phosphors, laser hosts and scintillators. A new field for the application of these materials has emerged a few years ago when a new generation of cryogenic detectors, offering the capability of discrimination between electron and nuclear recoils has been implemented in some particle physics experiments. The increasing interest in using $CaWO_4$ for rare events searches initiated research in the fundamental physical characteristics of this material over a wide temperature range. To address this problem we turned our attention to modelling techniques and recently it was demonstrated that quasiharmonic lattice dynamics and the static lattice minimization method are viable tools for the characterization of low temperature properties of calcium tungstate [1] and molybdate [2].
A high structural stability for both WO_4 and MoO_4 tetrahedra has been observed for $CaWO_4$ and $CaMoO_4$ by theoretical studies along with a pronounced anharmonicity of thermal expansion in both *a*- and *c*- directions of the tetragonal cell. To extend the knowledge about materials with scheelite structure as well as about the correlations between anisotropy of thermal expansion, structural parameters of $CaWO_4$ and thermal vibrations a number of structural studies of calcium tungstate has been performed.
These investigations were carried out by elastic neutron scattering and high-resolution synchrotron powder diffraction techniques. Low temperature (5 - 295 K) neutron diffraction studies were performed at instrument D2B (Institute Laue - Langevin, Grenoble, France), whereas structural studies at high temperatures (300 - 1773 K) have been performed at instrument SPODI (research reactor FRM-II, Technical University of Munich, Garching n. Munich, Germany). Additionally, high-resolution powder diffraction experiments were carried out at the beamline B2 of HASYLAB/DESY over the temperature range 12 - 295 K. The data were collected during cooling and heating of the samples in small temperature increments, using the image plate detector OBI.
All datasets collected on the different instruments and sources coincide well among themselves and are in good agreement with the lattice dynamical simulations reported in Refs. [1,2]. The origin of the anisotropy of the thermal expansion has been related to the variation of individual bond lengths, bond angles, anisotropic displacement parameters and anharmonic vibrations.

[1] Senyshyn A., Kraus H., Mikhailik V.B., Yakovyna V., *Phys. Rev.* B, 2004, 70, 214306. [2] Senyshyn A., Kraus H., Mikhailik V.B., Vasylechko L., Knapp M., *Phys. Rev.* B, 2006, 73, 014104.

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Superspace playground: on-line toys for aperiodic crystallographer

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The important development of computer graphics tools has provided an enormous boost to both structural research and teaching ... excepted for aperiodic crystallography. The reason is perhaps that higher-dimensional structures do not immediately appeal to our perception*)* as this is the case for conventional structures. A quick search on the Internet reveals the existence of numerous web sites presenting interactive applets for crystallography teaching, but none of them is devoted specifically to the concept of superspace.
Apart from tuition, practical work in the field also requires much more than simple descriptive data. For example, the list of space groups for incommensurately modulated crystals given in vol. C of the Int. Tables for Crystallography is not feasible for practical solutions unless there is a tool relating it to 3-dimensional groups.
The aim of the project [1] launched two years ago in our laboratory is to fill both didactical and practical gaps by providing tools for handling superspace embeddings *a la carte:* from the choice of an initial model to the generation of illustrations, without forgetting visual models for training newcomers.
Our latest tool, Superspace Harvester, is designed to uncover similarities in an *ensemble* of 3-dimensional structures. It simulates the diffraction pattern for each structure on a semi-transparent layer and superpose the layers to help in the identification of common spots. In the superspace approach, these intensities correspond to the same main reflection. All other peaks are expected to be satellites. Different colors attributed to patterns help to estimate roughly the modulation parameters for each particular case.
Another component of the project intended for teaching includes user-controlled simulations (developed on Macromedia Flash) of higher-dimensional structures. We propose to illustrate the use of the tools with a few examples drawn from various fields of crystal chemistry.

[1] http://superspace.epfl.ch/