MS15-P6 **Crystal structure of ~RCu₃S₃ and ~RCuTe₂ (R = Gd–Lu) compounds.** Marek Daszkiewicz,[a] Lubomir D. Gulay,[b] Anna Gągor,[a] Adam Pietraszko,[a] Vasylyna Ya. Shemet,[c] [a]*Institute of Low Temperature and Structure Research, Polish Academy of Sciences, P. O. Box 1410, 50–950 Wrocław, Poland* [b]*Department of Ecology and Protection of Environment, Volyn National University, Voli Ave 13, 43009 Lutsk, Ukraine,* [c]*Department of Chemistry, Lutsk National Technical University, L'vivska str. 75, 43018 Lutsk, Ukraine*
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Designing of new functional materials with increasingly complex compositions has become a primary direction in modern science and technology. Complex rare–earth–based chalcogenides are interesting due to their specific thermal, electrical, magnetic and optical properties [1]. Various chalcogenide materials have application in the field of infrared and nonlinear optics. Systematic investigation of complex chalcogenide systems is important way for searching of new materials with interesting properties [2]. Here we report several crystal structures obtained from the ternary R–Cu–S and R–Cu–Te systems. The crystal structures of ternary compounds $TbCu_3S_3$, $Dy_{1.06}Cu_{2.84}S_3$ (space group $R\bar{3}$), $Ho_{0.67}Cu_2S_2$ (space group $P\bar{3}m1$), $ErCu_3S_3$ (space group $P\bar{3}1c$), $Yb_{0.80}Cu_{1.60}S_2$, $Lu_{0.67}Cu_2S_2$, $TbCuTe_2$, $DyCuTe_2$, $Tm_{1.07}Cu_{0.78}Te_2$, $LuCuTe_2$ (space group $P\bar{3}m1$), $Gd_{0.75}Cu_{1.74}Te_2$ (space group $P\bar{3}1m$) were determined by means of X–ray single crystal diffraction. The S(Te) atoms are stacked in a close packed arrangement with the layers in the sequence *AB*. The R atoms are distributed over octahedral interstices whereas Cu atoms are located in tetrahedral interstices. Disorder of R and Cu atoms in studied chalcogenides is found. Crystal structure comparison showed that $TbCuTe_2$ and $DyCuTe_2$ crystalize as superstructure $2a \times 2a \times 2c$ to $CaAl_2Si_2$ structure type, whereas $Gd_{0.75}Cu_{1.74}Te_2$, $ErCu_3S_3$ and $TbCu_3S_3$ ($Dy_{1.06}Cu_{2.84}S_3$) have superstructure $\sqrt{3}a \times \sqrt{3}a \times n \cdot c$ with n=1,2,3 [3].

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M15-P7 **Towards the solution of challenging crystal structures using Laue Microdiffraction.** Catherine Dejoie,[a] Lynne B. McCusker,[a] Christian Baerlocher,[a] Martin Kunz,[b] Nobumichi Tamura,[b] Christine Beavers,[b] Simon Teat,[b] [a]*ETH Zurich, Laboratorium f. Kristallographie, Zurich, Switzerland,* [b]*Lawrence Berkeley National Laboratory, Advanced Light Source, Berkeley CA 94720, USA*
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The white-beam, Laue diffraction experiment is an attractive alternative to the more conventional monochromatic one for single-crystal structure analysis, because it takes full advantage of the X-ray energy spectrum at a synchrotron and requires no rotation of the crystal in the X-ray beam. By using a broad band-pass X-ray source, a large number of reciprocal lattice points can be recorded simultaneously in a single exposure. This is why just a single Laue pattern obtained using an area detector is sufficient to determine a crystal's orientation or to measure its distortion or strain in mapping experiments. For this, only the positions of the reflections are needed. However, using the intensities of the reflections, as would be required for structure analysis, is more complicated. In order to properly interpret the intensities, various issues such as harmonic identification, energy dependent correction factors (absorption, Lorentz coefficient) and a precise evaluation of the effective incident spectrum have to be addressed. If these issues can be resolved, the structures of very small crystals (ca. 1 μm), crystals embedded in a heterogeneous matrix, beam-sensitive crystals, or samples in environments with restrictive geometries (e.g. in a high pressure cell) could become more easily accessible. The potential of Laue diffraction was recognized and exploited by the protein community many years ago [1]. In their approach, the Laue specific problems were addressed by exploiting the redundancy of the data stemming from the large unit cells of typical protein crystals. Unfortunately, this approach cannot be applied to inorganic substances or small molecules, which generally have relatively small unit cells and correspondingly fewer reflections. Therefore, we are attempting to devise ways of extracting the integrated intensities from a Laue pattern when the number of reflections is lower than in the protein case. The Laue patterns were indexed using the XMAS software package [2] and reliable integrated intensities were extracted using the 'Seed-Skewness' method [3]. We determined an effective flux curve by comparing the measured Laue intensities of a well characterized standard crystal (calcite) with the corresponding calculated structure factors [4]. This normalized flux curve proved to be transferable to other measurements. In the first application, the microstructure of deformed quartz was investigated. The Laue diffraction data allowed the primitive trigonal unit cell to be indexed unambiguously and the corresponding trigonal stress tensor to be calculated. An experimental setup, sample mount and data collection strategy have already been developed for measuring very small crystals on Beamline 12.3.2 at ALS, and some data have been collected with this setup. However, various aspects still need to be optimized. To this end, a series of simulations using the structure of the zeolite ZSM-5 have been performed for different experimental setups. In this way, we hope to establish how a sufficient number of reflection intensities for structure solution can be measured efficiently using the Laue technique.

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