spectroscopy, X-ray diffraction (XRD), scanning electron microscopy (SEM) and pair distribution function analysis (PDF). The analyses show that, depending on the reaction conditions, different products are formed. Some of these are nanocrystalline.
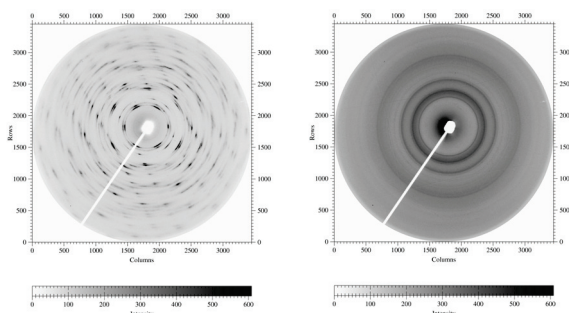

Fig. 1: Synchrotron X-ray diffraction patterns before (left) and after (right) laser heating W(CO)$_6$ in a diamond anvil cell.
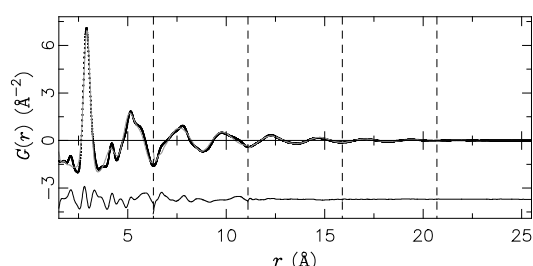

Fig. 2: PDF refinement results of the decomposition product obtained in the autoclave at lower pressures and temperatures. Note that the structural correlations end at about 2-2.5 nm.

[1] Porrati, F.; Sachser, R.; Huth, M.; *Nanotechnology*, 2009, 20, 195301.

Keywords: diamond anvil cells, decomposition, tungsten compounds

Full details of single crystal instrumentation and methodology are described in [3]. A sample was placed in a BGI design diamond anvil cell in ethanol:methanol (1:4) pressure transmitting media (steel gasket with a 350 microns hole preindented at 110 microns). For comparison, reference data were also collected for the same crystal at the same pressures using a Eulerian diffractometer equipped with a conventional X-ray source/optics [3]. The crystal size (180×120×50 mkm^3) was selected on the basis of its scattering power, such that the Bragg maxima were reasonably intense on the conventional system. In summary, we note that the lattice parameters measured using both diffractometers agree perfectly, lying within less than 2 estimated standard deviations.

Ultrasonic wave velocity measurements indicate that the dependency of the second order elastic stiffness tensor component C_{66} vs. P extrapolates to zero at 3.2 GPa [4]. The possibility of a phase transition was therefore suggested [4]. However, we observed no transition up to 7 GPa, which agrees with high pressure Raman scattering study [5]. F_E-f_E plot for Li$_2$B$_4$O$_7$ indicates a positive slop, therefore, a Birch-Murnaghan 3rd order EoS was fitted to the volume-pressure data (V_0=923.26(4) Å^3, K=46(1) GPa, K'=6.8(5)). Li$_2$B$_4$O$_7$ is more compressible along polar c-axis with $\beta_0 a$:$\beta_0 c$=1:3.04. Finally, relations between thermal expansion and compressibility of Li$_2$B$_4$O$_7$ will be presented.

[1] London D., Zolensky M.E., Roedder E., *Canadian Mineralogist*, 1987, 25, 173. [2] Trots D., Kurnosov A., Boffa Ballaran T., Frost D.J., *BGI Annual Report*, 2009, pp.187 -189. [3] Angel R.J., Downs R.T., Finger L.W., *Reviews in Mineralogy and Geochemistry*, 2000, 41, 559. [4] Sidek H.A.A., Saunders G.A., James B., *J. Phys. Chem. Solids*, 1990, 51, 457. [5] Li Y., Lan G., *J. Phys. Chem. Solids*, 1996, 57, 1887.

Keywords: high-pressure mineralogy-1, elastic properties-2, X-ray high-pressure techniques-3

FA2-MS19-P04

Compressional Behaviour of Diomignite, Li$_2$B$_4$O$_7$.

Dmytro M. Trots[a], Alexander Kurnosov[a], Tiziana Boffa Ballaran[a], Leonid Vasylechko[b], Marek Berkowski[c], Daniel J. Frost[a]. [a]*Bayerisches Geoinstitut, Universität Bayreuth, Deutschland.* [b]*Lviv Polytechnic National University, Ukraine.* [c]*Polish Academy of Sciences, Institute of Physics, Warsaw, Poland.*
E-mail: dmytro.trots@uni-bayreuth.de

Despite the fact that diomignite (Li$_2$B$_4$O$_7$, $I4_1cd$ symmetry) may control the physicochemical properties of highly fractionated late stage fluids in pegmatites [1], no diffraction studies concerning its compressional behaviour are available. In respect to technological importance, pegmatites are the primary source of lithium, which is widely employed in different fields of science and engineering (e.g. as a battery material, coolants for heat transfer applications etc.). Synthetic Li$_2$B$_4$O$_7$ can be implemented in acoustoelectronics, non-linear optics and piezotechnolodgy.

Compression of weakly scattering diomignite was also investigated for the purpose of commissioning an Eulerian single crystal diffractometer with an ultra high intensity rotating anode X-ray source equipped with multilayer optics [2]. This technique allows 8-position centring of Bragg reflections for accurate measurements of lattice parameters.

FA2-MS19-P05

Crystallographic Characterisation of Copper Based Shape Memory Alloys.

Osman Adiguzel, *Firat University, Department of Physics, Elazig/Turkey.*
E-mail: oadiguzel@firat.edu.tr

Shape-memory alloys are functional materials due to their unusual ability to "remember" the desired particular shapes at different temperatures. This ability arises from the characteristic microstructures in parent and product phases. These alloys exhibit a peculiar property called shape memory effect and involve the repeated recovery of macroscopic shape of material at different temperatures. The origin of this phenomenon lies in the fact that the material changes its internal crystalline structure with changing temperature.

Shape memory effect comprises crystallographically reversible transition from the high-temperature parent phase with high symmetry to low-temperature product phase, martensitic phase with low symmetry and exhibits dynamic recovery of the shape. This effect leads to a displacive transition, martensitic transition, which precedes through a series of metastable states in copper based shape memory alloys with changing temperature.

Copper-based alloys exhibit this property in β-phase field which has a bcc structure at high temperature parent phase. The high temperature bcc-structure undergoes two types of

ordering reactions called premartensitic transitions, bce→B2 and bcc→ DO_3, on cooling from high temperatures. On further cooling, martensitic transformation occurs by two or more lattice invariant shears on a {110}-type plane of austenite matrix called basal plane for martensite together with Bain distortion. Bain distortion consists of an expansion of 26% parallel to the $[001]_\beta$ axis and a compression of 11% normal to this axis, and a delineated fct unit cell in the long range order β-phase undergoes to the corresponding fcc lattice with this distortion.

Martensite phase has the unusual layered structures called as 3R, 9R or 18R martensites with low symmetry depending on the stacking sequences on the close-packed planes of the matrix.

The basal plane of martensite is subjected to the hexagonal distortion with martensite formation on which atom sizes have important effect. In case the atoms occupying the lattice sites have the same size, the basal plane of martensite becomes regular hexagon. Otherwise the deviations occur from the hexagon arrangement of the atoms in case atom sizes are different. martensite.

In the present contribution, x-ray diffraction and transmission electron microscopy (TEM) studies were carried out on two copper based ternary alloys, CuZnAl and CuAlMn.

Key Words: Shape memory effect, martensitic transformation, layered structures.

FA2-MS19-P06

Pressure-induced phase transition of KIO_3.
Lkhamsuren Bayarjargal[a], Björn Winkler[a], Alexandra Friedrich[a], Jasmin Biehler[a], Florian Schröder[a], Erick A. Juarez-Arellano[b]. [a]*Institut für Geowissenschaften, Goethe-Universität Frankfurt, Germany.* [b]*Universidad del Papaloapan, Tuxtepec, Mexico.*
E-mail: Bayarjargal@kristall.uni-frankfurt.de

KIO_3 is a promising material for optical applications as it is transparent in a large frequency range and shows significant non-linear optical effects [1-2]. KIO_3 crystallizes in space group *P1* [3]. The iodine atom environments consist of three oxygen atoms, defining a pyramidal IO_3 group, and three more distant oxygen atoms completing a distorted octahedron. There have been several studies of temperature-induced structural phase transitions in KIO_3 [4-6], but the response to pressure has not been investigated yet.

In this work we present the results of our investigation of the pressure induced phase transition of KIO_3 using X-ray diffraction, Raman spectroscopy, second harmonic generation (SHG) measurements and DFT-based calculations.

Powder X-ray diffraction has been performed on KIO_3 up to 20.9 GPa at the Advanced Light Source, ALS (Berkeley), on beam line 12.2.2 using 25 keV radiation. Raman spectra were collected with an in-house Renishaw micro-spectrometer. The pressure dependence of the SHG signals was measured with Nd:YLF laser (λ = 1054 nm).

The triclinic crystal structure of KIO_3 is stable up to 7 GPa where a phase transition is detected. The pressure at which the phase transition takes place obtained by X-ray diffraction agrees well with the pressure obtained by the Raman measurements. The lattice parameters and probable space group *P3* of the high-pressure phase were obtained from powder crystal data in situ at 10 GPa. The lattice parameters are *a* = 5.998(2) Å, *c* = 13.896 (2) Å, Z = 6 at 10 GPa. Atomic positions were then obtained using density functional theory.

A second phase transition is detected around 14 GPa. This transformation is followed by a continuous degree of amorphization upon increasing pressure. The ambient-pressure crystal structure is recovered once the pressure is released. The crystal structure determination of the first high-pressure phase and it's structural compression mechanism will be discussed.

[1] Bergman, J.G.; Boyd, G.D.; Ashikin, A.; Kurtz, S.K., *J. Appl. Phys.* 1969, 40, 2860. [2] Landolt–Börnstein, Vol. III/30b, Springer, 2000, 62. [3] Lucas, B.W., *Acta Cryst.* 1984, C40, 1989. [4] Herlach, F., *Helv. Phys. Acta.* 1961, 34, 305. [5] Maeda, M.; Takagi, M.; Suzuki, I., *J. Phys. Soc. Jpn.* 2000, 69, 267. [6] Kasatani, H.; Aoyagi, S.; Kuroiwa, Y.; Yagi, K.; Katayama, R.; Terauchi, H., *Nucl. Instrum. Meth. B:* 2003, 199, 49.

Keywords: high-pressure phase transformations, nonlinear optical materials

FA2-MS19-P07

New Layered High-Pressure Phase of AsS. N.B. Bolotina[a], V.V. Brazhkin[b], T.I. Dyuzheva[b], A.G. Gavriliuk[b], A.G. Lyapin[b], S.V. Popova[b], S. Samulski[c]. [a]*A.V. Shubnikov Institute of Crystallography RAS, Moscow, Russia.* [b]*Institute for High Pressure Physics RAS, Troitsk Moscow region, Russia.* [c]*Chemistry Department, University of Cambridge, UK.*
E-mail: bolotina@ns.crys.ras.ru

For arsenic sulfides, one layered covalent compound As_2S_3 and several molecular phases such as As_4S_4, As_4S_3 and others have been know so far. Under high pressures > 4 GPa and temperatures > 670 K the molecular phase As_4S_4 transforms into a new covalent modification with a layered orthorhombic structure (sp. gr. $Pbc2_1$; unit-cell values are a = 7.4537(7), b = 10.270(2), c = 18.258(1) Å). This high-pressure modification of AsS is metastable at normal pressure up to 530 K and represents a chemically stable narrow-gap (~0.8 eV) semiconductor. New structure is noticeable for the presence of covalent bonds between the same type of atoms (As-As) and anomalous weak covalent bonds between dissimilar atoms (As-S) with lengths (2.35 – 2.5 Å) "atypical" of this bond; some structure disordering has also been observed. Obviously, many of the known pseudo-molecular compounds such as As_4S_3, As_4Se_4, P_4S_3, P_4Se_4 and others should transform under high pressure to new covalent layered-structure modifications as well.

Keywords: high-pressure phases, structure analysis, layered compounds

FA2-MS19-P08

Structure mechanism of decomposition of $Mn_{3-x}Al_xO_4$ and $La_{1-x}Ca_xMnO_3$ solid solutions. Olga Bulavchenko[a,b], Evgeny Gerasimov[a,b], Svetlana Cherepanova[a,b], Sergey Tsybulya[a,b], Lubov Isupova[a]. [a]*Boreskov Institute of Catalysis SB RAS, Russia.*