

ordering reactions called premartensitic transitions, bcc \rightarrow B2 and bcc \rightarrow DO₃, 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] _{β} 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.

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Pressure-induced phase transition of KIO₃.

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KIO₃ 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]. KIO₃ crystallizes in space group *P1* [3]. The iodine atom environments consist of three oxygen atoms, defining a pyramidal IO₃ group, and three more distant oxygen atoms completing a distorted octahedron. There have been several studies of temperature-induced structural phase transitions in KIO₃ [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 KIO₃ using X-ray diffraction, Raman spectroscopy, second harmonic generation (SHG) measurements and DFT-based calculations.

Powder X-ray diffraction has been performed on KIO₃ 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 ($\lambda = 1054$ nm).

The triclinic crystal structure of KIO₃ 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 its structural compression mechanism will be discussed.

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Keywords: high-pressure phase transformations, nonlinear optical materials

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New Layered High-Pressure Phase of AsS. N.B.

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For arsenic sulfides, one layered covalent compound As₂S₃ and several molecular phases such as As₄S₄, As₄S₃ and others have been known so far. Under high pressures > 4 GPa and temperatures > 670 K the molecular phase As₄S₄ transforms into a new covalent modification with a layered orthorhombic structure (sp. gr. *Pbc2₁*; 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 As₄S₃, As₄Se₄, P₄S₃, P₄Se₄ and others should transform under high pressure to new covalent layered-structure modifications as well.

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

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Structure mechanism of decomposition of Mn₃

_xAl_xO₄ and La_{1-x}Ca_xMnO₃ 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.*