

patterns at high pressures and room temperature. We identified four Na-Au intermetallic phases (phases I ~ IV) in the pressure range up to 60 GPa.

The powder patterns taken at pressures lower than 3.5 GPa are complicated, showing phase mixture. Above about 3.5 GPa, we obtained clear diffraction patterns of single phase III. By decreasing pressure from phase III, we obtained single-phase patterns of phases II and I.

The first phase (phase I) exists below ~1.3 GPa. The critical pressure required for the solid-solid reaction of Na and Au is not well established, since some minimum pressure is necessary to seal the gasket of the DAC. Phase I is the known phase Na<sub>2</sub>Au with the CuAl<sub>2</sub>-type structure (*I4/mcm*, *Z*=4). It changes to phase II, which is stable between 0.7 and 3.6 GPa. Note that the pressure range includes the region of phase mixture with phase I or phase III. Phase II has the composition Na<sub>3</sub>Au with the AsCu<sub>3</sub>-type structure (*P-3c1*, *Z*=6). In this structure, a gold atom is coordinated by 11 sodium atoms. It should be noted that the compound Na<sub>3</sub>Au is not known at atmospheric pressure. Phase II further transforms to phase III above about 2.0 GPa. Phase III has again the composition Na<sub>3</sub>Au with the BiF<sub>3</sub>-type structure (*Fm-3m*, *Z*=4). The same structure has been found for K<sub>3</sub>Ag synthesized at high pressures [1]. Phase III is stable over a wide pressure range up to about 54 GPa, where it transforms to phase IV. Phase IV gives broad diffraction patterns, indicating large structural disorder. On decreasing pressure, phase IV is retained to at least 18 GPa. The powder pattern taken at 2.3 GPa shows the back-transformation to phase III. With further decrease of pressure, phase III changes to phase II and I, successively. Phase I seems to be stable at atmospheric pressure in agreement with the Au-Na binary alloy phase diagram [2].

The present finding suggests that the gold-alkali metal system may have a rich variety of intermetallic phases at high pressures.

[1] T. Atou, M. Hasegawa, L.J. Parker, J.V. Badding, *J. Am. Chem. Soc.* **1996**, *118*, 12104-12108. [2] T.B. Massalski, H. Okamoto, P.R. Subramanian, L. Kacprzak, *Binary Alloy Phase Diagrams*, 2nd ed. **1990**, (ASM International, Materials Park, OH).

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### Making use of topological similarities in HP structures

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As soon as we introduce a sample into a high-pressure device we lose information and it becomes increasingly difficult to derive models for high pressure phases; especially after phase transitions – when a new structure has formed. The effects of strain, scattering contrast, absorption, limited real-space resolution, high background, multiphase patterns *etc* can all contribute to rendering solution or refinement more difficult. Here we present examples of the potential for use of models derived from topologically similar features that may allow one to more readily identify structures and refine high-pressure datasets from them. Examples will be drawn from a variety of systems: *AX*<sub>2</sub> to complex minerals; from *OD*, polytypic and isomorphous structures and from materials science and mineralogical investigations at high pressure. These will be complemented by real powder data, collected from samples held in diamond-anvil cells or large-volume devices. We will also demonstrate typical code (none of which is the author's) that can allow one to manipulate structural assemblages, derive symmetry and a standardised structural description and how this can then be refined to

extract a complementary set of information on the state of the sample under extreme conditions.

**Keywords:** pressure, transition, systematics

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### The origin of memory glass effect in pressure amorphized rare earth molybdates

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A phenomenon called “memory glass effect” has been observed in AlPO<sub>4</sub>, Zeolite Y(Na-Y), clathrasils and some other materials, which have been subjected to pressure-induced amorphization. This effect is that the single-crystal/polycrystalline samples brought to the amorphous state due to applied pressure further restore the initial crystalline phase after pressure release. Moreover in the case of AlPO<sub>4</sub> it is argued that the single-crystal sample returns to a single-crystal state with the original crystal orientation. However the nature and possible mechanisms of this phenomenon are still not clear. In this work we report on studies of the memory glass effect in β'-Eu<sub>2</sub>(MoO<sub>4</sub>)<sub>3</sub> single crystal samples.

Early it was established [1] that powder samples of some rare earth molybdates undergo phase transformation from initial metastable crystalline β'-phase to the amorphous state at relatively moderate pressures ~7-9 GPa. However high pressure treatments of Eu<sub>2</sub>(MoO<sub>4</sub>)<sub>3</sub> single crystal samples in the same pressure range resulted in more complex structural states[2]. Here we carried out detailed structural analysis of the HP treated single crystal samples and structural transformations at subsequent annealing using XRD, HRTEM and HAADF STEM techniques. It was found that the “treated” sample structural state is complex and inhomogeneous: the most part of the sample has amorphous-like structure and this amorphous medium contains nano-sized inclusions of a crystalline phase distributed evenly over the medium, total content of the inclusions being a few percents. These crystalline domains are highly correlated in orientation over the sample, due to what they produce single-crystal diffraction patterns, in both XRD and TEM methods, relatively weak, along with intensive diffuse-like diffraction pattern from the amorphous part. The crystal structure of the domains corresponds to a new high pressure phase (HPP) of Eu<sub>2</sub>(MoO<sub>4</sub>)<sub>3</sub> (*P* > 2.1 GPa). Thus the nano-sized inclusions in the amorphous medium of the sample are in fact the residual islands of HPP. In the talk we are presenting the detailed picture of the structure transformations under high pressure treatment and following annealing illustrated by both X-ray single diffraction patterns and TEM/HRTEM images. These studies reveal the origin of memory glass effect to be result of the retention of the residual inclusions of HPP in the amorphous medium of sample.

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[1] V. Dmitriev et al., *Journal of Physics and Chemistry of Solids* **2003**, *64*, 307-312. [2] A.P. Kiselev, S.Z. Shmurak, V.V. Sinitsyn, S.S. Khasanov, B.S. Redkin, A.V. Alekseev, E.G. Ponyatovsky, *Bulletin of RAS:Physics* **2008**, *72* (9), 1297-1302.

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