

**MS22 P06**

**Simple metals at high pressure: the Hume-Rothery argument** Valentina F. Degtyareva, *Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Moscow district, Russia*. E-mail: [degtyar@issp.ac.ru](mailto:degtyar@issp.ac.ru)

**Keywords:** high-pressure structures, phase stability, crystal structure and properties

Under compression, simple s-bonded alkali metals pass through the sequence of phases characterized by lowering in symmetry, coordination number and packing density [1]. Structural transformations in these metals are controlled by the combined effects of electrostatic (Madelung) and electronic (band-structure) contributions to the crystal energy. The latter term increases with pressure yielding low-symmetry complex structures, such as Li-*cI16*, Rb-*oC52* and Cs-*oC84*. Stability of these structures can be supported by a Hume-Rothery argument when new diffraction plains appear close to the Fermi level [2]. Upon compression up to ~0.4 of initial volume, Cs and Rb form a very open structure *tI4* with coordination number 4+4 and packing density ~0.56. The transition to Cs-*tI4* is accompanied by an approximately 12% reduction in the atomic radius compared with Cs-fcc. Considering the Brillouin zone configuration with respect to the Fermi sphere one can conclude that the Hume-Rothery mechanism is effective if the number of valence electrons increases up to ~4 [2]. In the *tI4* structure the loss in the electrostatic energy compared with fcc should be compensated for by the gain in electronic energy that can occur by increase in the number of valence electrons due to the core overlap. The *tI4* and *oC16* structures in heavy alkalis Rb and Cs are similar to those in polyvalent group IV elements (Si, Ge and Sn) implying the similarity in the valence electron configurations in these two groups metals and supporting an assumption of core ionization in alkalis at much lower pressures than predicted by theory [3].

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**MS22 P07**

**Origin of unexpectedly high bulk modulus of Au and Ag nanoparticles** Qinfen Gu<sup>a</sup>, Guenter Krauss,<sup>a</sup> Fabian Gramm,<sup>b</sup> Antonio Cervellino,<sup>c</sup> Walter Steurer<sup>a</sup>

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**Keywords:** high pressure, nanocrystalline, gold and silver

We studied commercially available gold (30 nm, *n*-Au) and silver (10 nm, *n*-Ag) nanoparticles at high pressures up to 30 GPa using X-ray diffraction (XRD) and a diamond-anvil cell. Unexpectedly for that particle size, the nanoparticles show significantly higher bulk modulus than the corresponding bulk materials, i.e. about 60 % for *n*-Au and 20 % for *n*-Ag. The bulk modulus of *n*-Au,  $K_0 = 277(5)$  GPa, even surpasses that of ceramic materials such

as B<sub>4</sub>C (254 GPa), SiC (203 GPa), Al<sub>2</sub>O<sub>3</sub> (257 GPa) or TiB<sub>2</sub> (240 GPa). The structural characterization of both kinds of nanoparticles by XRD using a whole pattern-fitting method [1] and high-resolution electron microscopy (HRTEM) identified polysynthetic domain twinning and lamellar defects as described in [2] as the main origin of the strong decrease in compressibility. Free-surface effects do not play a significant role.

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**MS22 P08**

**Single crystal neutron diffraction** R. J. Nelves, J.S.Loveday, C.L.Bull, M.Guthrie, K.Komatsu and H. E. Maynard, SUPA, School of Physics and Centre for Science at Extreme Conditions, University of Edinburgh, Mayfield Road, Edinburgh, EH9 3JZ, UK  
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Although the pressures achieved routinely in high pressure neutron diffraction studies have reached to 30 GPa and beyond for almost twenty years this limit has applied only to powder diffraction studies. The limit for single crystal studies has remained at ~3 GPa which was achieved in the 1980's. This has meant that the advantages of neutrons for the study of problems like multisite disorder and anharmonic thermal motion have not been fully exploited beyond 3 GPa.

In this paper we will present developments made using the new VX Paris-Edinburgh cells which have extended the limit for neutron single crystal studies to almost 10 GPa. We will illustrate the power of high (real-space) resolution in studies of hydrogen bond centring in potassium dihydrogen phosphate and squaric acid as well as studies of multi-site disorder in ice VII.

**MS22 P09**

**Sixfold coordinated phosphorus by oxygen in AlPO<sub>4</sub> quartz homeotype under high pressure.** Alain Polian<sup>1</sup>, Julio Pellicer-Porres<sup>2</sup>, Antonino Marco Saitta<sup>1</sup>, Jean Paul Itié<sup>1,3</sup>, and Michael Hanfland<sup>4</sup>

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**Keywords:** high-pressure, phase transitions, X-ray diffraction, berlinite

AlPO<sub>4</sub> belongs to the berlinite quartz homeotype family, with potential applications as piezoelectric materials. We performed new angle dispersive x-ray diffraction experiments under high pressure combined with laser heating to relax the deviatoric stresses, complemented with *ab initio* calculations. We observed two phase transformations, and the structures were determined through Rietveld refinements. It is shown that AlPO<sub>4</sub>