FA2-MS18-P01

Compressed alkali and alkali-earth metals: Understanding structure through Jones zone activation. <u>Valentina F. Degtyareva</u>. Institute of Solid State Physics Russian Academy of Sciences, Chernogolovka, Russia. E-mail: <u>degtyar@issp.ac.ru</u>

Under compression, simple *s*-bonded alkali and alkali-earth metals pass through the sequence of phases characterized by lowering in symmetry, coordination number and packing density [1,2]. 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 *c1*16 in Li and Na, 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 [3]. Effect of *pressure induced Jones plane activation* was considered theoretically recently by Ashcroft and coworkers [4].

Upon further compression heavy alkalis Cs and Rb form a very open structure t/4 with coordination number 4+4 and packing density ~0.56. 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 from 1 up to 2 and higher values implying the transition of the outer core electrons into the valence band. Similar changes in the valence state are expected for compressed Na at the transition from c/16 to oP8 at pressures above 117 GPa [2,5]. Observations of the simple cubic structure in Ca (above 32 GPa) and the beta-tin structure in Sr (above 25 GPa) imply the increase in the number of valence electrons resulting from the core ionization.

McMahon M.I. and Nelmes R.J., *Chem. Soc. Rev.* 2006, 35, 943.
Gregoryanz E. et al., *Science* 2008, 320, 1054.
Degtyareva V.F, *Phys. Usp.* 2006, 49, 369.
Feng, J., Hoffmann, R., and Ashcroft, N.W., *J. Chem. Phys.* 2010, 132, 114106.
Degtyareva V.F. and Degtyareva O., *New J. Phys.* 11, 063037 (2009).

Keywords: high pressure, crystal structures, alkali metals