

MS20-P8 Structural complexity of dense lithium: electronic origin

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Lithium – the lightest alkali metal – exhibits unexpected structures and electronic behavior at high pressures [1,2]. As the heavier alkalis, Li is bcc at ambient pressure and transformed first to fcc (at 7.5 GPa). The high-pressure form Li-*cI16* (at 40-60 GPa) is similar to Na-*cI16*. The other high pressure phases found for Li (*hR1*, *oC88*, *oC40*, *oC24*) at pressures up to 130 GPa are specific to Li, whereas for heavier alkali metals there are several sheared forms. The different route of Li high-pressure structures correlates with its special electronic configuration containing the only 3 electrons (at 1s and 2s levels). Complex structures for Li are analyzed within the model of Fermi sphere – Brillouin zone interactions [3,4]. Stability of *post*-fcc structures for Li can be supported by Hume-Rothery arguments when new diffraction plains appear close to the Fermi level and characterized by pseudogap formation near the Fermi level decreasing the crystal energy. The filling of Brillouin-Jones zones by electron states for a given structure defines the physical properties as optical reflectivity, electrical resistivity and others. Recently found Li transformations metal-semiconductor-metal [2] are related to the Fermi surface – Brillouin zone configurations for corresponding structural states.

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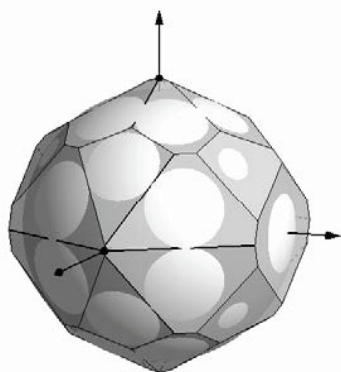


Figure 1. The Brillouin-Jones zone constructed for Li-*oC40* at 75 GPa is almost filled by electron states consisting with the experimentally found semiconducting properties of this Li phase.

Keywords: alkali metals, high pressure, crystal structures, Hume-Rothery effects

MS20-P9 Compressibility and pressure-induced deformation mechanisms in Si-Ferrierite

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Several experimental and theoretical studies have recently been performed in order to describe the compressibility and the pressure-induced deformation mechanisms (at the atomic scale) of nominally hydrophobic all-silica zeolites, compressed in penetrating or non-penetrating media (PTM)(i.e. [1-5]). In this paper, we explore - using penetrating and non-penetrating *P*-transmitting media - the crystal-fluid interaction upon pressure of an all-silica ferrierite-type zeolite [Si-FER: Si₃₆O₇₂]. Compression of Si-FER in silicon oil (as a non-penetrating medium) showed a remarkable flexibility of this framework in response to the applied pressure. A first displacive *Pmnn* to *P12₁/n1* phase transition was observed at ~ 0.7 GPa, followed by a second displacive transition to the *P2₁/n11* space group (via the intermediate *P-1* structure) at ~ 1.24 GPa. All the three observed polymorphs show a virtually identical bulk compressibility: the average β_V being 0.051(4), 0.056(9) and 0.055(3) GPa⁻¹, respectively. The structural deformation of the framework is mainly accommodate by the compression and the distortion of the 10- and the 8-ring channels running along *c* and *b*, respectively. The compression of Si-FER in three potentially penetrating media [i.e., methanol:ethanol:H₂O = 16:3:1 (mew), ethylene glycol (egl) and 2metil-2-propen-1ol (mpo)] showed evidence of crystal-fluid interactions at high pressure. Common features among the three experiments are: 1) the *Pmnn* to *P12₁/n1* phase transition at ~ 0.7 GPa (except for mew, where it occurs at ~ 1.5 GPa) and 2) the absence of the *P2₁/n11* polymorph (previously observed in silicon oil), coupled with a less pronounced compressibility compared to that in silicon oil, suggesting penetration of PTM molecules. For all the *in situ* experiments, the orthorhombic symmetry was restored after decompression.

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Keywords: Zeolite, high-silica ferrierite, compressibility, phase transition, penetrating PTM, non penetrating PTM, fluid penetration