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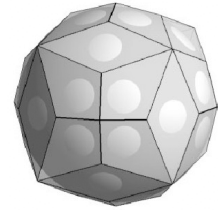
Crystal Structure of High-pressure Phases in Simple Metals: View from the Reciprocal Space. Valentina F. Degtyareva, Inst. of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Moscow region, 142432 Russia.

Recent high-pressure studies on simple metals yielded transitions from close-packed high-symmetry structures (like *fcc*, *bcc* and *hcp*) to complex, low-symmetry structures. Underlying physical reasons can be understood by Fermi sphere – Brillouin zone interactions (FS-BZ) within the nearly-free-electron model. Crystal structure energy is lowered by formation of the energy gap at BZ boundaries lying close to the Fermi level. The classical example of a crystal structure stabilized by FS-BZ effects is a Hume-Rothery gamma-brass phase Cu_5Zn_8 with 36-faced BZ polyhedron accommodating well the FS and filled by electron states to $\sim 93\%$ (upper figure). Similar Hume-Rothery effect is a characteristic of high-pressure structures of alkali metals as *Li-c/16* [1] and related structures of heavy alkalis. The BZ polyhedron of *Li-c/16* consists of 24 planes in contact with the FS and is filled by electron states to $\sim 89\%$ (lower figure). A program BRIZ is developed to visualize the FS-BZ configurations [2]. Several complex structures in *sp* metals at ambient and high pressure are considered with the electron contribution as a dominant part of the crystal structure energy.

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[1] Hanfland M, Syassen K, Christensen NE, Novikov DL, Nature 408, 174 (2000). [2] Smirnova I.S., Degtyareva V.F., *BRIZ – a program for the FS-BZ visualization*, Institute of Solid State Physics, Russian Academy of Sciences (2005).

gamma - brass Cu_5Zn_8



Li - c/16

