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Simple metals at high pressure: the Fermi sphere - Brillouin zone concept

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Crystal structure sequences at high pressure are analyzed for simple *sp*-elements and some binary alloys. Structure stability in these metals is related to effects of Fermi surface - Brillouin zone (FS-BZ) interactions [1]. These effects increase under pressure and lead to formation of structures with a decrease of symmetry and packing density. Structural similarities of alkali and alkali-earth metals to polyvalent group IV and V elements under pressure are considered. Correlations between structural and physical properties (resistivity and superconductivity) for these metals are discussed within the model of FS-BZ interactions. Complex high-pressure structure Li - *cI*16 [2] is considered as Hume-Rothery phase of gamma-brass type in the Cu-Zn alloy system. The underlying physics relates to formation of BZ by 24 planes with wave vector q_{211} close to $2k_F$ (here k_F is FS radius) accommodating well the FS (see Figure). The filling of BZ by electron states is ~89%. These characteristics define specific physical properties of the Li - *cI*16 phase.

[1] Mott N.F. and Jones H., *The Theory of the Properties of Metals and Alloys*, Oxford University Press, London, 1936.
[2] Hanfland M., Syassen K., Christensen N.E., Novikov D.L., Nature, 2000, 408, 174.

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BRIZ: a visualization program for Brillouin zone - Fermi sphere configuration

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The program BRIZ is developed for displaying of Brillouin zones and Fermi sphere geometry. The underlying physics relates to the nearly-free-electron model for simple sp-metals. Those planes are selected for construction of 'large' or Brillouin-Jones zones (called as BZ) that have wave vector q close to $2k_F$, where k_F is Fermi sphere (FS) radius. This condition provides formation of the energy gap on the BZ plane and leads to the lowering of structure energy [1]. A classical example of structure stabilization due to BZ-FS interactions is a gamma-brass in the Cu-Zn alloy system known as Hume-Rothery phase. The crystal structure is cubic with 52 atoms, and the BZ contains 36 planes accommodating well the FS (see Figure). The filling of the BZ by electron states is ~93%. These characteristics define specific physical properties of the gamma-brass phase.
The program BRIZ allowed one to visualize intersections of BZ planes and FS. Within the program is possible to vary the length of and axial ratio for non-cubic structures.

[1] N.F. Mott and H. Jones, *The Theory of the Properties of Metals and Alloys*, Oxford University Press, London (1936).