# Oral Contributions

**[MS20-05] Incommensurate Host-guest Structures in Compressed Elements: Hume-Rothery Effects as Origin.**

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Discovery of the incommensurate structure in the element Ba under pressure 15 years ago [1] was followed by findings of a series of similar structures in other compressed elements (see reviews [2,3] and refs. therein). Incommensurately modulated structures of host-guest (h-g) type consist of a tetragonal host structure and a guest structure in the form of chains embedded in the host atom channels so that the axial ratios of these subcells along c axis ($\gamma = c_{host}/c_{guest}$) are not rational. We consider here two types of the h-g structures: (1) the host cell with 8 atoms; (2) the host cell with 16 atoms; for both types the guest cells contain 2 atoms adding to the h-g cell ($2\bullet\gamma$) atoms. Examples are: (1) *t*I 11* in Bi, Sb, As and (2) *t*I 19* in Na, K, Rb, with the non-integer number of atom in cell. There is a close structural relationship of these h-g structures with the binary alloy phase $Au_3Cd_5$-tI32 [4], space group I4/*mcm*. Cd atoms in position 16k form octagon - square nets same as alkali - host atoms in *t*I19*. Au atoms in position 8h form square - triangle nets like Bi - host atoms in *t*I11*. Atoms Cd in 4b and Au in 4a relate to guest atoms in chains with increased interatomic distances forming a quest subcell with the incommensurate chost/ cguest ratio and reduced number of atoms in the structure to non-integer values. Axial ratio c/a ~ 0.5 for Au3Cd5 -tI32 is comparable with (c/a) host for tI11*and tI19*. The phase Au3Cd5-tI32 is related to the family of the Hume-Rothery phases that stabilized by Fermi sphere – Brillouin zone (FS-BZ) interactions where decrease in the electronic band structure energy occurs by the contact of the Fermi sphere (within the nearly-free electron model) and Brillouin planes [5,6]. An important characteristic is degree of BZ filling by electron states depended on zN, where z is the count of valence electrons per atom and N is the number of atoms in the cell. Configurations of BZ and inscribed FS are constructed with the program BRIZ [7]. For the $Au_3Cd_5$-tI32 structure the form of BZ consists of 32 planes with zN = 1.615•32 = 52 giving the BZ filling ~95% that satisfy well the Hume-Rothery effects. These parameters are used for the host-guest structures to evaluate the valence electron count per atom. Appropriate approximants for the host-guest incommensurate structures were used and additional BZ planes were constructed from superstructure reflections. One of consequences of this consideration for alkali elements is the necessity to assume the valence electrons band overlap with the upper core electrons and increase of the valence electron count from monovalent at ambient pressure to divalent [8] and even higher values [9] under compression.

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