Contribution ID: **533** Type: **Verbal**

Sublattices of actinide atoms in crystal structures

Thursday, May 17, 2018 2:00 PM (15 minutes)

As known, in classical crystal chemistry special attention is paid to closest sphere packings, which satisfy the Laves'maximum space filling (MSF) principle. The most important to crystal chemistry closest sphere packings are the face-centered cubic (fcc) and hexagonal close-packed (hcp) ones. In terms of such packings, atoms in crystal structures are treated as hard spheres of constant radius and realize coordination number (CN) equal to 12.

Extensive calculation of single-element sublattices in all crystal structures contained in ICSD and CSD in 2006–2008 allowed one to rethink the value of Belov's 12-neighbor rule. That project involved calculation of characteristics of Voronoi–Dirichlet (VD) polyhedra of more than 12 million crystallographically independent atoms. It revealed that the most common type of VD polyhedra for more than eighty chemical elements had 14 faces, while VD polyhedra with 12 faces were predominant for sublattices of only seven chemical elements: argon and six actinides (Ac, Pa, Am, Cm, Bk or Cf).

Increased prevalence of VD polyhedra with 14 faces was explained within the stereoatomic model of crystal structure, in which atoms are regarded as "soft" deformable spheres of constant volume. The total deformation of soft spheres forming the thinnest covering corresponding to VD tessellation is minimal in the case when the centers of the spheres form a body-centered cubic (bcc) lattice. As opposed to fcc and hcp lattices, the bcc lattice features CN equal to 14. As the number of structures of actinide containing compounds has risen up by a factor of 2-4 in the last ten years, it was interesting to check if the occurrence of VD polyhedra with 12 and 14 faces has changed, and to study the reasons of different CN's in sublattices of different elements.

In the course of this study, more than 18 thousand crystallographically independent atoms of 10 actinide elements from Th to Es were analyzed. It was shown, that VD polyhedra with 14 and 12 faces still remain the most common in actinide sublattices. Curiously, U-sublattices with 20 or more independent crystallographic sorts of U atoms feature VD polyhedra with 15 faces as the most common. Similar VD polyhedra with 15 faces are characteristic for the model system 'ideal gas', which lacks both short-range and long-range order. This similarity allows us to assume that sublattices of crystals containing 20 or more crystallographically nonequivalent A atoms have no short-range order but conserve long-range order. Thus, crystals with such sublattices can be treated as antipodes of quasicrystals, which feature short-range order, but lack long-range order.

The reported study was funded by RFBR according to the research project № 16-03-00200 a.

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Session Classification: TAN 3

Track Classification: Chemistry of Actinide and Trans-actinide Elements