Poster Presentations

[MS19-P01] 4-150-atom Lennard-Jones clusters in intermetallics

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We have performed comprehensive search for all energy-optimal conformations of 4-150-atom Lennard-Jones clusters as local atomic configurations in the crystal structures of intermetallic compounds. Crystal data have been taken from ICSD (release 2011/2) and Pearson's Crystal Data (version 2010/2011) with the TOPOS program package [1] by applying the algorithm for selecting finite subgraphs of any complexity in infinite periodic graphs.

As a result, we have found model nanoclusters containing from 4 to 74 atoms in 2067 crystal structures of intermetallics. Assembly mechanism of nanoclusters reveals a hierarchy of the sequence of the model clusters according to which each subsequent model cluster includes the previous one; this hierarchy characterizes the growth mechanism. Model clusters with more than 74 atoms are not realized in the structures of intermetallic compounds.

Using a recently developed algorithm of the nanocluster modeling [2] we have found three kinds of relations of the model nanoclusters and cluster building units in intermetallics: 1) full compatibility, when the model nanoclusters can be considered as building blocks forming the structure of the intermetallic compound; 2) partial compatibility, when the core of the cluster building unit corresponds to the model cluster; 3) total incompatibility of the model nanoclusters and cluster building units.

We have detected the atomic ensembles, which we called Centaur clusters because they consist of different nanoclusters to be fused without any distinct boundary. Thus Lennard-Jones clusters correspond to real atomic configurations and can describe the mechanisms of their growth.

[1] Blatov, V. A. (2006). *IUCr CompComm Newsletter,* 7, 4-38. http://www.topos.ssu.samara.ru.
[2] Blatov, V. A., Ilyushin, G. D., Proserpio, D. M. (2010). *Inorg. Chem.* **49**, 1811-1818.

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