MS13-O5 The nanocluster approach to elucidate complex intermetallics

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In the crystal chemistry of intermetallics, the classification in terms of atomic coordination polyhedra is traditionally used. However, the information about coordination of atoms does not determine the structure as a whole; therefore models that consider building blocks going beyond the first atomic coordination shell have been developed. The cluster model usually treats the structural fragments as nested polyhedra of a regular form that include atoms not necessarily connected to each other. The set of nested polyhedra does not always include all atoms and bonds of the structure; it usually describes only the general structural motif. In complicated and/or low-symmetrical (not only cubic) structures, the nested polyhedra cannot be selected unambiguously, and as a result, the same intermetallic compound can be described in several different ways. To resolve these problems, we have proposed the nanocluster method that implements a strict algorithm of searching for the structural units (nanoclusters) that model the entire crystal structure.[1] The method was realized in the program package ToposPro[2] and used to explore a number of complex intermetallics and the revealed nanoclusters were found in quite different compounds, even belonging to different structure types.[3,4] The work was supported by the Russian government (grant No. 14.B25.31.0005). [1] V.A. Blatov, G.D. Ilyushin, D.M. Proserpio., Inorg. Chem. 49 (2010) 1811-1818. [2] V.A. Blatov, A.P. Shevchenko, D.M. Proserpio, Cryst. Growth Des.,14 (2014) 3576-3586. http:/topospro.com [3] V.A. Blatov, G.D. Ilyushin, D.M. Proserpio., Inorg. Chem. 50 (2011) 5714-5724; [4] A.A. Pankova, V.A. Blatov, G.D. Ilyushin, D.M. Proserpio., Inorg. Chem. 55 (2013) 13094-13107.

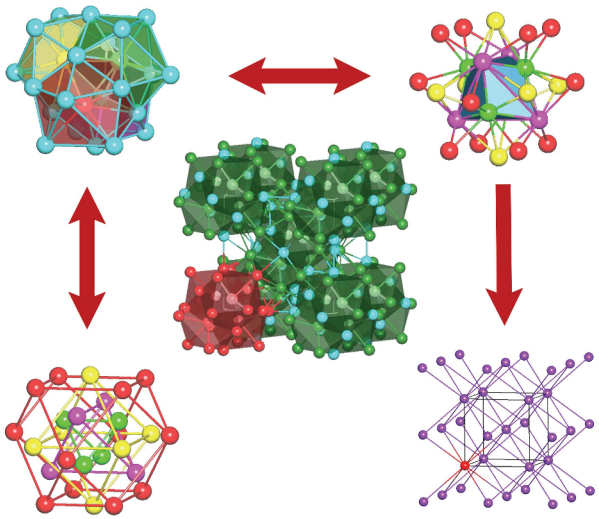

Figure 1.

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