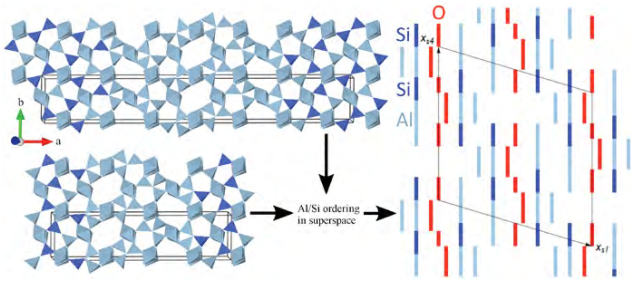
Figure 1: DFT relaxed models of mullite with x = 0.429 (upper left) and x = 0.5 (bottom left), and the common superspace model.



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Keywords: superspace, density functional theory, Al/Si ordering

MS14-O5

Nanocluster model and its application for crystal structure prediction of complex intermetallics

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One of the important thing to know about intermetallics is what they consist of and how building units connection is related to their structure and properties. An automatic procedure of representation of crystal structures as assembling of primary nanoclusters was developed and implemented into the ToposPro program package [1]. This approach is especially efficient to elucidate complex intermetallic structures. Thus, a collection of Topological Types of Nanoclusters (TTN) was created, which can be used for generating topological models of new intermetallics [2]. Further, the robustness of the obtained models can then be proved by quantum-mechanical calculations. In this work theoretical and experimental studies were successfully combined. Using the Nanoclustering procedure we found a group of intermetallics containing icosahedra and icosahedron-based two-shell Mackay clusters as primary building units. Among these the family of compounds belonging to $Sc_{57}Rh_{13}$ structure type (SG *Pm-3*) [3] seems to be incomplete since isostructural compounds are reported only for Sc-T systems where T = Rh, Ir, Ru, Pt. It is worth to note that one more structural type with stoichiometry 54:17 similarly composed from icosahedra and Mackay clusters arranged in the bcc mode (SG *Immm*) exists. Both cited structures can be considered as derivatives from an "ideal" cubic phase with 60:13 stoichiometry [3]. According to our DFT modeling and taking into account thermodynamics aspects, an intermediate phase of orthorhombic symmetry containing Mackay clusters of Pd@Sc12@Sc30Pd12 composition should exist. The Sc-Pd system was studied long ago, but only an approximate composition ~Sc_4Pd with no structural data was reported for the Sc-richest phase. Single crystals suitable for X-Ray investigation were mechanically extracted from the arc-melted alloys after the appropriate thermal treatment. Some disorder affects this orthorhombic structure of ~$Sc_{56}Pd_{15}$ composition, but Mackay clusters do not suffer from it. It is worth noting that new structure is quite unusual: the TTN collection includes merely 60 intermetallic compounds containing Mackay clusters as building units. The obtained results motivate us to continue a deeper exploration of related binary/ternary systems.

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