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Ab-initio and CVM calculations on the metastable fcc, hcp, and bcc Pb–Bi–Po and Pb–Bi–Te ternary systems

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Abstract

A molten Pb–Bi alloy will be used as coolant in MYRRHA (Multi-purpose hybrid research reactor for high-tech applications), a prototype of an accelerator-driven nuclear fission reactor ("generation IV reactor") that will be built at the Belgian Nuclear Research Center (start of construction in 2015, start of operation in 2025). Neutron capture by 209-Bi will inevitably lead to the appearance of 210-Po in the coolant (about 2 kg in the entire coolant volume of MYRRHA). In order to study interactions of Po with the coolant, knowledge of the Pb–Bi–Po phase diagram is required. Knowledge of the Pb–Bi–Te phase diagram is also desirable, since Po-containing systems, due to the high radiotoxicity of Po, are difficult to investigate experimentally. Therefore, analogies with the Pb–Bi–Te ternary system could lead indirectly to a better understanding also of the Pb–Bi–Po system.

The present work aims at determining overall trends in the Pb–Bi–Te and Pb–Bi–Po metastable fcc, hcp, and bcc phase diagrams. Ab-initio calculations at 0 K were performed in order to determine formation energies of several ordered compounds, in a simplified Cluster Expansion (CE) scheme. The ab-initio information was treated in a thermodynamic extrapolation to higher temperatures using the Cluster Variation Method (CVM). Binary and ternary phase diagrams were then compared at different temperatures, mainly to identify similarities and discrepancies between the systems.