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The role of lattice dynamics in phase stability of Fe-Sn binary systems

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For many technological applications, it is important to predict the physical properties at finite temperature. For example, magnetic materials suitable for permanent magnet applications must show large saturation magnetization and high magneto-crystalline anisotropy at elevated temperatures. Thus, predictions made by using DFT calculations at T=0˜K should be validated for finite temperatures. An interesting example is the Fe–Sn binary system with some phases, like Fe_3Sn, which is a ferromagnet, experimentally stabilized at temperatures above 750°C [1]. At finite temperatures one of the main contributions to the free energy is due to the atomic vibrations and it can be estimated, in many cases, within the quasi-harmonic approximation. In the case of Fe–Sn binary systems, however, the account of lattice dynamics is necessary for an accurate description of phase diagram even at T=0˜K. At low temperatures, there exist three experimentally observed structures: Fe_3Sn_2, FeSn, and $FeSn_2$. The DFT calculations at T=0˜K predict that enthalpy of formation of all these phases is positive. In this work, we show that these experimentally observed phases are energetically stabilized by phonons. We also calculate the finite temperature phase diagram at elevated temperatures.

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Refs

[1] C. Echevarria-Bonet {\it et al.}, {\it Structural and magnetic properties of hexagonal Fe_3Sn prepared by non-equilibrium techniques}, Journal of Alloys and Compounds {\bf 769}, 843 (2018).

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