Phonon effects in phase equilibria

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One of the most significant characteristic of metallic materials is the microstructure consisting of a few phases. Hence, many properties of metals cannot be understood from single crystals. The microstructure can be designed from the phase diagram that is determined from free energies of multiple phases. The free energy is decomposed into a few contributions, where the most important ones include the phonon effects and the configrational entropy. One of the problem in calculating the phonon free energy is the existence of the martensitic phase transition, where a high temperature phase is not stable at zero temperature exhibiting imaginary phonons. The self-consistent phonon (SCPh) method [1] can cure this problem.

In this project, we performed first-principles phonon calculations to evaluate free energies of metallic materials. Figure 1 shows calculated free-energy differences between the bcc and hcp phases for pure Ti and a Ti-Nb alloy. Since the bcc phase of Ti-based alloys exhibits martensitic phase transition, we performed SCPh calculations with the ALAMODE code [2]. In addition, we included effects of the electronic free energy, because we found it non-negligible. Even though binary Ti-Nb alloys has two-phase equilibrium regions in the phase diagram due to the digree of freedom in the composition variation, we fixed the composition so that the phase equilibrium occurs at a single temperature. The phase transition of the Ti-Nb alloy occurs at a lower temperature compared with pure Ti, consistent with an experimental fact that Nb is known as a bcc stabilizer in Ti-based alloys [3]. In addition, phase equilibria in permanent magnets were discussed through the CALPHAD approach with the first-principles cluster-expansion method [4].

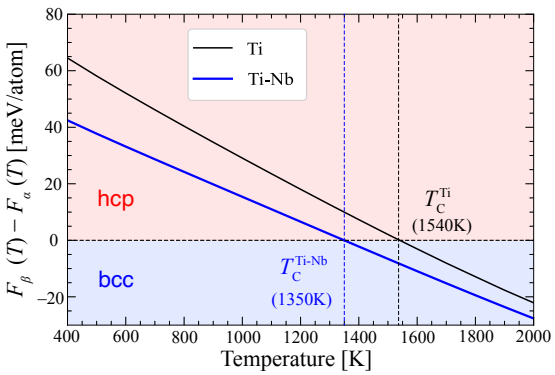

Figure 1: Calculated free-energy differences between the bcc and hcp phases for pure Ti and a Ti-Nb alloy as functions of the temperature T. $F_\alpha(T)$ indicates the free energy of the α phase, i.e., the hcp phase, whereas $F_\beta(T)$ is for the β phase, i.e., the bcc phase.

[1] T. Tadano and S. Tsuneyuki, Phys. Rev. B **92**, 054301 (2015).
[2] T. Tadano, Y. Gohda, and S. Tsuneyuki, J. Phys.: Condens. Matter **26**, 225402 (2014).
[3] K. Hashimoto, T. Tanaka, and Y. Gohda, in preparation.
[4] S. Enomoto, S. Kou, T. Abe, and Y. Gohda, J. Alloys Compd. **950**, 169849 (2023).