Vibration free energy of Cr_2Zr Laves phase

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Laves phases crystallize in cubic ($MgCu_2$, C15) or hexagonal ($MgZn_2$, C14 and $MgNi_2$, C36) type structures which differ only by a different stacking of the same four layered structural unit. In the Zr-Cr system, these three Laves phases appear in the phase diagram. Ab initio analysis of relative stability of Laves phase structures confirms the sequence of decreasing stability C15–C36–C14 [1].

In the present study, for discussing the finite temperature effect, we applied the quasi-harmonic approximation with the phonon-DOS calculations. Phonon-DOS calculations were performed by MedeA, which uses the first principle calculation code of VASP. Figure 1 shows the temperature dependency of vibration free energy change of $ZrCr_2$ Laves phases. The volumes are fixed at the equilibrium ones of the ground states. The C15 phase is correctly estimated to be the lowest energy at the low temperatures. The C14 phase is highly stabilized at the high temperatures, and the phase transition from C15 to C14 phases is predicted to occur at 1000K. The C36 phase is experimentally expected to be stable at the middle temperature range, but is not calculated yet.

References:

1 J. Pavlů, J. Vřešťál, M. Šob, CALPHAD, 33 (2009).

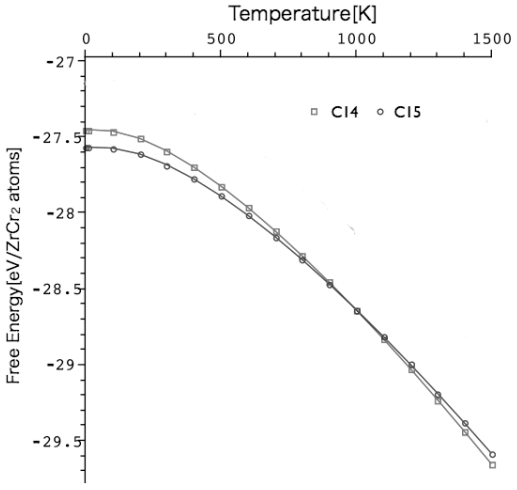

Fig.1 Temperature dependency of vibration free energy change of $ZrCr_2$ Laves phases.