Determination of thermodynamic properties using *ab initio* methods for the intermetallic compounds in Nd-Fe-B system

○Adie Tri Hanindriyo[1], Soumya Sridar[2], K. C. Hari Kumar[2], Kenta Hongo[3,4,5], and Ryo Maezono[3]
(1. Grad. Sch. Adv. Sci. Tech., JAIST, 2. Dept. Metal. Mater. Eng., IITM, 3. Sch. Info. Sci., JAIST, 4. NIMS, 5. PRESTO, JST)
E-mail: adietri@icloud.com
arXiv:1811.06744

Phase diagrams are indispensable to researchers and engineers working on materials processing and fabrication. It maps the phases in a certain system with the various thermodynamical parameters in which these phases are stable. The computational method CALPHAD can utilize relevant thermodynamic properties of phases to predict stability and calculate the phase diagram of a system.

The Nd-Fe-B system attracts a good amount of attention from researchers and engineers due to its magnetic properties. Perhaps most importantly, the ternary phase $Nd_2Fe_{14}B$ has become the base for a family of materials used in powerful permanent magnets available today. However, there is limited experimental data on some phases in this system, especially outside the binary Fe-B system. This presents an opportunity for *ab initio* methods to step in and provide valuable predictions as more data points for CALPHAD to work with.

We investigated several phases in the Nd-Fe-B system, using *ab initio* methods to calculate the enthalpy of formation and the specific heat (under constant pressure, or C_p) with respect to temperature. Density Functional Theory (DFT) with effective Hubbard U correction[1] was used in order to account for $4f$ electrons in Nd atoms, while vibrational contribution to C_p is calculated using phonon calculations. We found that the correction introduced by Hubbard U parameter generally produces more reliable values of enthalpies of formation compared to uncorrected DFT. C_p prediction has also been made for these phases, with a good reliability from 20 K $< T <$ 1000 K, due to the unaccounted contribution from magnetic ordering in the low temperature region.

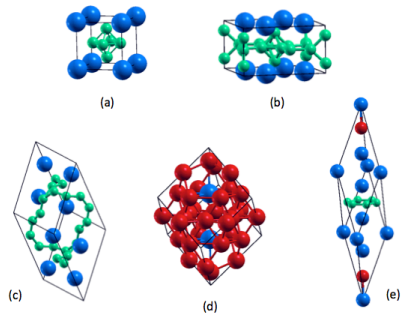

Figure 1: Nd-Fe-B phases investigated in this work, including (a) NdB_6, (b) NdB_4, (c) Nd_2B_5, (d) Nd_2Fe_{17}, and (e) $Nd_5Fe_2B_6$

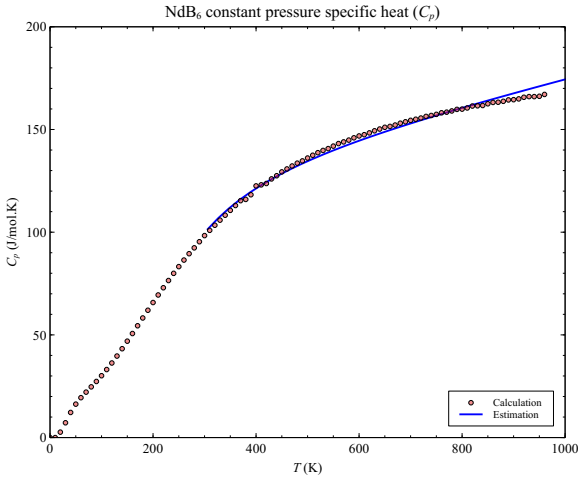

Figure 2: Calculated C_p data of NdB_6 ("Calculation") with theoretical estimation ("Estimation") from the work of Bolgar, *et al.*[2]

References

1. M. Cococcioni and S. de Gironcoli, Phys. Rev. B **71**, 035105 (2005)
2. A. S. Bolgar *et al.*, J. Alloys Compd. **201**, 127-128 (1993)