Progress in establishing QMC-CALPHAD Framework

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

The Nd-Fe-B system has generated high interest within both academic and industrial fields due to its application as a base alloy for strong permanent magnetic materials, specifically the ternary $Nd_2Fe_{14}B$ compound. This has fueled much of the research into the system, including in the construction of the phase diagram for Nd-Fe-B and its constituent binary systems of Nd-B, Nd-Fe, and Fe-B systems. The computational method CALPHAD has been regularly used to assess the phase diagrams of various systems, with Nd-Fe-B ternary phase diagrams having been studied in multiple past works [1-4] utilizing most recent information available (Figure 1).

In order to obtain more information for constituent phases, *a*b initio methods provide a lot of potential for use in CALPHAD due to its reliability and cost-effectiveness particularly compared to empirical measurements. Density Functional Theory (DFT) is generally used in order to investigate material properties pertaining to Gibbs energy modelling within CALPHAD, as an alternative to empirical measurements. Incorporating the Hubbard U correction to account for the strong correlation within these compounds, we have obtained such thermodynamic properties as enthalpies of formation and specific heat in constant pressure (Cp), as seen in Figure 2 for NdB_6.

We also see potential in the Quantum Monte Carlo (QMC) method in taking into account dynamic electronic correlation within certain classes of materials, such as Mott insulators or $3d/4f$ materials. These classes of materials are notoriously difficult to investigate with DFT as the electronic correlation is included within the exchange-correlation functionals, and are well-known to be poorly described with conventional functionals such as LDA and GGA. QMC can potentially answer the need for a reliable method of investigating strongly correlated systems such as rare-earth alloys in the Nd-Fe-B system. We present our work with the Nd-B binary system using DFT-CALPHAD framework with Hubbard U corrections, as well as our investigation into establishing QMC-CALPHAD framework.

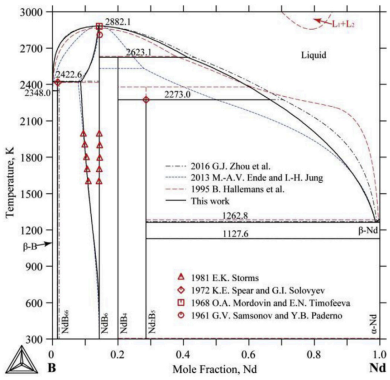

Figure 1: Nd-B phase diagram from CALPHAD assessment [4]

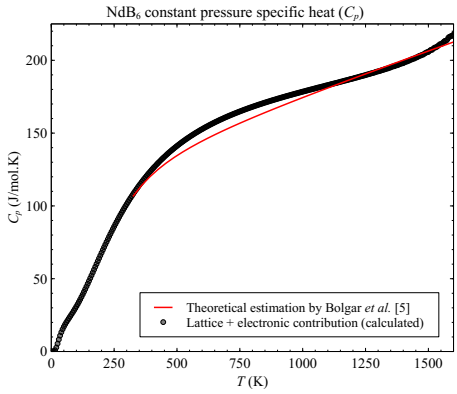

Figure 2: NdB_6 calculated specific heat (DFT)

1. B. Hallemans *et al.*, J. Phase Equib. **16**, 137 (1995).
2. M.-A. Van Ende and I.-H. Jung, J. Alloys Compd. **548**, 133 (2013).
3. G.J. Zhou *et al.*, J. Electron. Mater. **45**(1), 418 (2015).
4. T.L. Chen *et al.*, Calphad **66**, 101627 (2019).
5. A.S. Bolgar *et al.*, J. Alloys Compd. **201**, 127 (1993).