First-principles study on the nanoscale physics of $Nd_2Fe_{14}B$

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In 1970's, Re_2Fe_{17}, where Re represents rare earth elements, could be considered as permanent magnets. However, the Curie temperature (T_c = 330K) was not high enough for permanent magnets. B was introduced into Re_2Fe_{17} by Sagawa [1], who is the inventor of Nd-Fe-B sintered magnets, in order to increase the magnetic properties, for example, magnetic moment, magnetization, Curie temperature, etc. of Re_2Fe_{17}. This led to creating $Nd_2Fe_{14}B$ known as the main phase of Nd-Fe-B sintered magnets. However, the role of B in $Nd_2Fe_{14}B$ was not clearly studied from nanoscale physics.

We systematically studied the effects of B in $Nd_2Fe_{14}B$ on the magnetic properties and electronic states through first-principles calculations [2]. We used OpenMX [3] mainly on System B for the present study. In order to understand how B changes the magnetic moment and magnetization of $Nd_2Fe_{14}B$, we calculated these two physical quantities of $Nd_2Fe_{14}B$, $Nd_2Fe_{14}B_0$ and Nd_2Fe_{14}. $Nd_2Fe_{14}B_0$ has the same lattice parameters and the atomic positions of $Nd_2Fe_{14}B$, but B is not present in it. Nd_2Fe_{14} is a hypothetical material and its lattice parameters and atomic positions are optimized, therefore, these are not the same as $Nd_2Fe_{14}B$. We find that B does not increase the magnetic moment and magnetization of $Nd_2Fe_{14}B$. We check the stability of $Nd_2Fe_{14}X$ (X = B, C, N, O, F) by comparing the formation energies of $Nd_2Fe_{17}X$. We find that the formation energies of $Nd_2Fe_{14}B$ or $Nd_2Fe_{14}C$ become negative relative to that of $Nd_2Fe_{17}B$ or $Nd_2Fe_{17}C$ (see Fig.1). Our calculation result is in good agreement with the experimental fact that $Nd_2Fe_{14}B$ and $Nd_2Fe_{14}C$ stably exist. The main role of B in $Nd_2Fe_{14}B$ is not to increase the magnetic properties but stabilizes the structure of $Nd_2Fe_{14}B$ itself.

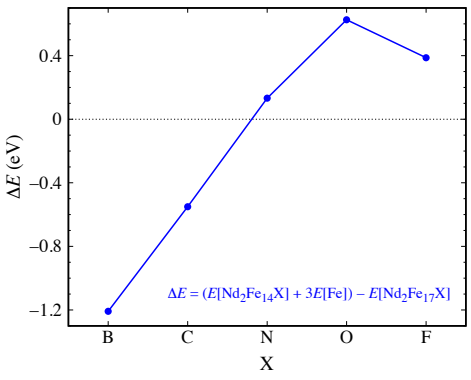

Figure 1. The formation energy of $Nd_2Fe_{14}X$.

References

[1] M. Sagawa *et al.*, J. Appl. Phys. **55**, 2083 (1984).

[2] Y. Tatetsu *et al.*, Phys. Rev. Mater. **2**, 0744100 (2018).

[3] http://www.openmx-square.org