Ab initio analysis on the stability of magnetic ternary alloys

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Adding a small amount of third elements in binary systems not only stabilizes system but also changes these physical properties. Recently, a new ternary alloy was discovered by introducing a third element of In into $L1_2$-$FePd_3$ by Teranishi's group in Kyoto University [1]. Other interesting example is Nd–Fe amorphous phases which can be crystalized after adding Ga in Nd–Fe–B sintered magnets. Although the physical aspects of these added elements are unclear and cannot be understood deeply only through experiments.

In this study, we conducted theoretical analyses for the stability of an In-doped novel Fe–Pd and Ga-dope Nd–Fe ternary alloys using OpenMX. The model structures for the calculations were based on the chemical composition ratio obtained from experiments.

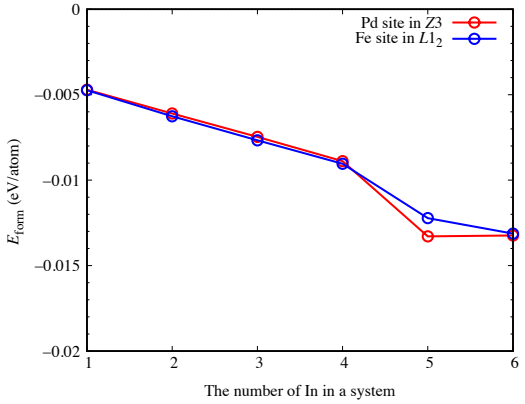

Figure: Formation energies for $L1_2$-(Fe, In)Pd_3 and $Z3$-Fe(Pd, In)$_3$.

For In-doped Fe–Pd ternary alloys, the In sites were chosen by replacing Fe or Pd sites with a special-quasirandom-structure method implemented in the Alloy Theoretic Automate Toolkit [3]. The figure illustrates the formation energies of $L1_2$-(Fe, In)Pd_3 and $Z3$-Fe(Pd, In)$_3$ when the number of In in a system takes from 1 to 6. By comparing these formation energies, $Z3$-Fe(Pd, In)$_3$ can be more stable than $L1_2$-(Fe, In)Pd_3 only in a narrow range of the In content. This tendency can be seen in the experimental results from XRD, EXAFS, and STEM-EDS analyses.

In Ga-doped Nd–Fe ternary alloys, we found that Ga is a key not only to stabilizing the fluorite-type crystal structure but also to suppressing its Curie temperature, which might be one of the reasons to explain why Ga-added Nd–Fe–B sintered magnets have high coercivity [4].

References

[1] K. Matsumoto, R. Sato, Y. Tatetsu, T. Teranishi, *et al.*, submitted.

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

[3] A. van de Walle *et al.*, Calphad Journal **42**, 13 (2013).

[4] Yuta Ainai *et al.*, Jpn. J. Appl. Phys., **59**, 06094 (2020)