First-principles study on the stability of magnetic alloys

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Transforming crystal structures of materials by adding pressure, heat, or other elements is one of the fundamental approaches to discover novel physical properties. Recently, a new *Z*3-type $Fe(Pd,In)_3$ crystal structure, was discovered by Teranishi's group in Kyoto University [1]. The new structure was obtained by introducing a third element of In into $L1_2$-$FePd_3$, which is the thermodynamically stable phase of binary Fe–Pd systems. Although the addition of In might be the key behind this new finding, the physical aspects of In in stabilizing the new structure is unclear and cannot be understood deeply only through experiments.

In this study, we performed theoretical analyses for the stability of an In-doped novel Fe–Pd phase to check the systems' formation energies using OpenMX. The model structures for the calculations were based on the chemical composition ratio of *Z*3-$FePd_3$ obtained from experiments. 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]. We investigated stable sites for In in the *Z*3-$FePd_3$ structure by comparing formation energies which is illustrated in the figure. We found that an In stably occupies the Pd site rather than the Fe site. There are two different Wyckoff positions of Pd labelled by 2e and 2g in *Z*3-$FePd_3$. From detailed analyses, we concluded that the new *Z*3-type $Fe(Pd,In)_3$ structure, in which a Pd atom at a 2e site is replaced with an In atom, is more stable than In-doped $L1_2$-$FePd_3$ structures. These results are consistent with the experimental results from XRD, EXAFS, and STEM-EDS analyses.

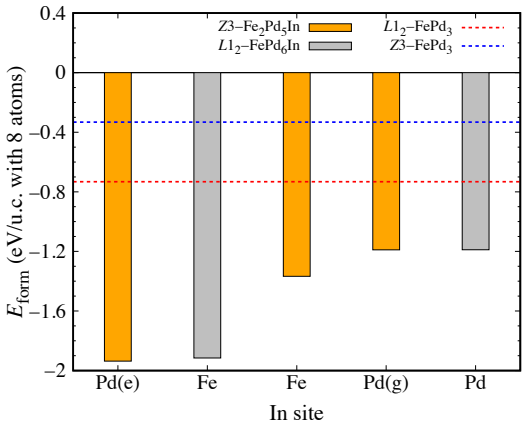

Figure : The comparison of the formation energies of In-doped *Z*3- and $L1_2$-type $FePd_3$.

References

[1] K. Matsumoto *et al.*, in preparation.

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

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