Site preference of ternary alloying addition (Ti, Fe, Co and Ni) in DO$_3$ Fe$_3$Al, Co$_3$Al and Ni$_3$Al - basic compound for alnico-8 magnetic materials

GERMAN SAMOLYUK, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, BALAZS UJFALUSSY, Research Institute for Solid State Physics and Optics of the Hungarian Academy of Sciences, Konkoly-Thege M. út 29-33., HU-1121 Budapest, Hungary, MALCOLM STOCKS, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA — We performed first-principles calculations to investigate the site preference of ternary alloying additions in DO$_3$ Fe$_3$Al, Co$_3$Al and Ni$_3$Al alloys. In Fe$_3$Al the discussed ternary elements are found to occupy the Fe sublattice. For both Fe-rich and Al-rich compounds, the ternary elements with fewer 3$d$ electrons than Fe (Ti) prefer to occupy $\alpha$-sites of Fe sublattice and elements with larger number of 3$d$ electrons - the $\gamma$-sites. In Fe-rich regions, the small enthalpy difference of Ti occupying $\alpha$-sites of Fe and Al sublattices, the site distribution of Ti varies with concentration and temperature. A similar dependency was obtained for Ni distribution between Co and Al sublattice in Co$_3$Al. Similar to the Fe$_3$Al alloy, the ternary element prefer to occupy Co sublattice with a change of preferred sites from $\alpha$ for Ti and Fe to $\gamma$ for Ni. In the Ni-rich Ni$_3$Al the ternary elements prefer to occupy the Al sublattice, while, in the Al-rich alloy the ternary elements prefer to occupy Ni sublattice in a similar fashion. The magnetic moments of transition metals in Fe$_3$Al and Co$_3$Al are ordered ferromagnetically, whereas the Ni$_3$Al is nonmagnetic unless the Fe or Co are added as a ternary element.

This work was supported by U.S. Department of Energy (DOE), Energy Efficiency and Renewable Energy.

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Date submitted: 15 Nov 2013

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