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Site preference of ternary alloying addition (Ti, Fe, Co and Ni) in DO_3 Fe_3Al, Co_3Al and Ni_3Al - basic compound for alnico-8 magnetic materials[1] GERMAN SAMOLYUK, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, BALAZS ÚJFALUSSY, 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_3Al, Co_3Al and Ni_3Al alloys. In Fe_3Al the discussed ternary elements are found to occupy the Fe sublattice. For both Fe-rich and Al-rich compounds, the ternary elements with fewer $3d$ electrons than Fe (Ti) prefer to occupy α-sites of Fe sublattice and elements with larger number of $3d$ electrons - the γ-sites. In Fe-rich regions, the small enthalpy difference of Ti occupying α-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_3Al. Similar to the Fe_3Al alloy, the ternary element prefer to occupy Co sublattice with a change of preferred sites from α for Ti and Fe to γ for Ni. In the Ni-rich Ni_3Al 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_3Al and Co_3Al are ordered ferromagnetically, whereas the Ni_3Al is nonmagnetic unless the Fe or Co are added as a ternary element.

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