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Ferro-to-antiferromagnetic transition in Gd(Fe,Ni)Si

Roman Mukhachev[1], Alexey Lukoyanov[1,2], Anatoly Kuchin[1], Sergey Platonov[1], Aleksey Volegov[1,2], Vasilii Gaviko[1,2] and Mari Yakovleva[1]

[1] M.N. Mikheev Institute of Metal Physics UrB RAS, Ekaterinburg, Russia
[2] Ural Federal University, Ekaterinburg, Russia

Ternary intermetallic RTX compounds are composed of R - a rare-earth metal and T, X - different d or p-elements [1]. This family of intermetallics has a wide range of possible applications, such as magnetocaloric cooling, gas liquefaction and others [2–4]. Experimentally and theoretically it was found that T-sublattice doping can significantly improve their magnetic and electronic properties [3], a composition-Induced magnetic transition was revealed in $GdMn_{1-x}Ti_xSi$ for x = 0−1 [4]. Therefore, further study of their properties may be useful for various environmentally sustainable applications.

In this work, the series $GdFe_{1-x}Ni_xSi$ compounds was synthesized and investigated for x = 0 - 0.4 due to the solubility limit [5]. The theoretical calculations were carried out for the tetragonal structure for x ranging between 0 and 0.5. The electronic structure, magnetic moments and types of magnetic orderings were investigated using the DFT + U method taking into account strong electron correlations in the 4f Gd shell [5]. In the self-consistent DFT + U calculations, the theoretical total magnetic moment of $GdFe_{1-x}Ni_xSi$ was found to be solely formed by the Gd ion, and Ni, Si are either non-magnetic or have small magnetic moments 0.02 μ_B at Si and 0.1 μ_B at Ni. In the calculations for x = 0–0.25, in GdFe1-xNixSi the ferromagnetic (FM) ordering of the Gd magnetic moments was found as the most stable. For $GdFe_{0.7}Ni_{0.3}Si$ and compositions with the larger content of Ni, the antiferromagnetic (AFM) ordering was found to be more preferable in total energy. Several types of AFM orderings were checked. The one with the Gd moments being aligned antiferromagnetically in ''W slabs'' and ferromagnetically in ''$BaAl_4$ blocks''. This type of AFM became more stable than the ferromagnetic one with the differences in total energy equal to 0.09 meV/f.u. (x = 0.3) and 0.29 meV/f.u. (x = 0.35). From experimental magnetic measurements, the behaviour of the magnetization curves and Curie temperature for $GdFe_{1-x}Ni_xSi$ differs from the one for V, Cr, Ti [4] with the Ni-doping and a decrease in interatomic distances. The magnetocaloric effect (MCE) of the $GdFe_{1-x}Ni_xSi$ systems changes with a change in composition from 3.8 (x = 0.1, T_C = 111 K) and 3.3 (x = 0.2, T_C = 104 K) J/kgK to 1.4 (x = 0.3, T_C = 106 K) J/kgK which can be attributed to the FM-AFM magnetic transition.

Thus, for the $GdFe_{1-x}Ni_xSi$ series, the transition from a ferromagnetic (low Ni content) to an antiferromagnetic ordering (x > 0.25) was identified using our first-principles calculations. The results are supported by the experimental magnetic data. The data obtained may indicate promising prospects of the GdTSi compounds studied in this work and the whole group of ternary intermetallic compounds with rare earth metals, which will motivate further research.

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