Magnetostriction in Fe1−x Gax M (M=Ni,Pr)

Talgat M. Inerbaev

L.N. Gumilyov Eurasian National University

inerbaev\_tm@enu.kz

**Absract:** The electronic structure of the FeGa alloy is investigated theoretically using methods of the density functional theory. The work aims to explain the difference in changes in the magnetostrictive properties of the material when using various types of doping elements. The effect of interest is explained by the dopant-caused variation of chemical bond character between the iron atoms of the first and second coordination spheres around the impurity atom. Strengthening the bonding nature electronic orbitals between these atoms leads to a decrease in the magnetostrictive effect, while its weakening leads to the opposite effect. In present work we performed computer simulations using the density functional theory of magnetostrictive properties of Ni and Pr of a modified FeGa alloy. It has been shown that the experimentally observed decrease (increase) in the λ001 coefficient upon the addition of Ni (Pr) dopants is due to an increase (decrease) in the anti-bonding nature of the chemical bond between the iron atoms in the first and second coordination spheres of the doping atom compared to the situation if, to enhance the magnetostrictive effect gallium was used. The hybridization makes the main contribution of the d-states of iron atoms. In the case of doping with Pr atoms, the effect of *f*-*d* hybridization is negligible due to the low density of states of the *f*-electrons below the Fermi level.

Keywords: magnetostriction, FeGa alloy, doping, computer modeling