Modeling of the magnetic and structural properties of Fe-Rh-Co and Fe-Rh-Pt by first principles method

Oksana Pavlukhina[1], Vasiliy Buchelnikov[1], Vladimir Sokolovskiy[1,2], Mikhail Zagrebin[1]

[1]Chelyabinsk State University, Chelyabinsk, Russia

[2]National University of Science and Technology "MIS&S", Moscow, Russia

Fe-Rh-based alloys is a promising material showing a metamagnetic first-order phase transition above room temperature that is of great interest for magnetic cooling and spintronics devices [1-3]. Technology of magnetic cooling is very promising technology. Fe-Rh alloys with almost equiatomic composition are ones of the best magnetocaloric materials showing a giant magnetocaloric effect close to room temperatures. For instance, the direct magnetocaloric effect measurements in $Fe_{51}Rh_{49}$ alloy [2] showed that the value of the adiabatic temperature change was found to be -13 K at the point 307 K with the magnetic field change from 0 to 2 T. This work is devoted to the investigation of structural and magnetic properties of $Fe_8Rh_{8-x}Co_x$ and $Fe_8Rh_{8-x}Pt_x$, (x = 0 − 3) alloys by first principles method.

In this study, the structural and magnetic properties of Co- and Pt-doped Fe-Rh alloys are investigated by using the density functional theory calculations as implemented in the Vienna Ab initio Simulation package (VASP). The generalized gradient approximation for the exchange correlation functional in the formulation of Perdew, Burke and Ernzerhof (PBE) was taken into calculations. The energy calculations were performed for $L2_1$ supercell ($Fe_8Rh_{8-x}Z_x$).

The ab initio calculations have been carried out by using the 16-atom supercell approach with different initial spin configurations. In the present work we calculated the total energies of the 16-atom supercells for $Fe_8Rh_{8-x}Z_x$ system calculated for different spin configurations as functions of the lattice parameter. For the parent Fe-Rh compound, the antiferromagnetic checkerboard-like spin configuration in a cubic cell is energetically favorable compared to other antiferromagnetic and ferromagnetic configurations. In this case, a total magnetic moment is found to be of 0 μ_B/f.*u.* To investigate the possibility of martensitic transformation in these alloys in dependence on the third element, we performed total energy calculations for tetragonal distortion of the cubic structure along *z* axis. The total energy differences between the tetragonal distorted and cubic phases for $Fe_8Rh_{8-x}(Co, Pt)_x$, (x = 0 − 3) compositions with the energetically favorable spin configuration as functions of *c*/*a* ratio was found. We note that the calculated optimized lattice parameter for Fe-Rh alloy is in a good agreement with experimental and other theoretical values [1, 3]. It is shown that a small variation of Pt or Co content leads to change the type of magnetic ordering.

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