Calculation of magnetic moments and lattice parameters Co-based Heusler alloys with determination of their energy favorable structure

M.V. Mamonova

Dostoevsky Omsk State University, Omsk, Russia

Cobalt-based full-Heusler compounds with composition Co_2YZ (where Y is a transition metal and Z is a main group element) are attracting attention due to their predicted half-metallic behaviour, a much desired property for spintronic devices[1-2]. Knowledge of the basic magnetic properties of these materials, especially in the form of thin films, is required both to exploit these promising materials and to understand the properties of magnetic multilayer structures based on them.

In this work we present results of structural and magnetic investigations of the Heusler compound by using VASP software package by means of the Projector Augmented Wave (PAW) method with generalized gradient approximation (GGA)[3]. From first principles the energy efficiency of the formation of various structures is investigated. The lattice parameters of Co_2FeAl(CFA), Co_2FeSi(CFS), $Co_2FeAl_{0.5}Si_{0.5}$(CFAS) Heusler alloys are calculated. The results of study magnetic properties of CFAS/Ag/CFAS multilayer structure are carried out.

Heusler compounds with the general formula Co_2YZ crystallize in the L21 and the B2 structures. At L21 structure the cubic unit cell consists of four interpenetrating fcc sublattices, two of which are occupied by Co atoms and the other two by the Y and Z atoms, respectively. At B2 structures in (0,0,0) and (1/2,1/2,1/2) sites are randomly occupied by Y and Z with an equal probability. The results of our calculations have shown that the bulk energy of CFA and CFS alloys in B2-type structure is greater than in the case of L21-type structure, this suggests that the L21-type structure is energetically more favorable. Also total magnetic moment in L21-type structure is greater than in the case of B2-type structure.

Investigation of the alloys lattice parameter dependence on the parameters of convergence made it possible to choose the optimal values of the plane waves cut-off energy Emax = 400 eV and Monkhorst Pack grid size 16x16x16. The optimized lattice constants for Co-based Heusler alloys a^{CFA} = 5.6965(9) Å, a^{CFS} = 5.6224(6)Å, a^{CFAS} = 5.5790(4) Å obtained by us are in good agreement with the experimental values.

In the case of CFAS/Ag/CFAS multilayer structure, the Ag lattice cell parameter is too small to accommodate a CFAS compound in the cube-on-cube epitaxial relationship. However, if the CFAS cube edge grows at an angle of 45° with respect to an in-plane Ag(001) direction, a good lattice match is obtained, enabling epitaxial growth. The supercell of CFAS/Ag/CFAS structure is consist of the 13 monatomic layers and vacuum layer with thickness 5Å. The layers of CFAS are placed on each side of the Ag five-layer slab. The magnetic moment of atoms is directed collinearly along the z axis.

Comparison of the values of the magnetic moment of CFAS atoms in the bulk and in the film adsorbed on Ag shows, that the Co atoms most distant from the substrate have greatest magnetic moment. For Fe atoms we obtained that magnetic moment for atoms in the bulk cell are slightly larger then magnetic moment for atoms located on substrate.

These results can be applied in numerical simulation by the Monte Carlo methods of the nonequilibrium behavior of multilayer magnetic superstructures[4].

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