Ab-initio calculations of magnetic moments and exchange integrals of $Co_{1-x}Ni_x$ alloy film on Cu(100) surface.

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One of the topical problems of modern physics is the investigation of the magnetic properties of multilayer structures in which the giant magnetoresistance effect is realized, because they prompt potential applications in data storage technologies [1]. Ni on Cu is a good epitaxial system since they both have the same fcc crystal structure with only 2.5% lattice mismatch. The growth of Co is more complicated than Ni since the equilibrium phase of bulk cobalt is hcp at room temperature. But $Co_{1-x}Ni_x$ alloy grows on Cu(100) in a well-ordered fcc structure via a layer-by-layer growth from 2 to 20 ML thickness [2].

In this work the results of a numerical first-principles calculations of the energy and magnetic characteristics for cobalt-nickel alloy on a copper surface by using VASP software package [3] by means of the Projector Augmented Wave (PAW) method are presented. The values of the total energy of various collinear spin configurations, the total magnetic moment and the magnetic moments of Ni and Co atoms are calculated. The exchange interaction integrals for the nearest and following nearest neighbors are calculated in the framework of the classical Heisenberg model.

We investigated a system consisting of a copper slab with the orientation of the surface face (100) and adsorbed on it from both sides by a ferromagnetic film of a cobalt-nickel alloy with the thickness of the films in three monoatomic layers. The multilayer structure was simulated using a periodic 2×2 36-atom supercell with the lattice constant corresponding to the copper substrate a = 3.6367 (5) Å, which we obtained as a result of calculations taking into account the optimization of the lattice parameters[4]. Ferromagnetic and six different anti-ferromagnetic configurations for "chess" and "interlaced" arrangement of Ni and Co atoms were considered. The results of our calculations demonstrates that the total energy of the multilayer structure in the ferromagnetic configuration increases with increasing Ni concentration in the alloy. The magnetic moments of atoms of both types take the greatest value in the ferromagnetic configuration in the atomic layer most distant from the substrate. The values of the exchange interaction integrals for the nearest J_1 and for the next nearest neighbors J_2 for pure metal films are positive and greater than the corresponding values in the bulk structure. From the calculation results of the exchange interaction integrals for the $Co_{0.5}Ni_{0.5}$ alloy film it follows that the constant J_1 contributes to the ferromagnetic ordering of the magnetic moments ($J_1 > 0$), and the exchange interaction constants depend strongly on the mutual arrangement of the atoms and on the choice of antiferromagnetic spin configurations.

These results can be applied in numerical simulation by the Monte Carlo methods of the nonequilibrium behavior of multilayer magnetic superstructures[5].

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