Enhancement of Fe Magnetic Moments in Fe/Co (001) Multilayers

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ABSTRACT

In order to investigate the electronic and magnetic properties of a bcc Fe/Co (001) multilayer, we have performed electronic structure calculations employing the total energy full-potential linear muffin tin orbital method. The magnetic moments of the layers are calculated. Based on these results, the magnetization profiles and the microscopic origin of the enhancement of Fe moments in the multilayers of the same Co content but with different interface qualities are reported. Large enhancement of magnetic moment is observed in the Fe monolayer located at the interface, and an even greater increase is obtained for the multilayer with one monolayer of intermixing between Fe and Co layers. The Co atoms were found to have similar magnetic moments in the bulk and at the interface.

INTRODUCTION

Thin films are well known to exhibit features that are not observed in bulk materials. A lot of work has been devoted to the study of bcc Co thin films and Fe/Co multilayers primarily for their great importance in investigating magnetism of surfaces and interfaces in unique structures. In this present work, the effects of interface quality to the magnetic moment of the constituent atoms in the multilayer are investigated. We have chosen to study magnetism in a multilayer consisting of Fe and Co, both of which are independently highly ferromagnetic, and their positions in the bcc lattice. An advantage of the Fe/Co system is that it makes it possible to investigate Co atoms in the bcc phase.

NUMERICAL METHOD

The computational method used is the full-potential linear muffin tin orbital (FP-LMTO) method based on the density-functional theory. This provides the basis set in which the wave functions are expanded by dividing the three-dimensional space into nonoverlapping muffin-tin (MT) spheres region and interstitial region. In each MT assigned to each atomic site, the density and potential are expanded using spherical harmonics, while outside the basis are expanded by means of Fourier series. The main input parameters are only the type of atoms and the structure of the system of atoms, which are information that have long been established or may be patterned from experimental results. The advantage of this method is that no approximation is made on the shape of the density or potential.

STRUCTURAL PARAMETERS

The supercell or the smallest volume of the infinitely periodic multilayer system is composed of eight atoms

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which are stacked along the (001) axis. The atoms form four conventional bcc unit cells with eight layers. The unit cell is perfectly cubic so the in-plane and out-of-plane lattice constants are equal at the numerically verified value of 5.20 Bohr. To simulate the experimentally observed imperfect interfaces in fabricated Fe/Co multilayers, the atoms in the supercell containing 25% Co concentration are rearranged such that Co atoms are intermixed within the Fe layers.

SUMMARY OF RESULTS

We have successfully verified theoretically the enhancement of the magnetic moment of Fe in Fe/Co (001) multilayer in the ground state without any restrictive assumptions. For multilayers with the same content concentration, the location of atoms in the multilayers affects the magnetic moment. Fe atoms that are sandwiched between two Co atoms show an even larger increase in magnetic moment than when placed adjacent to another Fe layer and Co. For the Fe monolayer, we have shown that this is due to the presence of a different kind of atom as its nearest neighbor. No significant change in Co moment is observed even when the number of neighboring Fe and Co atoms changes. These information are useful for multilayer devices where a large magnetic moment response is needed.