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Magnetic structure calculations of $Ir_{0.5}Mn_{0.5}$ over- and sub-layer at Co(001) surface

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ABSTRACT

Density functional theory calculations are performed to investigate the magnetic structure of $Ir_{0.5}Mn_{0.5}$ chemically alloyed over- and sub-layer at Co(001) surface. $Ir_{0.5}Mn_{0.5}$ exhibits ferrimagnetic ordering as the ground state for both systems. Alloyed $Ir_{0.5}Mn_{0.5}$ chemically ordered monolayer is found to be more stable at the surface rather than the sub-surface of Co(001). The magnetic moments of Mn surface atoms, Mn_I and Mn_{II}, in $Ir_{0.5}Mn_{0.5}$/Co(001) over-layer system are found to be 3.49 μ_B and −3.56 μ_B, respectively with intra-layer antiferromagnetic (AFM) coupling. While the Mn_I couples ferromagnetically with Co subsurface moment (1.68 μ_B), Mn_{II} couples antiferromagnetically. $Ir_{0.5}Mn_{0.5}$/Co(001) system exhibits a magnetocrystalline anisotropy energy (MAE) of −2.8 meV/cell (−0.7 meV/Mn atom), in the direction along [001]. The ferrimagnetic surface ordering and the high MAE of $Ir_{0.5}Mn_{0.5}$/Co(001) are believed to be promising for potential applications in perpendicular recording media.

1. Introduction

The exchange bias is a phenomenon that appears at the interface between antiferromagnet (AFM) and ferromagnetic (FM) layers. When these layers are cooled in a magnetic field below Néel temperature (T_N) of the AFM layer, where the Curie temperature (T_c) of the FM layer is larger than T_N [1], a magnetic anisotropy occurs at the AFM/FM interface causing a shift in the magnetic hysteresis loop [2,3]. This interface anisotropy contributes to phenomena such as interlayer exchange coupling, spin-tunneling, and giant magneto-resistance that have found their technological applications in devices such as spin-valve read heads [4] or magnetic random access memory (MRAM) [5].

It has been found that FeMn [6], IrMn [7], NiMn [8,9], MnPt [10], MnPd [11] alloys that possess $L1_0$ geometrical structure have antiferromagnetic ordering with high Nèel temperatures. Therefore, they attracted much of the scientific interest due to their promising applications such as exchange-biasing layers. However, low-dimensional overlayers of these alloys adsorbed on substrates such as Cu(001) are found to exhibit c(2 × 2) chemically ordered structures [12–20]. Therefore, these low-dimensional systems exhibit different magnetic orderings than their bulk.

The AFM alloy that exhibits the highest Nèel temperature among Mn-based alloyed systems is IrMn [21], which is considered to be promising for potential applications in recording media. Its interesting properties such as corrosion resistance, high blocking temperature (T_B=250 °C), and small critical thickness have stimulated much interest for experimental investigations [22,23,7]. The effect of decreasing the thickness of IrMn films to the Angström-scale on the exchange bias in spin valves has been investigated by Perdue et al. [24]. They found that the minimum required thickness of the antiferromagnet that retains the exchange bias is 4 Å. Using soft X-ray resonant magnetic scattering measurements, Hase et al. [25] have found a small magnetic moment on the antiferromagnetic IrMn pinning layer in a NiFe/Cu/Co/IrMn spin valve structure that lies antiparallel to the Co moment.

IrMn has also the highest magnetocrystalline anisotropy energy (MAE) as compared to MnNi, MnPd, MnRh, and MnPt [26]. This fact makes it promising for potential applications in spintronics devices since MAE is believed to be responsible for the exchange bias that shifts the hysteresis loop along the axis of an external field due to the interface coupling of FM and AFM layers. The exchange bias phenomenon has been reported for films of perpendicular easy axis [27–34]. IrMn has proven to be a good candidate to obtain exchange-bias in conjunction with perpendicular magnetic anisotropy, which has been evidenced in Co/Pt multilayers covered with IrMn thin films [7].

In spite of the abundance in the experimental studies for such a thin-film alloy, the theoretical investigations are still scarce. The aim of this paper is to provide a microscopic insight into the electronic and

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magnetic structures of IrMn alloyed over- and sub-layers at Co(001) substrate.

This paper is organized as follows: Section 2 contains the method of calculation, Section 3 includes the results and discussion, and Section 4 is devoted to the summary and conclusions.

2. Method of calculation

The calculations are performed using density functional theory (DFT) [35] based on the full-potential linearized-augmented plane-wave (FP-LAPW) [36,37]. The exchange-correlation functional is described using generalized-gradient-approximation (GGA) [38]. For the structural, electronic and magnetic properties calculations, the core states are treated fully relativistically, while the semi-core and valence states are treated by the scalar relativistic approximation (the spin–orbit interaction is ignored for the semi-core and valence electrons). However, the spin–orbit coupling is included in the calculations of MAE. I assumed a hypothetical face centered cubic (fcc) phase for bulk Co. The lattice constant of Co was optimized within a basis set of 16 Ry cutoff energy for the plane waves in the interstitial region between the muffin tins and 169 Ry for the potential. The wavefunction expansion inside the muffin tins were taken up to $lmax=10$ and the potential expansion up to $lmax=4$. The core energy cutoff was taken as -6.0 Ry. The k-point sampling in the irreducible part of the Brillouin zone is performed using a $(12\times12\times12)$ Monkhorst-Pack grid. Using this basis set, the bulk lattice constant of Co is obtained by structural optimization followed by fitting the obtained total energies with Murnaghan equation of state [39]. The convergence of the total energy in the self-consistent calculations was taken with respect to the total charge of the system with a tolerance of 0.0001 electron charges. The structure of Co(001) substrate was modeled using a supercell of seven atomic layers and a (2×2) unit cell. The $Ir_{0.5}Mn_{0.5}$ chemically ordered alloyed over- and sub-layer are placed at both sides of Co(001) surface. The vacuum is chosen to be equivalent to 10 interlayer spacings (about 34 Bohr), which is sufficient to prevent the overlap between atomic slabs. The basis set used in the calculations is as follows: 16 Ry cutoff energy, $(6\times6\times1)$ Monkhorst-Pack grid that corresponds to 18 k-points in the irreducible Brillouin zone (IBZ). The muffin tin radii are taken as 2.0 Bohr for Mn and Co atoms, whereas 2.4 Bohr is used for Ir to prevent spheres' overlap. The system is fully relaxed to allow the atoms to take the optimum positions with a convergence tolerance of 5 mRy/Bohr. The spin orbit coupling is included for the calculations of the magnetocrystalline anisotropy energy (MAE) for the Mn and Co magnetic moments using a denser mesh of 726 k-points in IBZ. The MAE is calculated using the following equation:

$$MAE = E^{001} - E^{100} \quad (1)$$

where E^{001} and E^{100} stand for the perpendicular and in-plane directions of the magnetic moments, respectively.

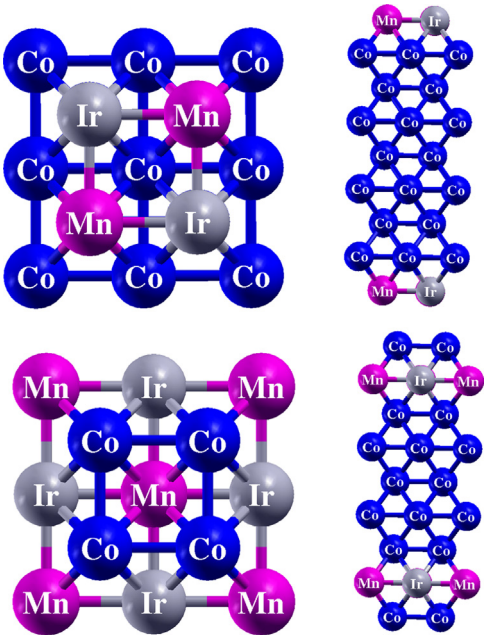

Fig. 1. The c(2×2) chemically ordered structures. The top view (upper left) and the side view (upper right) of $Mn_{0.5}Ir_{0.5}$/Co(001) surface. The top view (lower left) and the side view (lower right) of Co/$Mn_{0.5}Ir_{0.5}$/Co(001) surface.

3. Results and discussion

The hypothetical fcc phase of bulk Co is found to have a lattice constant 6.65 Bohr and a local magnetic moment of 1.68 μ_B in close agreement with previous LMTO calculations within GGA approximation that obtained 6.64 Bohr and 1.64 μ_B for lattice constant and local magnetic moment, respectively [41]. The $Ir_{0.5}Mn_{0.5}$ chemically (2×2) ordered alloyed monolayer is once placed on Co(001) surface and another buried below the surface layer (sub-surface), see Fig. 1. For each system we performed calculations for the FM and AFM in-plane spin orderings. The AFM ordering is found to be the stable solution for each system. The AFM solution is more stable than the FM by 120 meV/Mn atom for $Ir_{0.5}Mn_{0.5}$/Co(001) system and 38 meV/Mn atom for Co/$Ir_{0.5}Mn_{0.5}$/Co(001). This AFM behavior is the same as that obtained for Mn/Co(001) and Co/Mn/Co(001) systems [40,41]. The ordering of Co magnetic moments is FM for all cases, where no AFM solution could be stabilized for Co moments. Even though this FM coupling of Co moments could not affect the AFM coupling of Mn magnetic moments.

By comparing the AFM ground state solutions in both systems, $Ir_{0.5}Mn_{0.5}$/Co(001) is found to be more stable than Co/$Ir_{0.5}Mn_{0.5}$/Co(001) system by 437 meV/Mn atom. This indicates the surface preference of $Ir_{0.5}Mn_{0.5}$ rather than sub-surface. This is opposite to the case of buried Mn monolayer in Co/Mn/Co(001) system, which

Table 1
Spin magnetic moments of the stable structures of $Ir_{0.5}Mn_{0.5}$/Co(001) and Co/$Mn_{0.5}Ir_{0.5}$/Co(001) systems, Mn_I and Mn_{II} denote the two kinds of Mn atoms.

Structure	S element	μ_s (μ_B)	S−1 element	μ_s (μ_B)	S−2 element	μ_s (μ_B)
$Mn_{0.5}Ir_{0.5}$/Co(001)	Mn_I	3.49	Co	1.68	Co	1.71
	Mn_{II}	−3.56				
	Ir	0.25				
Co/$Mn_{0.5}Ir_{0.5}$/Co(001)	Co_I	1.82	Mn_I	2.61	Co	1.53
			Mn_{II}	−2.84		
			Ir	0.26		