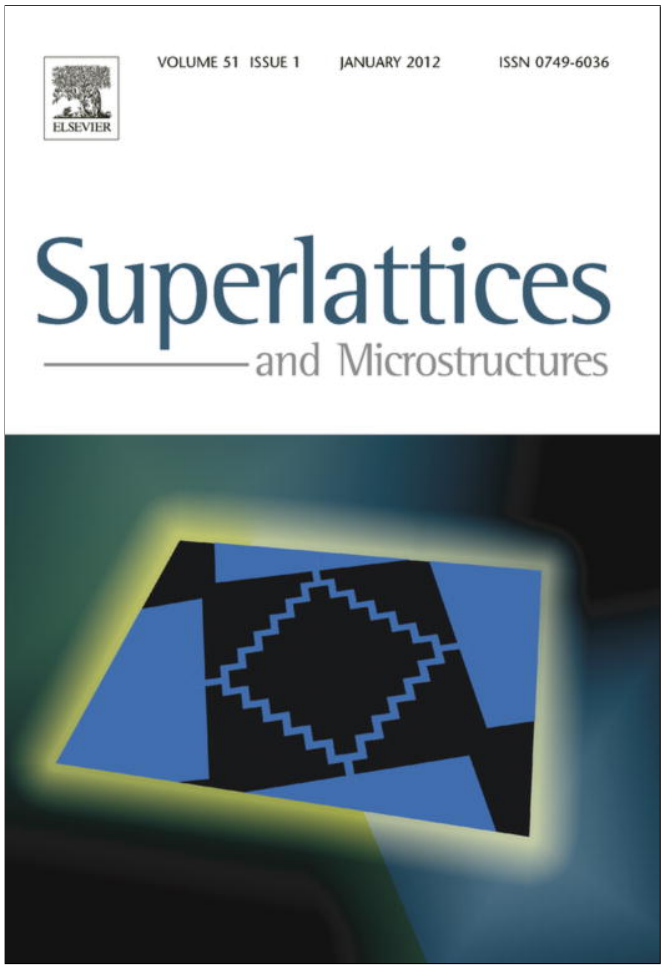

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First principles studies of Fe/Co superlattices and multilayers with bcc (001) and (110) orientations

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ABSTRACT

The layer resolved magnetic moments and magnetic anisotropy energy of Fe/Co superlattices and multilayers with bcc (0 0 1) and (1 1 0) orientations obtained from first principles simulations are reported here. The magnetic moment of Fe atoms are found to depend on the geometry, coordination number and proximity to Co atoms, whereas that of Co remains almost constant in the superlattices and multilayers. Mixing of atoms at the interface resulted in enhanced Fe magnetic moment while that of Co is unaffected. The magnetic anisotropy energy in superlattices and multilayers are found to be larger than the corresponding values of bulk counterparts. Calculated easy axis of magnetization is in the plane for all superlattice compositions considered in the study, while that in multilayers, changes with crystalline orientation and thickness of Co layers.

1. Introduction

Magnetic superlattices and multilayers are attracting considerable interest in recent years due to their interesting properties and applications in magnetic data storage. Magnetic storage media requires materials with enhanced magnetic moments and large magnetic anisotropy energy that can sustain magnetism over a long period of time [1]. The ferromagnetic Fe/Co alloy has been widely studied due to its unusual magnetic properties like high saturation magnetization at ambient conditions [2]. The spin moment of Fe, in these alloys increases from the bulk value of 2.2 μ_B to a maximum of about 3 μ_B for 50% Co concentration [3]. Apart from the bulk alloy, superlattices and multilayers of Fe/Co are also promising candidates in the search of materials with desirable magnetic properties

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[4–6]. Even though bulk Fe–Co alloy is of interest due to its high saturation magnetization at ambient conditions, its magnetic anisotropy energy is small due to the cubic symmetry. But it is possible to achieve high magnetic anisotropy energy by designing artificial structures like superlattices and multilayers where the cubic symmetry is broken [7]. Another interesting finding is that, the transition metal Co, which has hcp as the ground state structure can be stabilized as bcc in thin films and superlattices of Fe/Co having bcc (0 0 1) orientation [8,9]. Experimental studies on Fe/Co multilayers and superlattices are carried out by different techniques. Magnetization measurements on Fe/Co(0 0 1) superlattices using SQUID magnetometry and polarized neutron reflectivity showed enhanced Fe as well as Co magnetic moments compared to the bulk values [4], whereas, another study on similar samples with SQUID and X-ray magnetic circular dichroism (XMCD) measurements have not reproduced the increased moments [10]. Studies on Fe/Co multilayers have shown that at low concentration of Co, the average moments are lower than that of the bulk alloy, and at higher concentration, an opposite situation is found [11]. The experimental results on the magnetic moments of Fe and Co in multilayers and superlattices reported by different groups are not consistent [4,10,11]. This calls for a thorough theoretical investigation on the effects of parameters such as crystallographic orientation, mixing of atoms at the interface, and the thickness of the layers on the magnetic properties. In this work, we present a first principles study on the magnetic properties of both Fe/Co superlattices and multilayers.

A few theoretical studies on Fe/Co superlattices and multilayers also exist in the literature [12,13]. A magnetization profile at the Fe/Co interface in Fe/Co multilayers calculated using first principles linear muffin tin orbital (LMTO) method showed magnetic moment of 2.6 μ_B/atom for Fe and 1.75 μ_B/atom for Co [12]. First principles study by Bergman et al. [14] showed that magnetic moment of Fe/Co (0 0 1) superlattices show agreement with bulk Fe–Co alloys. They have seen that the magnetization in these superlattices prefer an in-plane easy axis, and the magnitude of magnetic anisotropy energy (MAE) obtained is about 50 μeV/atom. Another study also showed in-plane MAE of the order of about 50 μeV/atom in (1 1 0) oriented Fe_n/Co_n superlattices [15]. The experimental and theoretical studies conducted so far, using various methods do not address the change in properties that can arise out of the change in crystalline orientation and here we present a comparative study of both Fe/Co superlattices and multilayers oriented along bcc (0 0 1) and (1 1 0) orientations. We calculate the spin magnetic moments of superlattices and multilayers for different thicknesses of the Co layers, taking into account the full relaxation of the structure. By including spin–orbit coupling the orbital moments and MAE were also calculated, for some of the superlattice and multilayer configurations. Further, our calculations were extended to find out the effect of mixing of atoms at the interface on the magnetic moments. The changes in electronic structure caused by the mixing of atoms were analyzed through the calculation of the density of states.

2. Details of the calculation

In the present calculations, we have considered Fe_m/Co_n superlattices and multilayers, in the bcc (0 0 1) and (1 1 0) directions, as experiments report these two orientations for these systems [4,8,11]. The first principles density functional theory (DFT) calculations were done using the VASP code [16–18]. The Fe_m/Co_n superlattices (where $m + n = 4,8$) with bcc (0 0 1) and (1 1 0) orientations were constructed by supercell approach with the assumption of periodic boundary conditions (PBC) along the *X*, *Y* and *Z* directions with 4 atoms per layer of the unit cell. Schematic pictures of Fe_4/Co_4 superlattice in the bcc (0 0 1) and (1 1 0) orientations are shown respectively in (a) and (b) of Fig. 1. In multilayers too, the same geometry was taken along with the incorporation of a vacuum region of 15 Å along the *Z*-direction, following the atomic layers. This consideration ensures negligible interaction between the images arising from the periodic boundary condition along the *Z* direction. Structural optimization for both the superlattices and multilayers were carried out using the conjugate gradient method and optimization runs were stopped when the Hellmann–Feynman forces become less than 10 meV/Å. A tolerance of 10^{-7} eV in the energy was used for the self consistent iterations of the electronic structure calculations. The conduction electron–ion interactions were described by the projector augmented wave (PAW) method and PW 91 functional was used to describe the

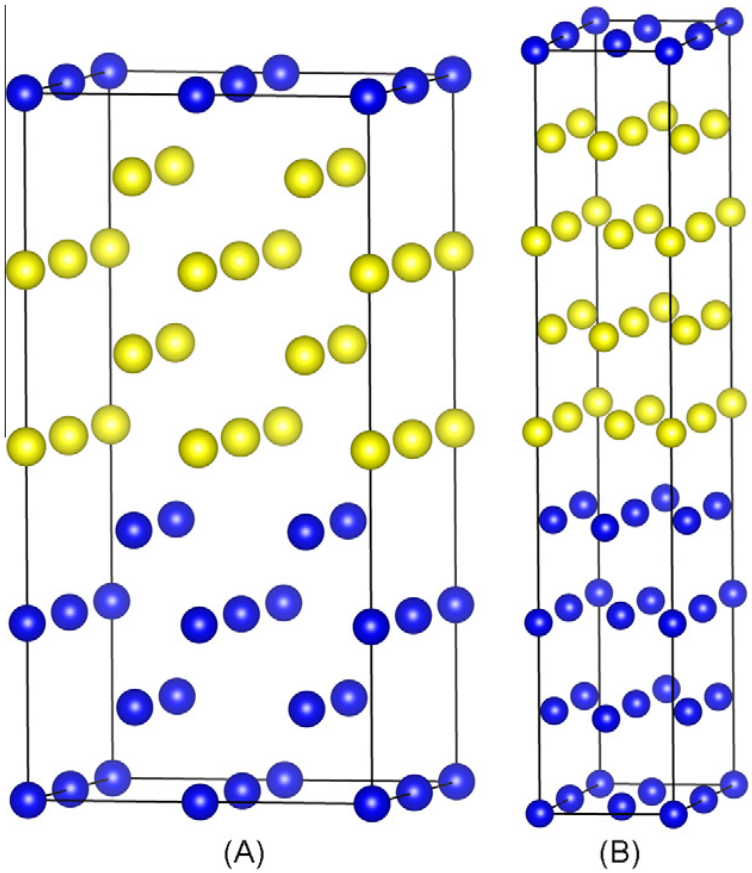

Fig. 1. (a) and (b) Represents Fe_4/Co_4 superlattices with bcc (001) and (110) orientation, respectively. The blue and yellow spheres represent Fe and Co atoms respectively. Each layer of the unit cell consists of 4 atoms in both (001) and (110) superlattices. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

exchange and correlation within the generalized gradient approximation [19]. The PAW approach produces the exact all electron potentials and charge densities without elaborate non-linear core corrections, hence it is particularly useful for magnetic elements [20]. Convergence tests were done to fix the k-grid for the Brillouin zone integration. In the case of Fe_m/Co_n superlattices, with $(m + n) = 4$ and 8, respectively $8 \times 8 \times 8$ and $8 \times 8 \times 4$ Monkhorst Pack k-grids [21] were chosen after convergence tests such that the stopping criterion for self consistent cycle is 10^{-7} eV and such highly accurate calculations were found to be essential to get reliable results for the MAE. In the case of Fe_m/Co_n multilayers, with $(m + n) = 4$ and 8, the k-grids used were $8 \times 8 \times 4$ and $8 \times 8 \times 2$, respectively, and chosen using the same criterion as that of superlattices. Convergence tests are done to fix the plane wave cut off and 450 eV was found to be adequate to describe the plane waves included in the basis set. The tetrahedron method with Blochl corrections was used for the density of states calculations [22]. Spin polarization was described using the spin interpolation proposed by Vosko et al. [23]. Spin orbit coupling was introduced to find out the magnetic anisotropy energy (MAE) and the spin–orbit coupling scheme used was that of Kresse and Lebacq as implemented in VASP [24]. In VASP, the Hamiltonian is represented as a 2×2 matrix in spin space. The non-diagonal elements arise from the spin–orbit coupling as well as from the exchange correlation potential when the system under consideration possesses a non-collinear magnetization density. Calculations including spin orbit coupling have, therefore, to be performed with the non-collinear method, and this was incorporated in VASP by using the prescription of Hobbs et al. [25] and Marsman and Hafner [26]. The MAE in superlattices and multilayers were obtained from the difference in total energies corresponding to magnetic moments lying in the plane and normal to it. The calculations for the MAE were performed in two steps. A collinear scalar relativistic calculation was carried out initially and the ground state resulted out of this calculation was used

to initialize the non-collinear calculation including spin orbit coupling. Orbital magnetic moments were calculated directly from the wave functions as the expectation value of the components of the angular momentum operator.

3. Results and discussion

3.1. Spin magnetic moments of superlattices and multilayers

The spin magnetic moment of Fe_2/Co_6, Fe_3/Co_5, Fe_4/Co_4, Fe_5/Co_3 and Fe_6/Co_2 superlattices and multilayers with bcc (001) and (110) orientations were obtained from spin polarized electronic structure calculations. The calculations were performed by considering ideal interfaces between Fe and Co layers without any mixing of atoms at the interface and the structures were fully optimized. The values of the layer resolved spin magnetic moments obtained from our calculations for the superlattices are shown in Fig. 2.

It can be seen from Fig. 2 that the magnetic moment of Fe atoms at the interface of both (001) and (110) superlattices are enhanced, compared to that in the middle Fe layers. It can also be noted from the panel (a) in the Fig. 3 that for the Fe_6/Co_2 superlattice, the Fe magnetic moment in the middle layers are close to the bulk value (2.2 μ_B/atom). Hence for low Co thicknesses, the magnetic moment of Fe atoms are almost bulk like. The Fe atoms in proximity to Co atoms show enhanced magnetic moments as large as 2.6 μ_B/atom in bcc (001) and 2.5 μ_B/atom in bcc (110) superlattices. The slight enhancement of magnetic moment of Fe atoms in bcc (001) superlattices compared to bcc (110) can be attributed to the changes in chemical environment arising from the geometry of the superlattice. This is similar to the observation of James et al. [28], in their calculations on $Fe_{50}Co_{50}$ alloy where the Fe

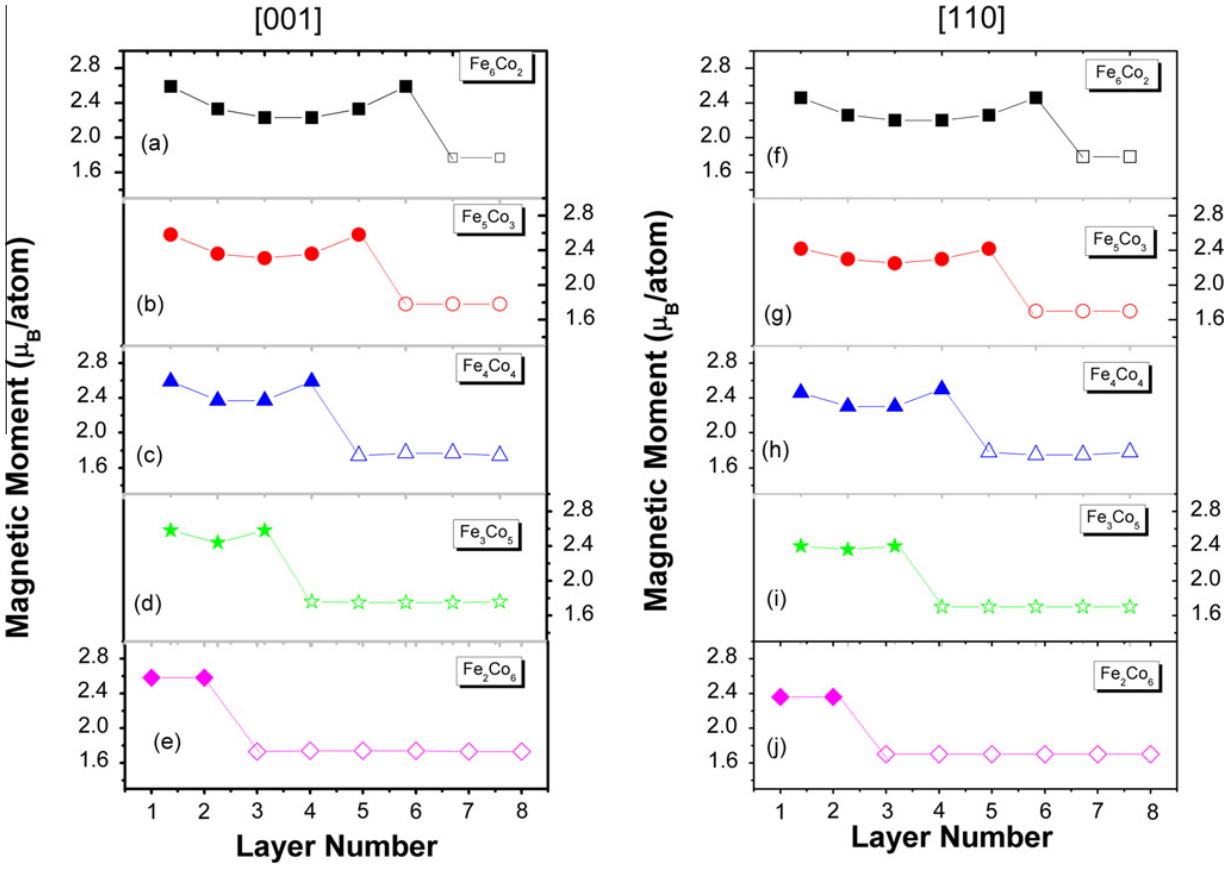

Fig. 2. The layer resolved spin magnetic moments of Fe and Co atoms in the Fe_2/Co_6, Fe_3/Co_5, Fe_4/Co_4, Fe_5/Co_3 and Fe_6/Co_2 superlattices with bcc (001) and (110) orientation. The filled and open symbols represent Fe and Co atoms, respectively. The location of the jumps from filled to open symbols represent the Fe–Co interface.

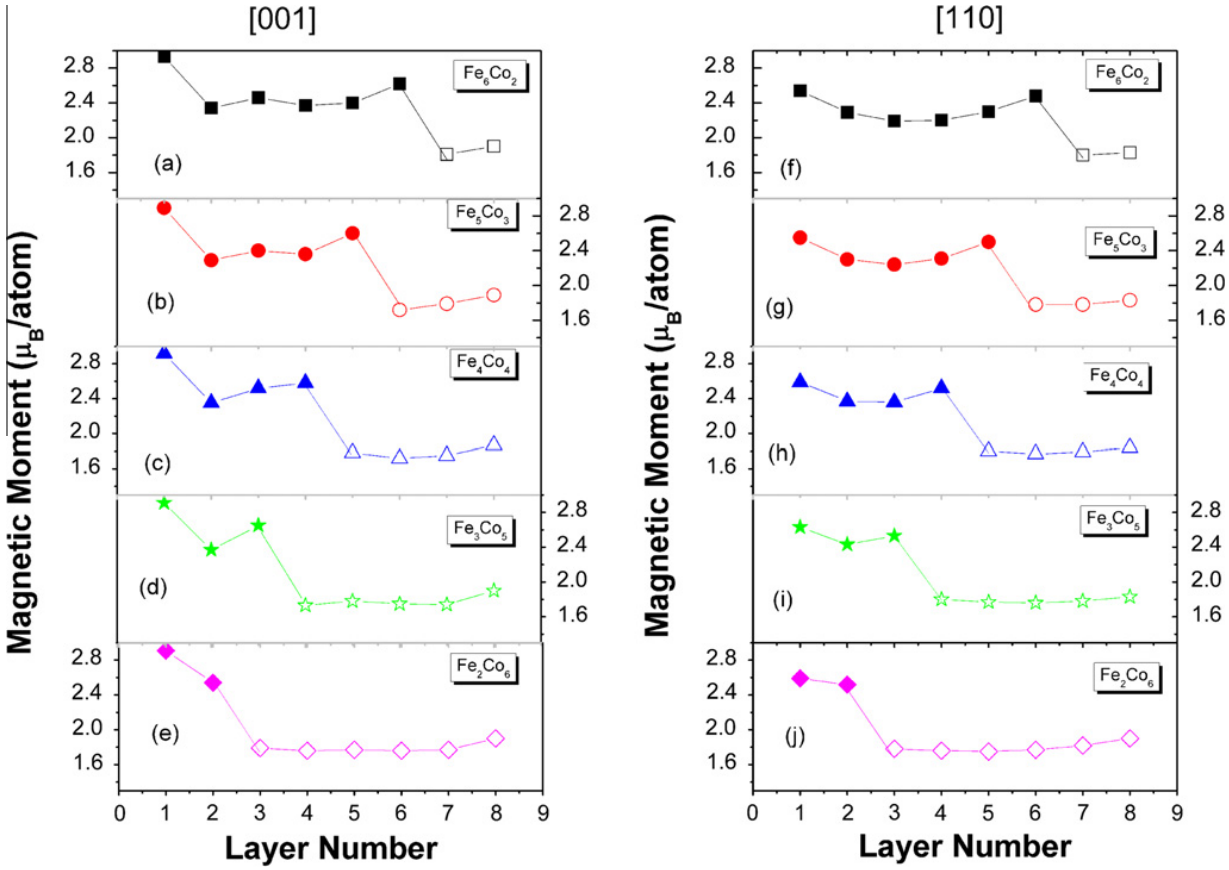

Fig. 3. The layer resolved spin magnetic moments of Fe and Co atoms in the Fe_2/Co_6, Fe_3/Co_5, Fe_4/Co_4, Fe_5/Co_3 and Fe_6/Co_2 multilayers with bcc (001) and (110) orientation. The filled and open symbols represent Fe and Co atoms, respectively. The location of the jumps from filled to open symbols represent the Fe–Co interface.

moment is seen to increase with the increase of Co atoms in the first shell. Since the Fe atoms at the interface have Co as the nearest neighbor on one side, the significant enhancement of the magnetic moment of Fe atoms at the interface is evidently due to the presence of Co atoms. The presence of Co at the interface will cause narrowing of Fe-d bands and it is found to enhance the spin moment [13]. It can also be seen from panels (d), (e), (i) and (j) of the Fig. 2 that the reduction in the thickness of the Fe layers enhances the Fe magnetic moment at the middle layers and it is again due to the increase of Co atoms in the environment of Fe atoms.

The magnetic moment of Co atoms in both the bcc (001) and (110) superlattices, on the other hand, does not show significant enhancement and it remains constant around 1.8 μ_B/atom in all the layers, reflecting the fact that the spin up band of Co is almost completely filled [13]. The maximum enhancement of Fe moments at the interface and almost constant Co moments in all layers in these superlattices are in agreement with other studies [10,14]. Bjork et al. [10] have reported enhanced magnetic moments of up to 3 μ_B/atom for the Fe atoms at the interface of Fe/Co superlattices and almost constant magnetic moment of 1.6 μ_B/atom for the Co atoms using the XMCD results. Our results are in agreement with these experimental results even though the magnitude of the magnetic moment of Fe atoms obtained from our calculations is smaller compared to the experimental value. Enhanced Fe moment of about 2.6 μ_B/atom and constant Co moment of 1.8 μ_B/atom were also obtained in Fe/Co (001) superlattices using RS-LMTO-ASA method with out considering any relaxation of atoms [14]. Experimental results on Fe–Co bulk alloys also showed enhanced magnetic moments for Fe atoms for 50% Co concentration while the magnetic moments of Co atoms are found to be almost constant [3].

Turning our attention to the magnetic moments of Fe/Co multilayers, as shown in Fig. 3, we have seen that for the (001) multilayer, the magnetic moment of Fe atoms at the surface layers are around 2.9 μ_B/atom. This enhancement can be explained as a consequence of the reduced coordination of the

surface layer that leads to narrowing of the d-bands and enhanced exchange splitting. But it is observed that the Fe magnetic moments at the surface layers of (1 1 0) multilayers are only slightly enhanced compared to that of (0 0 1) multilayers. The differences between the magnetic moment of Fe atoms at the surface layers of (0 0 1) and (1 1 0) multilayers is primarily due to the differences in the geometry corresponding to these two orientations. It is evident that surfaces with less packing will have more magnetic moment compared to surfaces with more packing. The magnetic moment of Fe atoms at the interface of both bcc (0 0 1) and (1 1 0) multilayers are around 2.6 μ_B/atom, and the middle layers posses reduced moments. It can be noted from the figure that the Co atoms in the surface layers of (0 0 1) multilayers show a slightly increased magnetic moment, compared to that of the other layers which may be attributed to the reduction in the coordination number of the surface layer. The magnetic moments of Fe and Co atoms obtained from our calculations agree with other calculations on Fe/Co multilayers [12,13]. The results obtained by Niklasson et al. [12] using the first principles Greens function techniques without considering the relaxation of atoms in Fe/Co multilayers showed an enhanced magnetic moment of about 2.5 μ_B/atom for Fe atoms at the Fe/Co interface and constant Co moment of 1.7 μ_B/atom in all layers. Calculations on Fe/Co multilayers using RS-LMTO-ASA method also showed the trend of a constant Co moment and increased Fe moments with increase in Co concentration [13]. As the enhancement of the magnetic moment of Fe atoms in these multilayers are due to the reduction in the coordination number and presence of Co atoms in the environment of Fe atoms, these two factors must be taken into account to obtain a qualitative understanding of the enhancement in the magnetic moment of Fe atoms in Fe/Co multilayers.

3.2. Effect of interface mixing on the magnetic moments

The influence of interface mixing on the magnetic properties and density of states are also investigated. In order to perform the calculations, Fe_2/Co_2 superlattices and multilayers were considered. Calculations were performed for the superlattices and multilayers with ideal interface (no mixing of atoms at the interface) as well as with 25% and 50% mixing of atoms at the interface. Mixing of atoms is carried out between the inter-facial layers designated as 2 and 3 in Fig. 4. They represent the Fe and Co layers at the interface of superlattice/multilayer. After mixing, for the Fe atom in the interface layer will have Co atom as the nearest neighbor, where as in the other layers, Fe atoms have Fe and Co atoms have Co as the nearest neighbor. Hence the symmetry of the supercell changes and hence the two Fe (Co) layers become in-equivalent. Thus the magnetic moments of these two layers will be different. To carry out the interface mixing calculations, we have considered only ordered structures and the mixing is restricted to the interface layers. However, we have exhausted all in-equivalent configurations arising out of mixing. These structures are then optimized to find out the configuration with lowest total energy. This is carried out for all superlattice/multilayer configurations and the magnetic moments of lowest energy configurations are reported here. The layer resolved magnetic moment of Fe_2/Co_2 superlattices and multilayers obtained from our calculations are shown respectively in the left and right panels of Fig. 4. It can be seen from the figure that the magnetic moment of Fe atoms even in the superlattice with ideal interface is larger compared to the bulk value and the presence of Co layer is the cause of this enhancement. Further enhancement in the magnetic moment of Fe atoms is observed when there is mixing of atoms (Fe atom moving to layer 3 and Co atoms moving to layer 2) at the interface. It is seen from the figures that the consequence of mixing is different in the (0 0 1) and (1 1 0) superlattices. The enhancement in the magnetic moment of Fe atoms in the third layer of the (1 1 0) superlattice is significant, whereas that of the (0 0 1) superlattice is marginal. The Fe magnetic moment in the second layer of the (1 1 0) superlattice also shows marginal enhancement whereas that of (0 0 1) shows a decrement. This difference in behavior of the magnetic moment can be understood from the changes in the geometry introduced by the mixing of atoms at the interface. It is straight forward to see that the Fe atom moving to layer 3 from layer 2 in (1 1 0) superlattice acquires increased Co coordination and it is the reason for the significant enhancement of the magnetic moment of this Fe atom. The magnetic moment of Co atoms, on the other hand, does not show significant variation when there is mixing of atoms at the interface. It is already known that the spin-up band of Co atoms in Fe/Co alloys is almost filled [27] and the magnetic moments are not affected by presence of Fe atoms. The observed behavior of the magnetic moment in the present study also

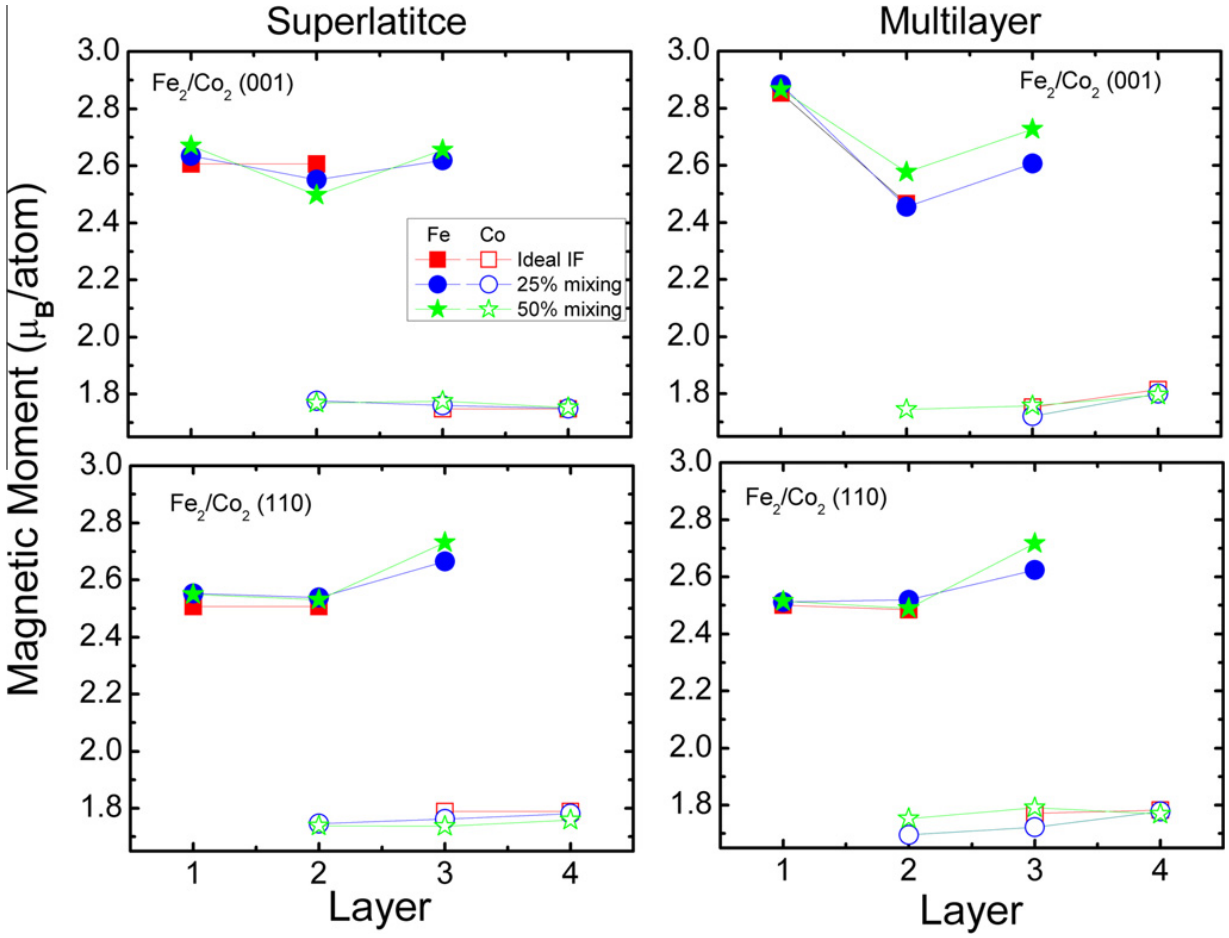

Fig. 4. The layer resolved spin magnetic moments of Fe_2/Co_2 superlattices (left panel) and multilayers (right panel) with ideal interface and with 25% and 50% mixing of atoms at the interface. The filled and open symbols represent Fe and Co atoms, respectively. For ideal interface, layer 1, 2 and 3, 4 consists of only Fe and Co atoms, respectively. Whereas, for 25% and 50% mixing of atoms at the interface, layers 2 and 3 contain both Fe and Co atoms together.

indicates this behavior, which will be discussed in the subsequent section where we present the atom-decomposed density of states.

The magnetic moments obtained for the bcc (001) and (110) multilayers are shown in the right panel of Fig. 4. As the two Fe (Co) layers of the multilayer even with out any mixing of atoms at the interface are in-equivalent, the magnetic moments in these two layers are different. It can be noted from Fig. 4 that the magnetic moment at the surface of (001) multilayer is large compared to that of the (110) multilayer. The Fe magnetic moment is found to be enhanced when there is mixing of atoms at the interface. The enhanced magnetic moment at the interface in the case of (001) multilayer is smaller than that at the surface layer whereas in the case of (110) multilayer it is larger than that at the surface layer. In addition to the reduced coordination number of atoms at the surface, the geometry of the (001) multilayer provides larger inter-atomic separation compared to that of (110) and it is the primary reason for the larger magnetic moment in the surface layer of (001) multilayer. The Co moment, on the other hand remains almost constant in these multilayers, like in the case of superlattices. This indicates that the reduced coordination in multilayers is not affecting the magnetic moment of Co atoms, reflecting the fact that the spin-up band of Co is almost completely filled and which is not affected by the changes in the local environment.

Enhanced Fe magnetic moment of about 2.7 μ_B/atom and the trend of a constant Co moment around 1.7 μ_B/atom is seen in un-relaxed Fe/Co interface calculated with first principles Greens Function studies [12]. We have seen an enhancement of Fe magnetic moment of about 0.2 μ_B/atom at the Fe/Co(001) superlattice after mixing whereas, Bergmann et al. [14] found an increase of only about 0.04 μ_B/atom for Fe/Co(001) superlattice without considering relaxation of atoms. The increased value

seen in our calculations may be due to the effect of atomic relaxations undertaken. However, our computed values of magnetic moments were not as large as 3 μ_B/atom for Fe and 2.1 μ_B/atom for Co atoms at the interface noticed experimentally [4].

In order to get further understanding of the enhancement of the magnetic moments of Fe atoms in these superlattices and multilayers we have calculated spin polarized density of states (DOS) and integrated DOS. The DOS and integrated DOS corresponding to a Fe and Co atom at the interface of bcc (1 1 0) Fe_2/Co_2 superlattice corresponding to the situation of ideal interface and with 50% mixing are shown in top and bottom panels of Fig. 5, respectively. It is seen from the figure that there is a reduction in the band width of Fe-d bands when there is mixing of atoms at the interface. The reduction in the symmetry at the interface caused by the mixing in the superlattice leads to the narrowing of Fe-d bands which gives rise to the enhanced splitting between the spin-up and spin-down states, forcing Fe to behave as a stronger ferro magnet compared to bulk Fe. The effect of this feature can be clearly seen from the integrated DOS shown in the figure. The integrated DOS of Fe atoms show distinct changes when there is mixing of atoms at the interface and it is the reason for the significant enhancement of the magnetic moment of Fe atoms at the interface after mixing. The behavior of Co-d bands, on the other hand, is found to be different. It can be seen from the figure that the spin-up band of Co atoms are almost filled whereas the spin down band is partially filled. The spin dependent integrated DOS of the Co atoms obtained from our calculations do not show significant changes when there is mixing of atoms at the interface and it is the reason for the Co moments to remain almost unaltered.

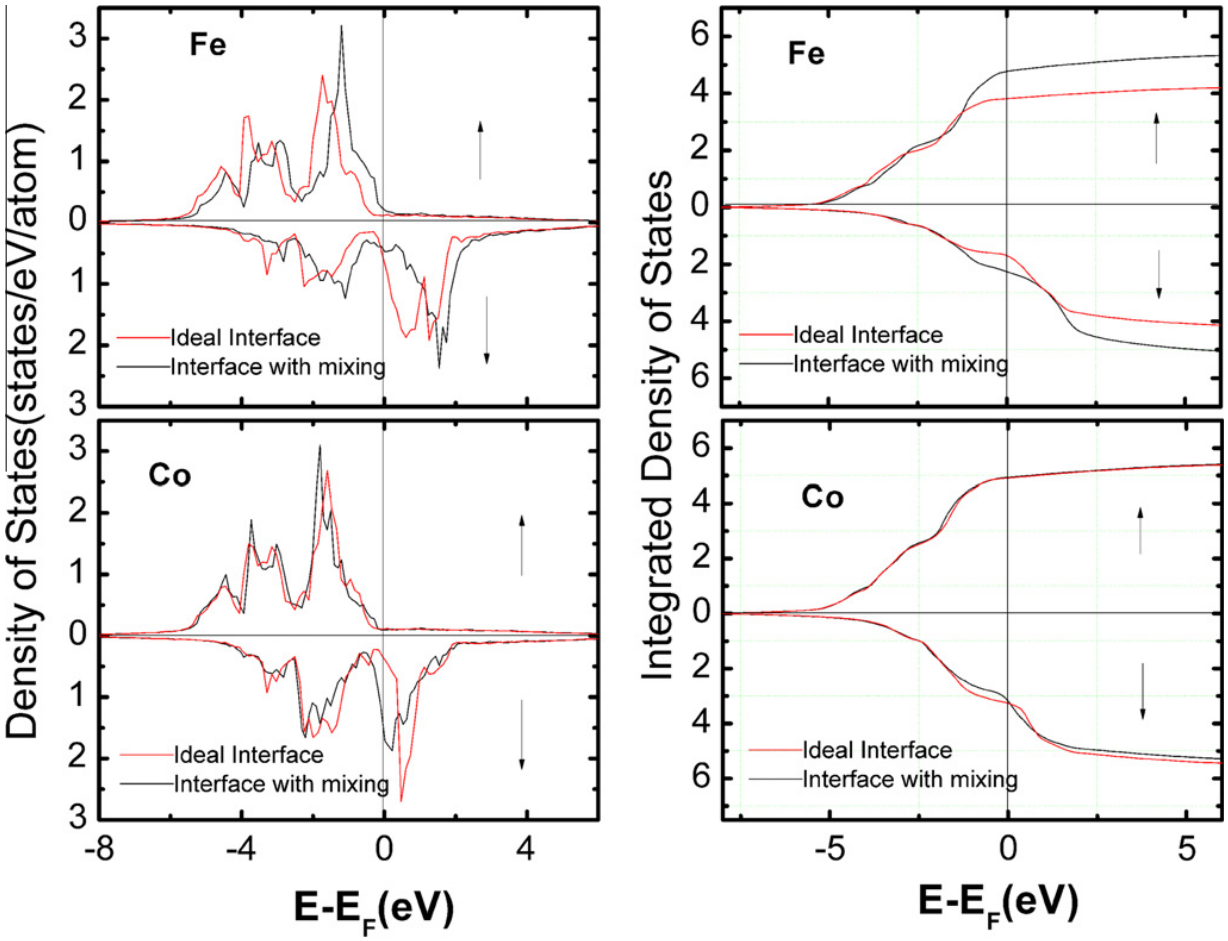

Fig. 5. Spin-polarized density of states (DOS) (left panel) and integrated DOS (right panel) corresponding to a Fe and Co atom in the Fe_2/Co_2 (1 1 0) superlattice for an ideal interface and with 50% mixing of atoms at the interface. The difference in DOS caused by the mixing of atoms can be noted from the DOS and integrated DOS of Fe atom. Compared to the Fe atom at the interface, Co is not showing much change in the DOS and integrated DOS before and after mixing, and this indicates an almost constant magnetic moment for Co. The straight line at the zero energy corresponds to the Fermi level.

3.3. Magnetic anisotropy energy (MAE)

The magnetic moments in a magnetic system often align along certain preferred direction with respect to the crystalline orientation called the easy axis. The energy required to rotate the magnetization from the easy axis to another direction is called the MAE. In low dimensional transition metal systems spin–orbit coupling (SOC) is the major cause of MAE and hence we have carried out calculations with the inclusion of SOC to obtain the MAE as well as the orbital moments. We have calculated the MAE as the difference in total energies corresponding to magnetization lying in the plane ($E_{||}$) of the superlattice/multilayer and normal to the plane ($E_{\perp}$).

$$\mathrm{MAE} = E_{||} - E_{\perp}$$

A negative value of MAE thus means that the magnetization prefers to orient along an in-plane axis, and a positive value means out-of plane orientation. MAE was calculated for the Fe_3/Co_1, Fe_2/Co_2 and Fe_1/Co_3 superlattices and multilayers with ideal interfaces taking into account the full relaxation of atoms. The initial inter-planar distances for the (0 0 1) and (1 1 0) superlattice/multilayer are taken as 1.433 Å ($a_0/2$) and 2.026 Å ($a_0/\sqrt{2}$) respectively, where a_0 = 2.866 Å, the lattice parameter of bcc Fe. We have seen that the Fe–Co inter-planar distance before and after relaxation are different and this is shown in the Table 1. The Fe–Co inter-planar distance is found to be reduced with decrease in number of Co layers and with increase in number of Co layers, the distance increases. We have calculated the MAE for these relaxed structures and the results are shown in Tables 2 and 3. Here our aim is to study the effect of Co layer thickness and the influence of layered structure on the MAE.

It can be seen from the Table 2 that the magnitude of MAE is found to be larger in (1 1 0) superlattices compared to that of (0 0 1) superlattices. There exist in the literature, reports on in-plane MAE of the order of 50 μeV/atom in (1 1 0) oriented Fe_n/Co_n superlattices [15]. It can be noted that the magnitude of MAE of the Fe/Co superlattices with (0 0 1) orientation obtained from our calculations agree with other first principles calculations [14].

For the superlattices, MAE is negative for all compositions. Even though the magnitude of MAE is different in (0 0 1) and (1 1 0) orientations, it can be seen from Table 2 that both these superlattices prefer an in plane easy axis irrespective of the Co layer thickness and the (1 1 0) orientation, having a larger MAE appears more favorable. On the other hand, advanced recording techniques require a magnetization orientation perpendicular to the surface, i.e. an out of plane orientation of magnetic moments. This out of plane orientation of magnetic moments is desirable for use in perpendicular magnetic recording media, as opposed to longitudinal magnetic recording. It can be seen from Table 3 that some of the multilayers considered in our study show an out of plane magnetization. The bcc (0 0 1) multilayers always favor out of plane magnetization whereas in bcc (1 1 0) multilayers, a cross-over from in-plane to out of plane orientation occurs with the increase in the number of Co layers. Since positive MAE implies perpendicular orientation of moments giving a higher packing density, for the multilayers, (0 0 1) configurations appears more favorable. It can be seen from the Table 3 that the orbital moments corresponding to perpendicular orientation also increase with increase in number of Co layers. Our results on bcc (1 1 0) Fe–Co multilayers also show large values of MAE with out of plane orientation of magnetization and the values can be seen in the Table 3. There exist experimental reports by Moulas et al. [7] in which Fe–Co films on Pt(1 1 1) showed out of plane orientation of

Table 1
The Fe–Co interplanar distance (in Å units) of superlattice/multilayer after relaxation, without any mixing of atoms at the interface. The initial values of inter-planar distances for the (0 0 1) and (1 1 0) superlattice/multilayer are taken as 1.433 Å ($a_0/2$) and 2.026 Å ($a_0/\sqrt{2}$), respectively, where a_0 = 2.866 Å, the lattice parameter of bcc Fe.

	Superlattice		Multilayer	
	bcc (0 0 1)	bcc (1 1 0)	bcc (0 0 1)	bcc (1 1 0)
Fe_1Co_3	1.896	2.061	1.418	1.996
Fe_2Co_2	1.644	2.054	1.401	1.992
Fe_3Co_1	1.405	1.971	1.382	1.985

Table 2
Calculated orbital moment per atom (m_L) along two different magnetization directions and magnetic anisotropy energy per atom (MAE) for the Fe/Co superlattices. The MAE is negative for all configurations, indicating the in-plane easy axis of magnetization. Hence the magnetization prefers an in-plane easy axis, irrespective of the number of Co layers.

Superlattice	bcc (001)			bcc (110)		
	MAE (meV)	$m_{L\|\|}$ (μ_B)	$m_{L\perp}$ (μ_B)	MAE (meV)	$m_{L\|\|}$ (μ_B)	$m_{L\perp}$(μ_B)
Fe_1Co_3	−0.053	0.07	0.08	−0.159	0.07	0.08
Fe_2Co_2	−0.058	0.06	0.07	−0.222	0.06	0.07
Fe_3Co_1	−0.051	0.06	0.07	−0.217	0.05	0.06

Table 3
Calculated orbital moment per atom (m_L) along two different magnetization directions and magnetic anisotropy energy per atom (MAE) for the Fe/Co multilayers. It can be seen that the MAE is positive for all multilayers with (001) orientation, indicating an out-of plane easy axis of magnetization whereas in (110) multilayers, the MAE changes sign with respect to the Co layer thickness. Hence the magnetization changes from in-plane to out of plane with increase in number of Co layers.

Multilayer	bcc (001)			bcc (110)		
	MAE (meV)	$m_{L\|\|}$ (μ_B)	$m_{L\perp}$ (μ_B)	MAE (meV)	$m_{L\|\|}$ (μ_B)	$m_{L\perp}$ (μ_B)
Fe_1Co_3	0.051	0.1	0.09	0.175	0.08	0.07
Fe_2Co_2	0.099	0.08	0.07	−0.02	0.07	0.08
Fe_3Co_1	0.129	0.08	0.07	−0.011	0.06	0.07

magnetization for all Co compositions, with large MAE of about 400 μeV/atom. They have also showed agreement of these experimental results with MAE calculated by KKR Greens Function methods. The experimental study by Yildiz et al. [29] using XMCD measurements on $Fe_{(1-x)}Co_x$ alloy films on Rh(100) substrate, indicate again large MAE of the order of 300 μeV/atom for the composition range $x = 0.3$–0.6, with out of plane orientation of magnetic moments. The observation of positive MAE (out of plane orientation of magnetization) of about 70–300 μeV, is also seen in FLAPW study of FeCo films on Pd(001) surface [30] for multilayers consisting of 2–5 monolayers, and hence support our finding of perpendicular anisotropy in multilayers. Further it is to be noted that in the above study, negative MAE is shown by a single monolayer only and no systematic of MAE with increase in monolayer thickness is seen.

We have analyzed the anisotropy of orbital moments to understand the observed variation of MAE with respect to thickness of Co layer in the superlattices and multilayers. It is seen from the Tables 2 and 3 that the magnitude of orbital moments calculated with magnetization oriented parallel and perpendicular to the superlattice/multilayer orientation are not the same. This anisotropy in orbital moments (Δm_L) is calculated as difference in the orbital moments corresponding to the parallel and perpendicular orientation of magnetization,

$$\Delta m_L = m_{L||} - m_{L\perp}$$

We find a linear relation between the orbital moment anisotropy and MAE. This is in accordance with the model proposed by Bruno [31]. We have seen that the anisotropy of orbital moments calculated in all superlattice configurations were $-0.01\,\mu_B$/atom which is consistent with the fact that the MAE is also negative. The Δm_L for Fe_2/Co_2 and Fe_3/Co_1 multilayers with bcc (110) orientation is $-0.01\,\mu_B$/atom whereas the Δm_L values for all other multilayers are $0.01\,\mu_B$/atom. It can be seen from Table 3 that for Fe_2Co_2 and Fe_3Co_1 multilayers with (110) orientation, the MAE also shows a negative value. Therefore in these configurations, the magnetization will be in-plane. In the bcc (001) oriented multilayers, both the MAE and Δm_L shows a positive value which indicates that the out-of plane orientation of magnetic moments are preferred. Apart from the large value of MAE, significant orbital moments were also shown by the superlattices and multilayers. These un-quenched values of orbital moments, compared to bulk, arise due to the asymmetric interactions present in the superlattices and multilayers which give rise to d-electron localization that leads to finite orbital moments.

4. Conclusions

The influence of layer thickness and interfacial mixing of atoms on the magnetic moments of bcc Fe/Co (0 0 1) and (1 1 0) superlattices and multilayers were studied using first principles simulation techniques. The spin magnetic moments of Fe atoms are found to be affected by the geometry, coordination number and the thickness of the Co layers whereas that of the Co atoms is found to remain almost constant. The mixing of atoms at the interface is found to enhance the spin magnetic moment of Fe atoms which was analyzed by calculating the spin polarized density of states. The magnitude of the spin magnetic moments of Fe atoms exhibit variations with respect to the geometry of the superlattices/multilayers. The spin magnetic moments of Fe atoms at the surface of the (0 0 1) multilayers is found to posses' significant enhancement which is found to be larger than that caused by the interface mixing. The large reduction in the coordination number of the atoms at the surface is the cause of this enhancement. The magnetic anisotropy energy of superlattices and multilayers were obtained by performing non-collinear calculations with spin–orbit coupling. The magnetization of both the (0 0 1) and (1 1 0) Fe/Co superlattices are found to prefer the in-plane easy axis irrespective of the Co layer thickness. On the other hand, Fe/Co multilayers prefer both in-plane and out of plane orientations of the magnetization depending on the Co layer thickness. Calculations carried out by including spin–orbit coupling showed that superlattices and multilayers exhibit significant orbital moments and there exist a direct relation between the MAE and orbital moment anisotropy.

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