Ab initio calculation of structural and magnetic properties for Fe mono- and bilayers on Mo(1 1 0)

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Abstract

The atomic structures were optimized and magnetic moments calculated for the pseudomorphic Fe overlayers on Mo(1 1 0) substrates employing the all-electron full-potential linearized augmented plane-wave (FP-LAPW) method. Three slabs were considered: (i) 5 monolayer (ML) Mo(1 1 0) substrate, (ii) and (iii) 1 and 2 ML pseudomorphic Fe overlayers on each side of 5 ML Mo(1 1 0) substrate. We found that for the bare Mo substrate, the top Mo–Mo interlayer spacing is contracted by 4.8% with respect to the theoretical bulk Mo(1 1 0) interlayer distance of 2.238 Å. For the 1 ML Fe coverage, the Fe–Mo interlayer spacing has a contraction of 10.3% with respect to the calculated bulk Mo(1 1 0) interlayer spacing, while, for the 2 ML Fe, it is reduced by 9.5%. The Fe–Fe interlayer spacing is also contracted by as much as 11.4% with respect to the theoretical bulk Fe(1 1 0) interlayer distance of 2.004 Å. The inner Mo–Mo interlayer spacings are slightly expanded ($<0.5\%$). The magnetic moment for the 1 ML Fe overlayer on top is enhanced to 2.59 μ_B compared to the bulk value of 2.2 μ_B. For 2 ML Fe coverage, the magnetic moments are 2.81 μ_B and 2.32 μ_B for the surface and interface Fe layers, respectively. © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction

The structural and magnetic properties of Fe thin films on substrates especially on noble metals have been studied widely [1–11] because of their unique magnetic behaviors such as perpendicular magnetic easy axis, enhanced surface magnetic mo-ment and giant magnetoresistance (GMR). Magnetic thin films on noble metal substrates were well characterized both experimentally [1–9] and theoretically [10,11]. Recently, however, Fe thin films on W(1 1 0) and Mo(1 1 0) substrates have been paid a lot of attention due to their thermostability [12,13] and the pseudomorphic layer-by-layer growth [13–19] of Fe films up to 2 ML on these substrates.

Mo and Fe metals have a BCC ground state lattice structure. Their lattice constants are 3.147 and 2.86 Å [20], respectively. Mo belongs to the 6B

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group of transition metals. Its valence electronic configuration is $4d^5 5s^1$. Due to the large lattice mismatch ($\sim 9\%$) between the Fe thin film overlayer and the Mo substrate, there is a large driving force for structure relaxation and possible magnetic reorientation due to the magnetoelastic effect even for ultrathin Fe films of thickness less than 2 ML.

It was found that Fe thin films grow pseudomorphicaly on the flat Mo(1 1 0) substrate up to 2 ML at room temperature [14,19]. Dislocations start to set in close to the completion of second monolayer growth of Fe on Mo(1 1 0) [14,19] substrate. No surface reconstruction was observed for the clean Mo(1 1 0) substrate, and for 1 and 2 ML Fe/Mo(1 1 0). It is well known [21] that metal surfaces tend to relax inward for the top layer in most of the cases and slightly outward or inward for the second layer. However, the actual amount of relaxation for the 1 and 2 ML Fe thin films on Mo(1 1 0) is still a controversy that needs to be resolved. Surface techniques such as low-energy electron diffraction (LEED) and photo-electron or Auger-electron diffraction (PED or AED) could provide such information. But so far, no experimental data are available concerning the vertical relaxation for these thin film structures.

In this paper we present ab initio results on the atomic structures of 1 and 2 ML Fe thin films on a Mo(1 1 0) substrate, i.e. the amount of relaxation, and the magnetic moments of the overlayer Fe atoms. The ab initio calculations were used to obtain these quantities.

2. Method

These calculations were performed by employing the WIEN97 code. The code was developed by Blaha, Schwarz and coworkers [22] and is based on the full-potential linearized augmented plane-wave (FP-LAPW) method. It has the additional capability of computing atomic forces [23–25] which makes the structure optimization much more efficient compared to the total energy only calculations. As described in Ref. [26], the FP-LAPW method is based on the density functional theory [26–29] solving Kohn–Sham equations. It adopts different representations for wave functions,

charge density and potential inside the muffin-tin sphere and in the interstitial region. The spherical harmonics were expanded up to $1 = 10$ inside the muffin-tin for the wave functions. The orbital basis was expanded up to $1 = 4$ for the interstitial region. The fully relativistic calculations solving the Dirac equation were included for the core electrons. The scalar relativistic calculations including the *velocity* and the *Darwin* terms were adopted for valence electrons. Spin–orbit coupling for the semi-core and valence electrons was not included for the structure optimization. It will be added later on to orbital moment calculations for electrons inside the muffin-tin sphere. Pulay corrections [24,30] to the Hellmann–Feynman forces were calculated which makes the structure optimization highly accurate. The improved tetrahedron method [31] was used for the integrations.

Three different slabs: (i) 5 ML Mo(1 1 0) substrate, (ii) 1 ML pseudomorphic Fe overlayer on each side of 5 ML Mo(1 1 0) substrate, and (iii) 2 ML pseudomorphic Fe overlayers on each side of 5 ML Mo(1 1 0) substrate were studied. A schematic picture of the system is shown in Fig. 1. Both 1 and 2 ML Fe overlayers were investigated because the structure relaxation and a possible magnetic reorientation occur between 1 and 2 Fe overlayers. The bare Mo substrate was studied to test our theoretical accuracy since reliable experimental data [32] are available and theoretical calculations are abundant [23–25]. Eight vacuum layers were incorporated in the supercell to separate the slabs in order to minimize any Coulomb and exchange interactions between the slabs as was commonly done previously [23–25] in these comparable slab calculations. Furthermore, slabs are symmetric with respect to the central substrate layer to avoid any charge accumulation on the surfaces. Thus the contribution to the total energy
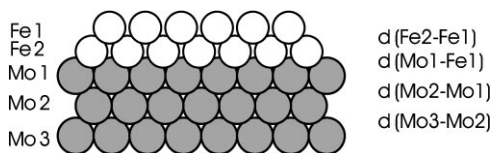

Fig. 1. Schematic picture of 2 ML Fe on 5 ML Mo(1 1 0) (upper half of the slab only).

from the electric-dipole interaction between the supercells in negligible compared to the contributions from within the supercell. Furthermore, only real wave functions are needed for the calculations because of the presence of inversion symmetry. The Fe layers on each surface are ferromagnetically coupled. The spin-polarized calculations were applied. The in-plane lattice parameters were kept constant using the theoretical bulk Mo(1 1 0) lattice value of 3.164 Å. Because of the two-dimensional (in-plane) translational invariance and only one atom on each layer in the supercell, there is no in-plane component of the force and therefore no in-plane lattice relaxation. In our calculations, we assume a periodic 1×1 in-plane translational symmetry, thus the in-plane components of the forces are non-existent. There are only vertical components of the forces. The use of the fixed in-plane lattice constant is reasonable since there is no reconstruction observed experimentally on the clean Mo(1 1 0) surface [14]. We assume bulk termination of the surface. As stated earlier, pseudomorphic Mo growth was observed for Fe layers on the flat Mo(1 1 0) substrate up to the completion of the second monolayer at room temperature [14]. In our calculations, the vertical lattice spacings are allowed to relax simultaneously according to the sign and magnitude of the force (there is only the vertical components of the force present) on each atom. The optimized structures and corresponding magnetic moments were obtained with the same converged spin-polarized self-consistent calculations.

In order to obtain the theoretical lattice constants for the bulk BCC Mo and Fe, total energies E_{tot} were calculated as a function of the lattice parameter a. As was done previously [23–25], the muffin-tin radii were chosen to be 1.27 Å for Mo and 1.164 Å for Fe. This choice of the muffin-tin radii is a good compromise between accuracy (smaller muffin-tin radii desirable) and efficiency (larger muffin-tin radii desirable). The calculations were done by choosing different k-point sets, the plane-wave and kinetic-energy cut-offs and different exchange potentials, GGA (generalized gradient approximation) [33] or local spin density approximation (LSDA) [34]. Convergence was achieved when the total energy and charge differences between two consecutive iterations are less

than 5×10^{-5} Ry and 1×10^{-4} e/(a.u.)^3, respectively. The magnetic moments were calculated as the differences between the spin-up charge and spin-down charge for these converged results. Orbital moments were evaluated when spin–orbit coupling was included in the final step of the calculations. The magnetization direction was chosen to be perpendicular to the film plane. Orbital polarization was not adopted in the calculations. Orbital moments are normally quenched in the bulk. For the free-standing Fe monolayers, it was estimated that the orbital moment of the Fe atom is around 0.1 μ_B [35] without orbital polarization. In our slab calculations, the orbital moment contribution to the total moment would be even smaller because of the presence of the substrate. Therefore we will not take into account the contribution of the orbital moment to the total magnetic moments here.

For the slab calculations, the GGA exchange potential and scalar-relativistic treatment were used. As was stated earlier, the theoretical equilibrium bulk Mo lattice constant ($a = 3.164$ Å which will be discussed later on the bulk Mo and Fe results) were used as the in-plane lattice constant for the slabs. The Fe overlayers are pseudomorphic to the substrates which means that these Fe overlayers have the same in-plane lattice constant as the substrate. The force (vertical component only) on each atom is computed and the vertical lattice spacings are relaxed accordingly. The two-dimensional k-point meshes are 21×21 for 5 ML Mo(1 1 0), 22×22 for 1 ML Fe on 5 ML Mo(1 1 0), and 23×23 for 2 ML Fe on 5 ML Mo(1 1 0). The slight difference among these two-dimensional meshes are due to the different vertical length of the unit cell. The numbers of k-points in the irreducible part of the Brillouin zone (IBZ) ($\frac{1}{4}$ of BZ) are 121, 132, and 144, respectively. The plane-wave cut-offs are 14 Ry for the 5 ML Mo substrate and 11 Ry for the 1 and 2 ML Fe overlayers on top. The kinetic energy cut-offs are 256 Ry for the Mo substrate and 100 Ry when there are Fe overlayers. The difference in these cut-off parameters is due to the CPU time required for the iterations.

The structures are optimized when the force on each atom is less than 1 mRy/(a.u.). For the total energy and magnetic moment calculations, the same convergence criteria are applied, i.e. the

differences in total energy and charge are less than 5×10^{-5} Ry and 1×10^{-4} e/(a.u.)^3, respectively between two consecutive iterations.

3. Results

3.1. Bulk properties for BCC Mo and Fe

Both ground state of Mo and Fe bulk metals have a BCC structure. Theoretical bulk equilibrium lattice constants were determined by the minima of the total energies. The total energy E_{tot} was calculated by varying the lattice parameter a. Standard parabolic behaviors are observed for E_{tot} versus a. The GGA exchange potential was employed. The plane-wave cut-offs are 17.36 Ry for Mo and 20.66 Ry for Fe. The kinetic energy cut-offs are 256 Ry in both cases. Scalar-relativistic calculations were used.

In the case of Mo, the lattice constant at 3000 **k**-points is 3.164 Å which is 0.5% higher compared to the experimental value of 3.147 Å. This slight overestimation of the lattice constant is most likely due to the use of the GGA exchange potential which is known to increase the equilibrium lattice constants for the heavy atoms.

In the case of Fe at 3000 **k**-points, the lattice constant is 2.834 Å which is 0.9% lower than the experimental value of 2.860 Å. The magnetic moment is 2.172 μ_B without orbital moment in close agreement with the experimental bulk value of 2.2 μ_B.

3.2. Structural results for Fe/Mo(1 1 0)

The structure optimization for the slabs was done by giving an initial guess of the interlayer spacings. As described earlier, the in-plane lattice constants are not allowed to relax due to the two-dimensional translational invariance and the fact that there is only one atom on each layer in the unit cell. The direction and degree of relaxation for the vertical interlayer spacings depend on the magnitude and sign of the forces present. The optimized interlayer spacings are listed in Table 1 for Mo with three different slabs. Also listed in the table is the LEED experimental data [32].

For the bare 5 ML Mo(1 1 0) substrate, the surface layer is relaxed downward by 4.82% compared to the theoretical bulk interlayer spacing. The first interlayer spacing is reduced from 2.238 to 2.131 Å. This is in very good agreement with the recent experimental LEED results [32] in which a 4.0% downward relaxation was observed. The LEED experiment yields a first Mo–Mo interlayer spacing of 2.137 Å. For the second Mo–Mo interlayer distance, we find only a very slight change from the theoretical bulk value. It is slightly expanded by 0.26% to 2.244 Å. It is also in good agreement with the LEED results which give a 0.2% expansion to 2.230 Å from the experimental bulk value of 2.226 Å. Our results also agree well with the previous calculations by Kohler et al. [23] employing the WIEN95 code. They also tried 7 and 9 ML Mo(1 1 0) slabs, the results are essentially the same as the 5 ML slab calculations. Thus our 5 ML Mo(1 1 0) substrate is a reasonable choice for the slab calculations.

For the slab of 1 ML Fe on each side of the 5 ML Mo(1 1 0) substrate, we find a significant downward relaxation of 10.3% for the Fe–Mo interlayer spacing compared to the bulk Mo(1 1 0) interlayer spacing. The Fe–Mo spacing is relaxed from the bulk value of 2.238–2.008 Å. The second and third Mo–Mo interlayer spacings are slightly expanded by 0.28% and 0.45%, respectively.

Table 1

Structural results (the layer spacings are given in Å. The relative changes as compared to the bulk Mo layer spacing are given in parentheses. The percentage of Fe–Fe contraction is relative to the bulk Fe–Fe interlayer spacing.)

	$d(Fe_2–Fe_1)$	$d(Mo_1–Fe_1)$	$d(Mo_1–Mo_2)$	$d(Mo_2–Mo_3)$
5 ML Mo(1 1 0)			2.131(− 4.82%)	2.244(0.26%)
1 ML Fe/Mo(1 1 0)		2.008(− 10.3%)	2.244(0.28%)	2.248(0.45%)
2 ML Fe/Mo(1 1 0)	1.775(− 11.4%)	2.026(− 9.5%)	2.243(0.23%)	2.242(0.17%)
Mo(1 1 0) (Exp. [32])			2.137(− 4.0%)	2.230(0.2%)

Table 2
Magnetic spin moments

	1 ML Fe/Mo(1 1 0) (μ_B)	2 ML Fe/Mo(1 1 0) (μ_B)
Fe(2)		2.807
Fe(1)	2.593	2.322
Mo(1)	− 0.104	− 0.099
Mo(2)	− 0.002	0.004
Mo(3)	− 0.003	− 0.001
Interstitial	− 0.055	− 0.04
Fe(2) (Exp. [39] Fe/W(1 1 0))		2.77
Fe(1) (Exp. [38] Fe/W(1 1 0))	2.53	

For the slab of 2 ML Fe thin films on both sides of the 5 ML Mo(1 1 0) substrate, we find contractions for both the Fe–Fe and Fe–Mo interlayer distances. The Fe–Fe interlayer spacing is reduced by 11.4%[1] from the bulk Fe(1 1 0) interlayer spacing of 2.004–1.775 Å. The Fe–Mo interlayer distance is contracted by 9.5% compared to the bulk Mo(1 1 0) value. The Fe–Fe interlayer spacing can also be estimated from the elastic theory [36] assuming a Mo(1 1 0) in-plane spacing. The elastic theory gives a Fe–Fe interlayer spacing of 1.844 Å, a contraction of 8% in reasonable agreement with our result. We have to bear in mind that the estimation assumes a small in-plane strain and a linear elastic response which may not be true in our case since we have a significant 9.4% misfit. Albrecht et al. [37] found a contraction of 10.4% for the Fe–Fe interlayer spacing with $d_{\text{Fe–Fe}} = 1.82$ Å. This seemingly smaller Fe–Mo contraction compared to the 1 ML case is reasonable considering that there is an additional Fe layer present [21]. The neighboring Mo–Mo interlayer spacing is slightly expanded by 0.23% similar to the previous 1 ML case. The inner Mo–Mo interlayer distance has virtually no relaxation.

3.3. Magnetic results for Fe/Mo(1 1 0)

The magnetic moment (only spin moment considered) of Fe atoms for the relaxed 1 ML layer Fe

on 5 ML Mo(1 1 0) is 2.59 μ_B, an enhancement of 18% compared to the bulk moment of 2.2 μ_B. This agrees well with the experimental results of 2.53 μ_B found by Elmers et al. [38] using torsion oscillation magnetometry (TOM). In earlier calculations on the 9 ML Fe(1 1 0) slab [11], a magnetic moment of 2.65 μ_B was obtained, which is in good agreement with our results and the experimental data. Nevertheless, no relaxation was considered in this 9 ML slab calculation. In our calculations of 1 ML Fe/5 ML Mo(1 1 0), we allow all the atoms to relax simultaneously and therefore the true minimum can be reached. From our results shown in Table 2, the Fe atoms are ferromagnetically coupled. However the neighboring Mo atoms acquire a small spin moment of 0.1 μ_B. In addition, the Mo atoms are antiferromagnetically coupled to their neighboring Fe atoms. Fig. 2 shows the spin-density (spin(↑)–spin(↓) in e/Å^3) for the system as shown in Fig. 3. The main peaks are the spin-densities of the Fe atoms. The smooth region between the two rows of Fe atoms is the vacuum space. The very small valleys are the spin-densities of the neighboring antiferromagnetically coupled Mo atoms. The projections on the bottom plane are the contour plot of the Fe spin-density. Mo atoms are invisible here because their spin-densities are at least 20 times smaller than those of the Fe atoms.

The orbital moment for the Fe overlayer was found to be 0.067 μ_B when the magnetization direction is perpendicular to the film plane. The neighboring Mo substrate layer also exhibits a small orbital moment of 0.005 μ_B. We can see that the orbital magnetic moment is rather small compared

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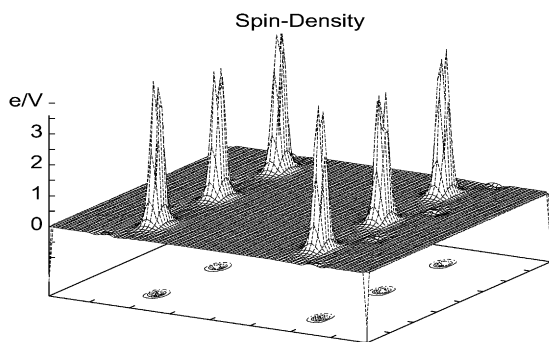[1] The Fe–Fe interlayer distance is contracted by 20.7% with respect to the Mo–Mo interlayer spacing.

Spin-Density

Fig. 2. Spin-density of the 1 ML Fe on each side of 5 ML Mo(1 1 0) for the (1 0 0) surface.
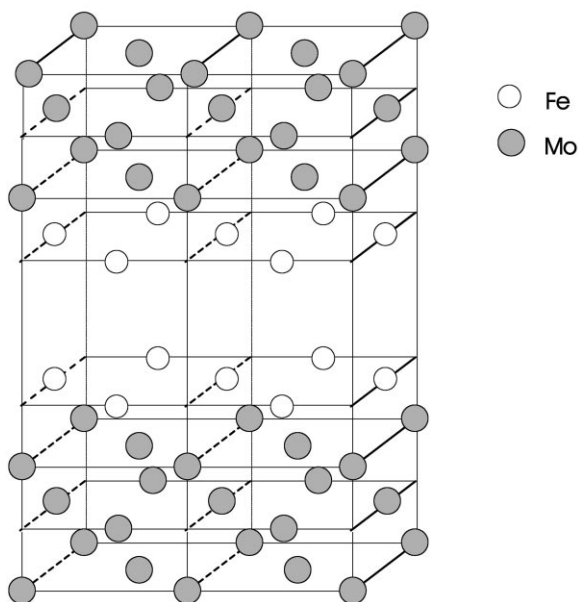

○ Fe
● Mo

Fig. 3. Unit cells of the 1 ML Fe on each side of 5 ML Mo(1 1 0).

to the spin magnetic moment. It is therefore not taken into account for the total Fe magnetic moment. Both Fe and Mo orbital moments are parallel to their corresponding spin moments. They are antiferromagnetically coupled to each other as the spin moments are.

For the 2 ML Fe thin films on 5 ML Mo(1 1 0), the magnetic moment for the top layer Fe is 2.81 μ_B, a significant enhancement of 28% from the bulk value. This result also agrees well with the

experimental measurement by Gradmann et al. [39] for the thicker Fe films on W(1 1 0) substrate. Their experimental estimation is 2.77 μ_B. Our calculation shows that the second Fe layer, i.e. the interface Fe layer, has a much reduced magnetic moment of only 2.32 μ_B. This again agrees well with the earlier calculation by Freeman et al. [11] for the 9 ML Fe(1 1 0) slab. They obtained a moment of 2.37 μ_B for the second layer of Fe next to the surface layer. Our results show that the interface Mo atoms also acquire a slight spin moment of 0.1 μ_B and are antiferromagnetically coupled to the neighboring Fe atoms.

As in the previous case, the orbital moments were obtained without orbital polarization and the magnetization is taken in the vertical direction. We found that the orbital moments for the surface and interfacial Fe layers are 0.062 and 0.052 μ_B, respectively. They are parallel to their spin moments and are ferromagnetically coupled to each other. The neighboring Mo layer acquires a very small orbital moment of 0.0019 μ_B and is antiferromagnetically coupled to the Fe layers.

Acknowledgements

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