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Magnetism at the V/Gd interface

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Abstract
Recent experimental investigations into the magnetic properties of V/Gd bilayers have shown that vanadium, which is nonmagnetic in the bulk, can acquire a magnetic moment in such systems. We have performed *ab initio* pseudopotential calculations to examine the magnetic behavior of V(110)/Gd(0001) bilayers for V layers with thicknesses up to 4 monolayers (ML). We considered both abrupt and atomic intermixed V/Gd interfaces. In both cases, the magnetic moment of the V layer is found to align antiparallel to the moment of the Gd layer, consistent with the experimental observation. However, the magnitude of the V moment at the abrupt interface is considerably smaller than the moments reported experimentally. In the presence of atomic intermixing, instead, substantially larger V moments are found, closer to the experimentally reported moments. On the basis of the calculated atomic and spin resolved density of states, we discuss the possible mechanism responsible for the observed Gd–V antiferromagnetic coupling.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Layered structures composed of ferromagnetic and nonmagnetic metals have been the focus of intensive research, motivated on one hand by a fundamental interest in the physics of low-dimensional systems and interfacial magnetism, and on the other hand by their promising potential applications in the area of magnetic storage, read heads, and magnetic sensors [1, 2]. Experimentally, the availability of techniques such as x-ray magnetic circular dichroism (XMCD), x-ray magnetic scattering, and polarized neutron reflectivity (PNR) has made possible the investigation of the magnetic properties of such systems with element specificity and monolayer sensitivity.

Most of the experimental work has been focused on layered structures composed of magnetic 3d and nonmagnetic 3d or 5d transition metals (TMs). In the case of the 5d elements Pt, W, and Ir, for example, XMCD results for multilayers [3, 4] have shown an induced magnetic moment of 0.17–0.29 μ_B/atom for Pt at the Ni/Pt interface, and of 0.2 μ_B/atom for W and Ir at the interface with Fe. Pt and Ir were found to couple ferromagnetically with the Ni and Fe moments, while antiferromagnetic coupling was reported for W with Fe. For the nonmagnetic V 3d TM, an induced moment was also reported at the V/Fe interface, coupled antiferromagnetically to the Fe moment. However, the induced moment across the Fe/V interface differed significantly between Fe/V/Fe trilayers (0.5 μ_B/atom) and Fe/V multilayers (0.9 μ_B/atom) [4]. V films grown on Fe substrate have also been studied experimentally [5, 6] and results have shown an induced magnetic moment (0.3–1.0 μ_B/atom), which in the coverage range of the first monolayer is oriented antiparallel to the moment of the substrate. For Fe/V layered structures, theoretical [7, 8] and experimental [9] studies showed that interface roughness and atomic interdiffusion play a key role in the enhancement of the V magnetic moments.

In a recent PNR study, Baczewski *et al* have shown that V can also acquire a magnetic moment at the interface with the rare-earth (RE) ferromagnetic metal Gd [10]. The experiments were performed on V(110)/Gd(0001) bilayers for V films of nominal thicknesses between 4 and 11 ML of V. The bilayers were fabricated by molecular-beam epitaxy, by first depositing the V layer on a Mo(110) buffer and then growing a Gd film (∼20 ML thick) on the V layer. The PNR study indicated that about 4 ML V become magnetic with an average magnetic moment as large as 0.8 μ_B/atom, aligned antiferromagnetically with the moment of the Gd

layer. Ferromagnetic TMs such as Fe and Co also show antiferromagnetic coupling across the Gd/Fe and Gd/Co interfaces, and with the Gd atoms in their alloy phases (see, e.g., [11–14]).

The interfaces between magnetic and nonmagnetic TM metals have been the subject of extensive theoretical study, in particular using first-principles calculations (see, e.g., [7, 8, 15]). At such interfaces, the magnetic exchange interaction takes place via direct coupling by hybridization between the d orbitals that carry the magnetic moments. Fewer theoretical investigations have been devoted instead to RE/TM interfaces or layered structures (see, e.g., [13]), and to the best of our knowledge there has been no *ab initio* study. The coupling in this case is bound to be indirect, as the overlap between the RE 4f and TM 3d orbitals is negligible. The RE–TM magnetic coupling is generally ascribed to an exchange interaction mediated by the RE 5d states, via 4f–5d direct exchange and 5d–3d hybridization [16]. However, the details of the mechanism responsible for the large V magnetic polarization and the origin of the observed antiferromagnetic Gd/V coupling are not yet fully understood.

Here we address the magnetic properties of V(110)/Gd (0001) bilayers by means of *ab initio* calculations. We investigate the influence of the interface atomic structure on the magnetic properties of the bilayers and the possible mechanism responsible for the antiferromagnetic Gd–V coupling. This paper is organized as follows: in section 2 we give a brief description of the computational approach used in this work. In section 3, we address the magnetic properties of the isolated Gd and V layers. Our results for the V/Gd bilayers are presented and compared to experiment in section 4. In section 5, we analyze the microscopic origin of the trends, while a summary and conclusions are given in section 6.

2. Methodology and calculational details

Our *ab initio* calculations are performed within the generalized-gradient approximation (GGA) to density functional theory (DFT), using the Perdew–Burke–Ernzerhof exchange correlation functional [17]. A plane-wave-basis set is used together with Vanderbilt ultrasoft pseudopotentials, as implemented in the PWSCF code [18]. For V, we employ the pseudopotential available from the QUANTUM-ESPRESSO library [18][5]. For Gd, we generated the pseudopotential using the Vanderbilt code [19], with the semicore 5s and 5p states treated as valence states[6]. The non-linear core correction is included in the calculations, both for V and Gd.

The computations of the V bulk and surface properties are performed with a kinetic-energy cutoff of 30 Ryd. For the Gd systems and V/Gd bilayers we use a kinetic-energy cutoff of 60 Ryd. The integrations in the Brillouin zone (BZ) for the bulk materials are carried out using a (18, 18, 18) k-point grid for bcc V and a (24, 24, 16) grid for hcp Gd. For the surfaces and interfaces, we employ a (24, 24, 1) k-point grid. The Fermi energy is determined using a Gaussian broadening scheme [20], with a broadening of 0.02 Ryd.[7] With these parameters, the numerical accuracy of the total energy is estimated as ∼1 mRyd/atom. The theoretical equilibrium lattice parameters are $a_{\mathrm{V}} = 2.99$ Å, $a_{\mathrm{Gd}} = 3.65$ Å, $c_{\mathrm{Gd}} = 5.85$ Å, with a zero magnetic moment for V and a ferromagnetic moment of $\mu = 7.60\ \mu_{\mathrm{B}}$/atom for Gd[8]. These calculated values are in good agreement with the experimental values: $a_{\mathrm{V}}^{\mathrm{exp.}} = 3.02$ Å, $a_{\mathrm{Gd}}^{\mathrm{exp.}} = 3.64$ Å, $c_{\mathrm{Gd}}^{\mathrm{exp.}} = 5.79$ Å, and $\mu^{\mathrm{exp.}} = 7.63\ \mu_{\mathrm{B}}$/atom.

We model the isolated V(110) and Gd(0001) surfaces and the V(110)/Gd(0001) bilayers using slab geometries in periodically repeated supercells. For the surfaces, we employ a symmetric slab including seven atomic layers, in the case of both V(110) and Gd(0001). We use a vacuum region of at least 14.8 Å to separate the periodic images of the slab. For the abrupt V(110)/Gd(0001) interface, we use a slab including seven atomic layers of Gd and 1–4 ML of V. A vacuum region of 18.4 Å is used to separate the periodic images of the V/Gd slab.

Experimentally, the alignment of the in-plane directions of the Gd(0001) overlayer and V(110) film is found to be Gd [1 1 $\bar{2}$ 0] ∥ V [001] [10]. The lattice mismatch, along that direction, between the experimental (theoretical) in-plane lattice parameters of Gd and V is 18% (17%) (between a_{Gd} and a_{V}) and 33% (32%) in the perpendicular in-plane direction (between $b_{\mathrm{Gd}} = \sqrt{3}a_{\mathrm{Gd}}$ and $b_{\mathrm{V}} = \sqrt{2}a_{\mathrm{V}}$). In order to simulate the V(110)/Gd(0001) interface, we need a commensurate interface atomic structure with a reasonably small interface unit cell dimension. We therefore elected to coherently strain the Gd overlayer to the V(110) in-plane lattice parameters.

In figure 1, we illustrate the atomic geometry considered in this work for the abrupt pseudomorphic V(110)/Gd(0001) heterostructure with in-plane directions Gd [1 1 $\bar{2}$ 0] ∥ V [001]. The epitaxial alignment of the Gd on V is made by positioning the atoms of the first Gd(0001) layer, adjacent to the V, in the continuation of the V(110) bcc lattice and using, for the V–Gd interlayer distance, the average between the bulk V–V interlayer distance and the bulk strained Gd–Gd interlayer distance. The subsequent Gd layers of the film are left in their bulk strained hcp positions. The strained hcp Gd film is elongated by ∼12% along c, following macroscopic elasticity theory and using the measured values of the Gd elastic constants[9].

In our study we use the theoretical values of the V and Gd lattice parameters. Unless otherwise specified, the moments

[5] The V 2s and 2p states are treated as core states.

[6] The all-electron calculations for the generation of the Gd pseudopotential were performed for the reference atomic configuration [X_e] $4f^7 5d^1 6s^2$. We generated the pseudopotential using the core-cutoff radii $r = 1.9$ au for the s, p, d components and $r = 2.0$ au for the f component. The reference energies used for the s, p, d, and f components were (−3.66, −0.27) Ryd, −2.00 Ryd, −0.19 Ryd, and (−0.63, 0.20) Ryd, respectively.

[7] Decreasing the broadening from 0.02 Ryd to 0.002 Ryd changes the magnetic moments of the V and Gd interface atoms of the 4 ML V(110)/7 ML Gd (0001) bilayer system, in table 2, from −0.07 to −0.05 μ_{B} and from 7.12 to 7.13 μ_{B}, respectively.

[8] The Gd magnetic phases with ferromagnetic and antiferromagnetic Gd-plane stacking along c are found to be degenerate in energy within our numerical uncertainty of ∼1 mRyd/atom. This remains true also for the bulk strained Gd considered in sections 3 and 4.

[9] We used the values of the measured elastic constants at low temperature from [21].

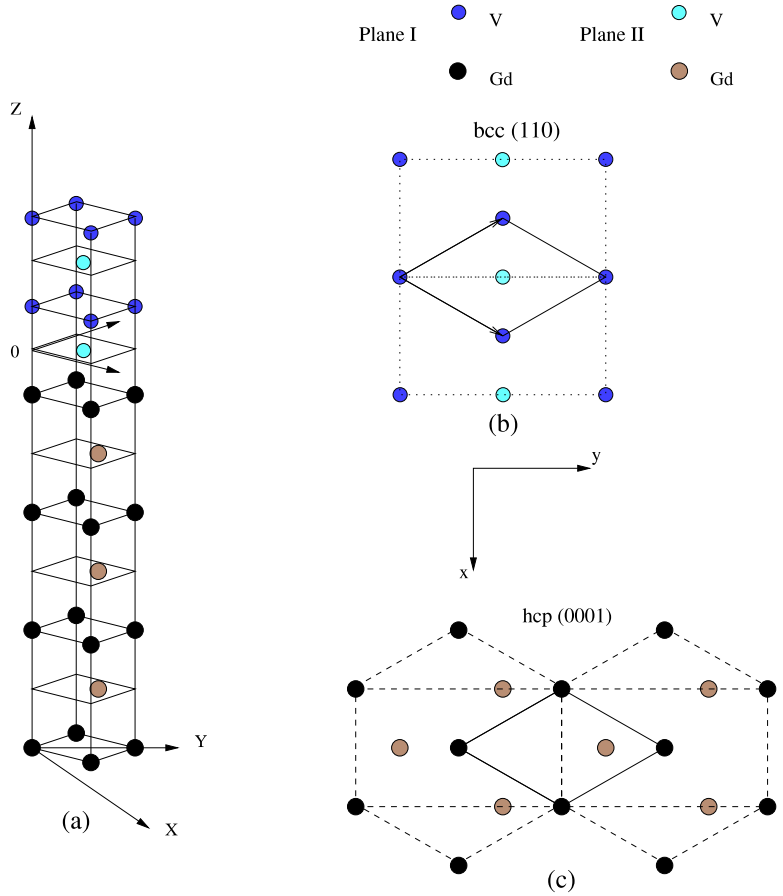

Figure 1. Plot of the atomic arrangement at the abrupt V(110)/Gd(0001) interface considered in this work. (a) Side view of the supercell including four planes of V atoms (small circles) and seven planes of Gd atoms (large circles). (b) Top view of the surface unit cell of V(110) (solid lines). (c) Top view of the surface unit cell of strained Gd(0001) (solid lines).

are calculated for unrelaxed atomic geometries. Relaxation of the atomic structure at the abrupt interface was found to change the magnetic moments by less than 0.01 μ_B.

3. Isolated surfaces and free-standing V monolayer

We first examine the magnetic properties of the isolated V(110) and Gd(0001) surfaces and of the free-standing V(110) monolayer. Vanadium is one of those paramagnetic metals that can exhibit magnetism under certain conditions, including loss of coordination, due to its large paramagnetic susceptibility. It is therefore important to first assess whether the isolated V(110) surface and the extreme case of a single isolated V(110) monolayer remain nonmagnetic within the GGA calculations. Recent experiments indicated that the clean V(001) surface is nonmagnetic, within the experimental uncertainty [22]. Hence, the more closely packed V(110) surface is expected to be nonmagnetic.

From the 7 ML V slab calculations, we indeed find that the V(110) surface is nonmagnetic within the GGA approach. In figure 2 we show the total energy computed for the ferromagnetic and nonmagnetic free-standing V(110) monolayer, as a function of the lattice parameter a. For values of the lattice parameter smaller than 3.08 Å, the isolated

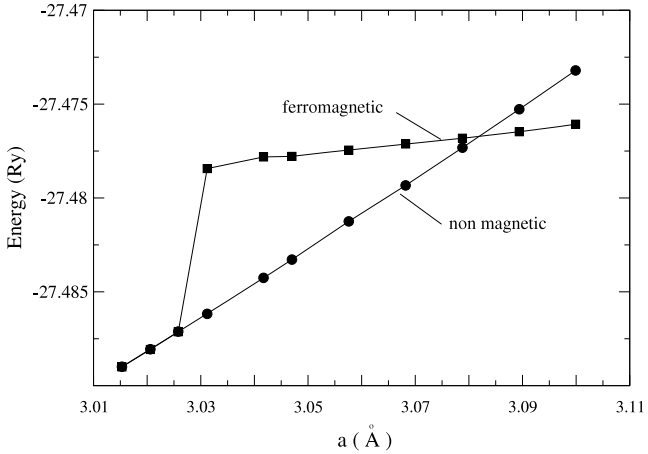

Figure 2. Comparison between the total energies of the ferromagnetic and nonmagnetic states of the V(110) free-standing monolayer as a function of the lattice parameter. For lattice parameters smaller than 3.03 Å, the ferromagnetic state could not be stabilized in the calculations and relaxed to the nonmagnetic state.

monolayer has a nonmagnetic ground state. The free-standing monolayer is thus nonmagnetic at the bulk lattice parameter of V. In figure 3 we display the moment as a function of a

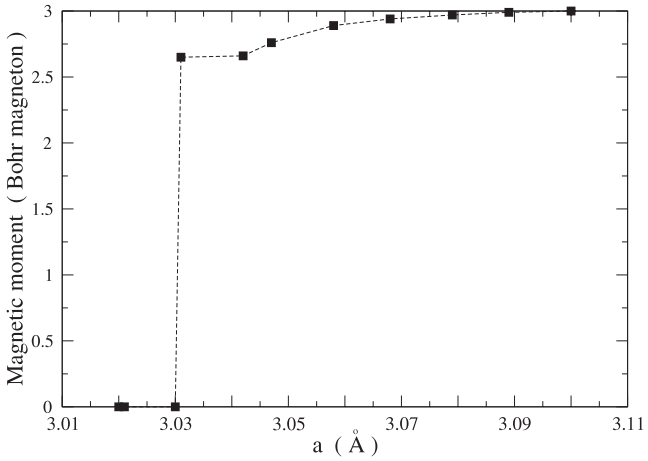

Figure 3. Magnetic moment per atom of the free-standing V(110) monolayer in the ferromagnetic phase (see also figure 2), as a function of the lattice parameter.

Table 1. Calculated magnetic moments for the free-standing seven-layer Gd(0001) film in the unstrained and strained configurations. The magnetic moments are in units of μ_B. The layer labeled 'S' is the surface layer, while the other sublayers are labeled according to their position from the surface and Gd(C) is the layer in the center of the film.

7 layer Gd(0001)	Gd(C)	Gd(S-2)	Gd(S-1)	Gd(S)
Unstrained film	7.55	7.59	7.57	7.75
Strained film	7.15	7.15	7.13	7.29

obtained from the calculations for the ferromagnetic phase. For $a > 3.08$ Å, when the ferromagnetic state is the ground state, the magnetic moment per V atom has a value of $\sim$3.0 μ_B.

The magnetic moments of the Gd atoms in the 7 ML Gd(0001) free-standing film with the bulk Gd lattice parameter are reported in table 1. The moment of the surface atom is 7.75 μ_B, which is about 3% larger than the moment of 7.55 μ_B of the atom in the central part of the slab. We also report in table 1, for comparison, the corresponding moments per atom in the Gd film coherently strained to the V(110) in-plane lattice parameters. The magnetic moments are reduced in this case—as expected due to the in-plane lattice and volume contraction—by $\sim$6% (to 7.29 μ_B) for the surface atom and by $\sim$5% (to 7.15 μ_B) for the atom at the center of the slab.

4. V(110)/Gd(0001) interface

In table 2, we present the magnetic moments of the Gd and V atoms calculated for the n ML V(110)/7 ML Gd(0001) ($n = 1, 2, 3, 4$) systems with an abrupt interface. In all cases, the V ML at the interface has a moment coupled antiferromagnetically to the moment of the Gd layer and is the dominant contribution to the total moment of the V layer. The moment of the V atoms in contact with the Gd is -0.21 μ_B in the case $n = 1$ (surface atom), and decreases in magnitude, as the V film thickness increases, to a value of $-0.07\mu_B$ at the interface for $n = 3, 4$. The V induced moment also decreases strongly in magnitude when going away from the interface within the V film. In particular, for $n = 3, 4$, the atoms of the second layer from the interface have a moment which is smaller in magnitude than 0.02 μ_B. For the Gd film, the magnetic moment of the atoms at the interface (7.12 μ_B) is slightly reduced as compared to the magnetic moment in the bulk part (7.14 μ_B).

The moment we find for the V atoms at the abrupt interface is about one order of magnitude smaller than the moment of about -0.8 μ_B/atom reported from polarized neutron reflectivity measurements for V layers with a nominal thickness of 4 ML [10]. Atomic relaxation has a very small effect on the magnetic moments at the interface (the moment of the V atoms at the interface increases by 0.006 μ_B upon structural relaxation, corresponding to a 1.7 % increase in the V–Gd interlayer distance and a 2.3 % reduction in the interlayer distance between the V layer at the interface and its neighboring V layer).

To understand what could be the possible origin of this discrepancy with experiment, we have investigated the effect of atomic intermixing at the interface. The V(110)/Gd(0001) interface is indeed known experimentally to be a rough interface [10]. We considered two intermixed ML in the following configuration: 3 ML V(110)/2 ML $V_{0.5}Gd_{0.5}$/6 ML Gd(0001), using a (1×2) lateral unit cell. The magnetic moments obtained for this intermixed bilayer are reported in figure 4, where we show a sketch of the interface atomic structure in the yz plane (see figure 1) with the moments of the corresponding Gd and V atoms.

Atomic intermixing significantly increases the magnitude of the magnetic moments of the V atoms closest to the Gd, which change from -0.07 μ_B at the abrupt interface to -0.46 and -0.21 μ_B in the intermixed case, i.e. to an average value of about -0.33 μ_B/atom of the nominally first deposited V monolayer. Intermixing can thus account for some of the difference with respect to the measured moment[10]. The calculated moments of the V atoms, however, are still significantly smaller than the measured moments. For comparison we also performed calculations for the limiting case of a V impurity in the Gd ferromagnetic bulk, under the same strain conditions. The calculations were performed using a $(3 \times 3 \times 1)$ Gd(0001) unit cell (18 atoms), with one Gd atom replaced by V. From these calculations we find an antiferromagnetic alignment of the V moment with respect to the Gd moments, with a value of -1.66 μ_B for the V moment.

In the experiment the V films were grown on a molybdenum buffer with a lattice parameter that is 4.3% larger than that of V. For ultrathin V films (4 ML or less) one may thus

[10] In order to obtain an estimate of the energy cost for intermixing, comparing the energy of the intermixed interface (in figure 4) with that of the abrupt interface, we performed additional calculations that include the effect of the local strain release with atomic relaxation (as the intermixing energy is much more sensitive to atomic relaxation than the magnetic moments). Such relaxation calculations (performed for both the intermixed and abrupt interfaces) had to be carried out with a somewhat reduced k grid (lateral sampling reduced from 24 to 20), as they are computationally very expensive. The resulting energy cost is $\sim$0.35 eV (with an estimated uncertainty of about 0.1 eV) per pair of exchanged Gd–V atoms, for the intermixed configuration considered in figure 4. For this configuration, we also find that the associated reduction (increase) of the magnetic moments of the V (Gd) atoms within the intermixed layer due to atomic relaxation is of the order of 0.01 μ_B.

Table 2. Magnetic moments of the Gd and V atoms calculated for the abrupt V/Gd systems composed of n V(110) ML ($n = 1, 2, 3, 4$) and 7 Gd(0001) ML. Magnetic moments are in units of μ_B. The atomic layers labeled 'I' are interface layers, while the other atomic layers are labeled according to their position from the interface or from the surface. The Gd(C) and Gd(S) are the atomic layers which are respectively at the center and at the surface of the Gd film.

n	Gd(S)	Gd(S-1)	Gd(S-2)	Gd(C)	Gd(I-2)	Gd(I-1)	Gd(I)	V(I)	V(I-1)	V(I-2)	V(I-3)
1	7.29	7.13	7.14	7.14	7.13	7.12	7.13	−0.21			
2	7.29	7.13	7.15	7.14	7.14	7.13	7.12	−0.08	−0.02		
3	7.29	7.13	7.15	7.14	7.14	7.13	7.12	−0.07	0.01	0.01	
4	7.29	7.13	7.14	7.14	7.14	7.13	7.12	−0.07	0.01	0.00	0.00

Table 3. Magnetic moments of the Gd and V atoms calculated for the abrupt n ML V(110)/7 ML Gd(0001) bilayer system ($n = 1, 2, 4$) coherently strained to the Mo(110) in-plane lattice parameters. Magnetic moments are in units of μ_B. The layers labeled 'I' are interface layers, while the other layers are labeled according to their position from the interface or from the surface. The Gd(C) and Gd(S) are the atomic layers which are respectively at the center and at the surface of the Gd film.

n	Gd(S)	Gd(S-1)	Gd(S-2)	Gd(C)	Gd(I-2)	Gd(I-1)	Gd(I)	V(I)	V(I-1)	V(I-2)	V(I-3)
1	7.63	7.36	7.35	7.34	7.34	7.32	7.39	−1.29			
2	7.63	7.36	7.36	7.35	7.35	7.35	7.33	−0.06	0.05		
4	7.63	7.36	7.35	7.35	7.35	7.35	7.32	−0.09	0.05	−0.02	0.02

Table 4. Magnetic moments of the Gd, V, and Mo atoms calculated for the abrupt 3 ML Mo(110)/1 ML V(110)/7 ML Gd(0001) heterostructure coherently strained to the Mo(110) in-plane lattice parameters. Magnetic moments are in units of μ_B. The layers labeled 'I' are Gd–V interface layers, while the other layers are labeled according to their position from the interface or from the surface. The Gd(C) and Gd(S) are the atomic layers which are respectively at the center and at the surface of the Gd film.

Gd(S)	Gd(S-1)	Gd(S-2)	Gd(C)	Gd(I-2)	Gd(I-1)	Gd(I)	V(I)	Mo(I-1)	Mo(I-2)	Mo(I-3)
7.63	7.36	7.36	7.35	7.35	7.34	7.31	−0.09	0.01	0.00	0.00

expect the V film to be coherently strained to the Mo lattice parameter. We therefore investigated whether such an epitaxial strain could explain some of the remaining discrepancy with experiment. We also note that with a 4.3% increase in the lattice parameter ($a \approx 3.12$ Å), the free-standing V(110) monolayer is predicted to be magnetic (see figures 2 and 3).

In table 3, we show the magnetic moments obtained from the calculations for the abrupt bilayers coherently strained to the Mo(110) in-plane lattice parameters. The corresponding elongation (contraction) of the Gd (V) film determined from macroscopic elasticity theory (see footnote 9) for $n > 1$ is 10% (4%). For 1 ML of V (surface atom), the magnitude of the V magnetic moment is found to increase to 1.29 μ_B. For thicker V layers, however, the magnitude of the moments of the V atoms at the interface remains essentially one order of magnitude smaller than the measured value. We also investigated the case of the supported Gd/V bilayer, including a single ML of V, on 3 ML of Mo(110).[11] The magnetic moments are reported in table 4. The results show that the magnetic moment of the V atoms at the interface in the 3 ML Mo(110)/ 1 ML V(110) /7 ML Gd(0001) system (−0.09 μ_B) is identical to the moment of the V atoms at the interface in the 4 ML V(110)/7 ML Gd(0001) system, and hence one order of magnitude smaller than the experimentally reported value.

[11] The Vanderbilt pseudopotential for Mo was generated using the reference atomic configuration [Kr] $4d^5 5s^1 5p^0$. For the core-cutoff radii we employed: $r_s = 2.2$, $r_p = 2.4$, and $r_d = 1.6$ au, and the reference energies used for the s, p, and d components were −0.3 Ryd, −0.08 Ryd, and (−2.7, 0.2) Ryd, respectively. The non-linear core correction was included in the calculations. The resulting theoretical equilibrium lattice constant for bulk bcc Mo was found to be 6.00 au.

We then examined the effect of atomic intermixing for the bilayer coherently strained to the Mo substrate. We considered in this case a 4 ML V(110)/7 ML Gd(0001) bilayer with two intermixed MLs at the interface with stoichiometry $Gd_{0.5}V_{0.5}$. The results for the magnetic moments are displayed in figure 5, together with the interface atomic structure. The moment of the V atoms closest to the Gd have values of −1.13 μ_B and −0.11 μ_B. This corresponds to an average value of −0.62 μ_B for the atoms of the first deposited V monolayer and hence to an increased moment of the V layer, when the Mo(110) in-plane lattice parameters are used.

The presence of atomic interdiffusion and inhomogeneity thus enhances the amplitude of the V moment and tend to bring it closer to what has been reported experimentally. Other features, not accounted for in our calculations, are also expected to increase the magnitude of the V moments. In particular, with lattice misfits as large as ∼15 and ∼30% (relative to Mo), the Gd film is not expected to adopt a pseudomorphic configuration. With such misfits, the film is expected to recover the bulk values of the Gd lattice parameters within a few ML at most from the interface. Calculations for such incommensurable interface atomic structures are not affordable within our *ab initio* approach. The increase in the Gd in-plane lattice parameters, however, is expected to increase the Gd moments and (in view of the decreased atomic packing at the interface and increased Gd moment) is also expected to increase the amplitude of the V moment at the interface. Corrections to the GGA approach may also be significant (see, e.g., [23] and [24]). Improvements relative to DFT local-density approximation (LDA) or GGA results, were obtained, for instance, using the DFT plus onsite Coulomb

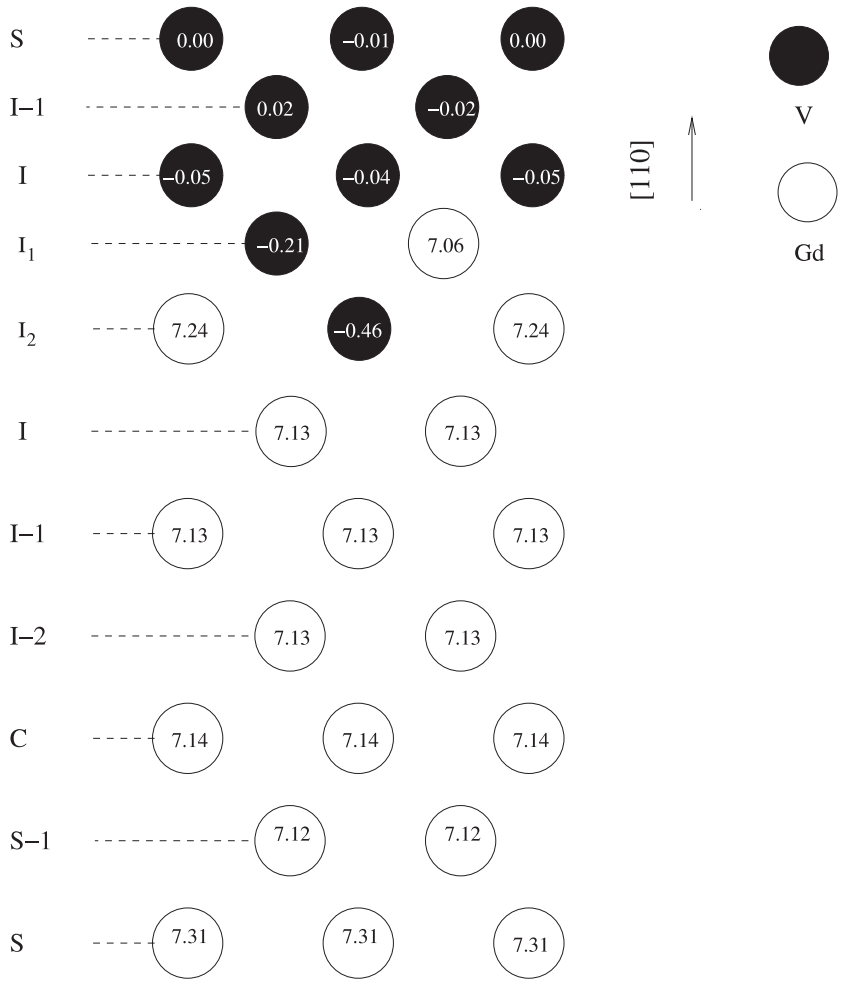

Figure 4. Sketch of the atomic structure in the yz plane (see figure 1) of the 4 ML V(110)/7 ML Gd(0001) bilayer with two intermixed MLs at the interface. Filled and open circles correspond to Gd and V atoms, respectively. The magnetic moment is reported for each atom (in Bohr magnetons).

interaction approach (DFT+U) for bulk and surface properties of Gd [23]. The DFT + U approach tends to increase the magnetic moments, and hence would also tend to bring the theoretical results for V closer to experiment.

5. Discussion

The induced moment on V as well as its antiparallel coupling to the Gd moment can be understood as a direct consequence of the Gd–V hybridization at the interface. In figure 6, we display the spin resolved projected V 3d, Gd 4f, and Gd 5d local density of states (LDOS) for the V and Gd atoms at the V/Gd intermixed interface. The corresponding LDOS for the bulk V and Gd atoms are shown in figure 7. The Gd 4f spin-up states are fully occupied, corresponding to the LDOS peak located ∼3.5 eV below the Fermi energy in our GGA calculations, while the empty 4f spin-down states are located about 2 eV about the Fermi energy[12]. The Gd 5d spin-up states experience a direct intra-atomic exchange interaction with the 4f spin-up electrons, which pulls down in energy the 5d spin-up band by about 1 eV with respect to the 5d spin-down band.

The Gd 5d states are located somewhat higher in energy than the V 3d states (considering the centers of mass of their respective DOSs) and are mostly empty. Hybridization between the Gd 5d and V 3d states is generally thus expected to induce, in both spin channels, an increased Gd 5d and decreased V 3d LDOS in the high-binding energy part of the spectrum. Furthermore this behavior is expected to be stronger in the spin-up channel than in the spin-down channel, since the V 3d states are closer in energy to the Gd 5d spin-up states than to the Gd 5d spin-down states. Such trends are indeed observed

[12] The energy position of the Gd minority-spin (majority-spin) 4f states is known to be underestimated (overestimated) within the LDA/GGA approach (see, e.g., [23] and [24]). In LDA calculations [24], the peak of the minority-spin 4f states is located only ∼0.2 eV above the Fermi level, with a non-negligible density of 4f minority-spin states at the Fermi energy, which is responsible for a layered antiferromagnetic ground state for bulk Gd in these calculations. In this case, the correct ground state can be obtained by either treating the Gd 4f states as core electrons [23] or using the LDA+U method [24]. In our GGA calculations, however, the peak of the minority-spin Gd 4f states is located about 2 eV above the Fermi energy, and the ferromagnetic state is actually slightly lower in energy than the layered antiferromagnetic state in the bulk strained Gd (although the energy difference is within our numerical accuracy of ∼1 mRyd per atom and we report these configurations as degenerate in energy; see footnote 8.)

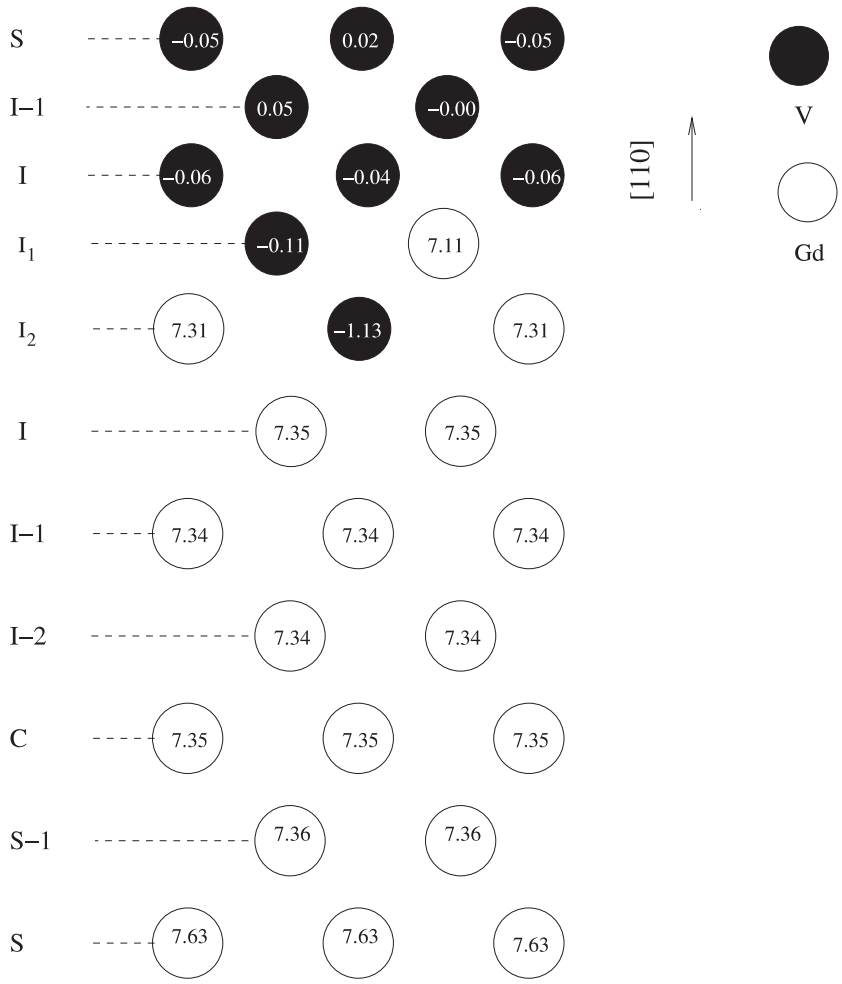

Figure 5. The same data as in figure 4, but for the bilayer coherently strained to the Mo(110) in-plane lattice parameters.

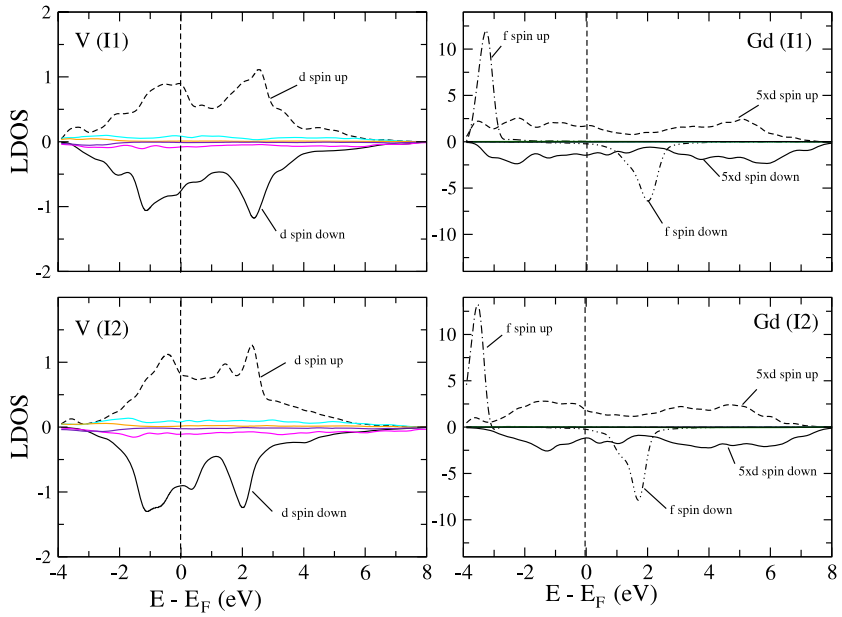

Figure 6. Projected V 3d (left panel) and Gd 5d (right panel) atomic local density of states (LDOS) for atoms at the V/Gd intermixed interface. Other components of the projected atomic densities of states are also displayed (light solid lines: V 4s and 4p components), but are essentially negligible in the energy window considered.

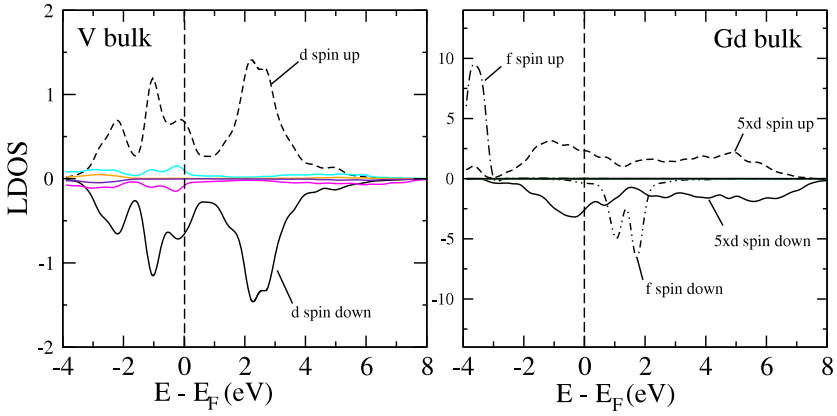

Figure 7. The same data as in figure 6, but for atoms in the bulk V and bulk (strained) Gd.

Table 5. Separate contributions from valence s, p, d, and f electrons to the magnetic moment of V and Gd atoms at the intermixed interface. The contributions for a Gd atom in the bulk (strained) Gd are also shown. Moments are given in units of μ_B.

	μ (s)	μ (p)	μ (d)	μ (f)	Total μ
V(I_1)	0.00	−0.01	−0.20	—	−0.21
Gd(I_1)	0.02	0.05	0.31	6.68	7.06
V(I_2)	−0.02	−0.01	−0.43	—	−0.46
Gd(I_2)	0.03	0.04	0.41	6.76	7.24
Gd(bulk)	0.04	0.05	0.33	6.72	7.14

by comparing the bottom parts of the d bands in figures 6 and 7. These trends are expected to give rise to a negative spin polarization of the V 3d states and to an increased positive spin polarization of the Gd 5d states.

In table 5 we display, for the V and Gd atoms at the V/Gd intermixed interface, the separate contributions of the valence s, p, d, and f (for Gd) electrons to the magnetic moments. We also display the moment decomposition for a Gd atom in the bulk part of the strained Gd slab. As expected, s and p contributions are minute, and the V 3d electrons show a significant negative moment. Comparing the moments of the Gd(I_2) and Gd(bulk) atoms, an increased 5d spin polarization is indeed found for the Gd (I_2) atom at the intermixed interface relative to the bulk Gd atom. Similarly to the Gd bulk atom, the Gd (I_2) atom is located at a hcp site of the lattice, and the moments can thus be directly compared to assess the effect of the hybridization with neighboring V atoms. In the case of the Gd(I_1) atom, instead, the moment contributions in table 5 are generally reduced compared to the bulk Gd atom. This is because the Gd(I_1) atom is located at a bcc lattice site where atomic packing is increased.

6. Summary

We have examined by means of *ab initio* pseudopotential calculations the magnetic behavior of V atoms at the V(110)/Gd(0001) interface. The V atoms at the interface exhibit a negative magnetic polarization relative to the Gd moments, consistent with the experimental observation. The amplitude of the V polarization at the abrupt interface, however, is much smaller than reported for the experimental V/Gd bilayers. Interface atomic intermixing together with epitaxial strain for growth of the bilayers on a Mo buffer increase the magnitude of the V magnetic moments and tend to bring the moments closer to values reported in PNR experiments. The induced moment on the V at the interface as well as its antiparallel coupling to the Gd moments can be understood as a direct consequence of the Gd–V 5d–3d hybridization at the interface and of the Gd 5d magnetic polarization by the 5d–4f intra-atomic exchange.

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