PHYSICAL REVIEW B, VOLUME 63, 104424

Magnetization profile and magnetocrystalline anisotropy of ferromagnet-semiconductor heterostructure systems

I. Cabria
Institut für Physikalische Chemie, Universität München, Butenandtstrasse 5-13, D-81377 München, Germany

A. Ya. Perlov*
MPI für Physik Komplexer Systeme, Nöthnitzerstrasse 38, D-01187 Dresden, Germany

H. Ebert
Institut für Physikalische Chemie, Universität München, Butenandtstrasse 5-13, D-81377 München, Germany

(Received 5 June 2000; published 20 February 2001)

Ab initio linear-muffin-tin orbital calculations of the magnetization profile and the magnetic anisotropy of ferromagnetic-semiconductor (FM/SC) multilayers, bcc Fe/Ge (001) and bcc Fe/GaAs (001), have been carried out to find out the microscopic origin of these properties. The electronic magnetic anisotropy energy (MAE), computed with the force method, was found to favor a magnetization perpendicular to the plane of the layers and to increase with the thickness of the ferromagnetic layers. The anisotropy of the energy, i.e., the MAE, as well as the anisotropy of the orbital magnetic moment turned out to depend only slightly on the type of semiconductor, Ge or GaAs, and to come mainly from the interface Fe layers. In particular, it was found that the relationship between the electronic MAE and the anisotropy of the orbital moment proposed by van der Laan is very well satisfied in these systems. According to that relationship, the magnetic anisotropy of these FM/SC multilayers is mainly due ($\sim$80–90%) to a delicate rearrangement of the occupations of certain $3d$ spin down levels in the interface Fe layers caused by the change of the magnetization direction.

DOI: 10.1103/PhysRevB.63.104424 PACS number(s): 75.30.Gw, 75.70.Cn, 75.50.Pp, 71.70.Ej

I. INTRODUCTION

A new field of interest in solid state physics was opened in the 1980s by the deposition of magnetic materials on semiconductors. This allowed the synthesis of a number of new artificial materials with potential applications in magnetoelectronics.[1–3] In particular, ferromagnetic-semiconductor (FM/SC) heterostructures have a potential use in devices based on the TMR (tunneling magnetoresistance). In particular, Fe deposited on GaAs (001) is a promising system, because epitaxial growth of bcc Fe on (110) and (001) surfaces of GaAs can be achieved due to the lattice constant of bcc Fe (2.87 Å) being about half that of GaAs (5.65 Å).[4,5] Accordingly, several experiments have been reported on the structural and magnetic properties of Fe layers on GaAs and similar systems.[6–15] Concerning possible TMR devices the transport properties of these systems are the most important ones, but these are intimately related to the magnetization profile and magnetic anisotropy, among other magnetic properties.

Band structure calculations allow one to connect the properties of these materials with peculiarities of their electronic and/or geometric structure and thus to undertand the origin of these properties. So far, there are few theoretical investigations on the magnetic and transport properties of FM/SC structures. Pickett and Papaconstantopoulos performed parametrized tight-binding calculations of the Fe/Ge (110) interface.[16,17] Continenza *et al.* studied the magnetic and the electronic properties of Fe/ZnSe superlattices obtained by means of the full-potential linearized augmented-plane-wave (FLAPW) method.[18] Schilfgaarde and Newman made *ab initio* linear-muffin-tin orbital (LMTO) calculations of the electronic structure of ideal metal-GaAs interfaces, bcc Fe among other metals.[19] Butler, MacLaren and co-workers have calculated the electronic structure of the spin-dependent tunneling structures Fe|Ge|Fe,[20] Fe|GaAs|Fe,[20] and Fe|ZnSe|Fe (Refs. 21,22) to understand the origin of the TMR in these structures, using the Layer KKR method. They found that the density of states and the net charge of the interfacial metal layer is very different from the other metal layers. This effect could be larger for physical magnitudes more sensible to the geometrical structure, as the anisotropy energy and orbital moment of the interface metal layer of similar systems.

Following that line of research, in this paper we present the results of *ab initio* spin-polarized fully relativistic (SPR) LMTO calculations[23,24] of the magnetization profile (spin and orbital moments), magnetic anisotropy energy and magnetic anisotropy of the orbital moment of bcc Fe/Ge and bcc Fe/GaAs (001) multilayers, using the von Barth-Hedin parametrization for the exchange-correlation potential[25] and the atomic sphere approximation (ASA). Particular attention has been paid to the convergence of the MAE with respect to the number of $\vec{k}$ points required for the Brillouin-zone integration. The underlying geometrical model for the FM/SC multilayers used in our calculations is described in the next section.

The method used to calculate the magnetocrystalline anisotropy energy is outlined in Sec. III. In particular, the force theorem method to calculate the electronic part of this energy. The results of the calculations are presented and discussed in Sec. IV. The magnetization profile (spin and orbital moment per layer and atom) and the magnetocrystalline anisotropy (energy and orbital moment) depend only slightly

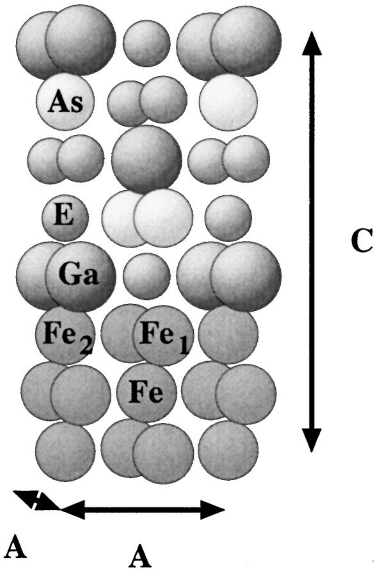

FIG. 1. Unit cell of the $Fe_3/(GaAs)_5$ multilayer. In this figure the c axis is oriented vertically. $A=\sqrt{2}a_{Fe}$ and $C=4a_{Fe}=2a_{GaAs}$.

on the kind of semiconductor. The orbital moments have been calculated in a spin-resolved way, which allowed us to test the relationship proposed by van der Laan between the MAE and the anisotropy of the orbital moment. The calculations have confirmed this relationship and therefore clarified to some extent the intertwining of MAE, orbital moment, spin-orbit interaction, and spin-polarization. In the last subsection this relationship is used to investigate the microscopic origin of the magnetic anisotropy of these FM/SC heterostructures.

II. GEOMETRICAL MODEL

The FM/SC multilayers were simulated as superlattices, using always five layers of GaAs (or GE) with a zinc-blende (or diamond) structure, and an odd number x of Fe layers per unit cell ($x=1$, 3, 5, 7, and 9) to keep the bcc structure of the Fe layers. These structures are denoted as Fe_x/Ge_5 and $Fe_x/(GaAs)_5$. This notation also means that the interface Fe layers are in contact with Ge and Ga atoms, respectively. The corresponding unit cell of the $Fe_3/(GaAs)_5$ multilayer is shown in Fig. 1, with the plane of atomic layers oriented horizontally. Several so-called empty spheres have been added for the LMTO calculations to represent some open regions of the unit cell. For all multilayers, the same lattice parameters, $a_{Ge}=a_{GaAs}=5.65$ Å and $a_{Fe}=2.825$ Å, have been used, assuming a perfect matching of the bcc Fe layers and diamond Ge or zinc-blende GaAs layers, respectively.

III. CALCULATION OF THE MAE

The magnetocrystalline anisotropy energy is the energy change due to a change of the magnetization direction and determines the spontaneous direction of the magnetization. There are two contributions to the magnetocrystalline anisotropy energy: the magnetic dipolar and the electronic band structure. The first comes from the classical magnetic dipolar interaction and, except for systems with a large anisotropy, it is much smaller than the second one. Van Vleck already pointed out that the physical origin of the electronic magnetocrystalline anisotropy energy and the orbital moment is the spin-orbit coupling.[26] Brooks and Fletcher applied the ideas of Van Vleck to itinerant ferromagnets using a semiempirical band structure model.[27,28] Nowadays it is well established that the electronic contribution and the orbital moment come from the simultaneous occurrence of spin-orbit coupling and spin polarization. For that reason, calculations of the orbital moment and the electronic magnetocrystalline anisotropy energy of bulk materials,[29–37] transition-metal thin film monolayers and multilayers,[34,38–44] and transition-metal alloys[45–47] from first principles became possible only after the development of spin-polarized relativistic band structure methods.

The experimental results of the MAE for bulk materials,[48,49] transition-metal thin film multilayers[50,51] and transition-metal ordered alloys[52,53] and the calculations of the MAE of these materials showed the smallness of the anisotropy energy, about 10^{-6} eV/atom for bulk Fe, Co, and Ni and 10^{-3}–10^{-4} eV/atom for transition-metal multilayers and ordered alloys, and also showed that this quantity is very sensitive to the details of the electronic structure. As a consequence, it depends on the approximations and numerical techniques used.

The electronic magnetocrystalline anisotropy energy, also called spin-orbit induced electronic MAE, is the difference between the total electronic energies for two different magnetization directions. In the case of magnetizations $\vec{M}$ parallel and perpendicular to the c axis $\hat{c}$ of the studied multilayers (this axis is perpendicular to the plane of the layers) the electronic magnetocrystalline anisotropy energy is given by

$$\Delta E=E(\vec{M}\|\hat{c})-E(\vec{M}\perp\hat{c}). \tag{1}$$

A straightforward calculation of the electronic MAE would require the self-consistent calculation of the total energy in the spin-polarized fully relativistic scheme, for both directions of the magnetization, which is a very demanding computational task for these FM/SC multilayers. Instead of the total energy method, the so-called force theorem method has been used.[54,55] This approximate method consists in computing the electronic MAE as the difference between the band energies for two different magnetization directions, obtained in calculations which consist in performing only one spin-polarized fully relativistic iteration, but using the charge density obtained in a self-consistent spin-polarized scalar relativistic calculation. The band energy is the sum of the occupied single-particle energies. In our case we have calculated the band energy with the Blöchl corrections.[56] Then, neglecting terms in second order on the change of the density, the electronic MAE is given by

$$\Delta E=\sum_{i,\vec{k}}^{\text{occ}}\epsilon_i(\vec{M}\|\hat{c},\vec{k})-\sum_{i,\vec{k}}^{\text{occ}}\epsilon_i(\vec{M}\perp\hat{c},\vec{k}), \tag{2}$$

where $\vec{k}$ is a Bloch vector in the full BZ.[32,54,55] The orbital moments and their anisotropy have been also calculated in the same way as the band energies. In the literature the anisotropy energies obtained from the force theorem method and also from self-consistent calculations of the total energy are very similar to the experimental values for some cases, but also are a factor of 2 or 4 larger or smaller than the experimental values for other cases, or even they have the wrong sign. In general, the theoretical results agree more with the experimental ones for transition-metal thin film multilayers.

One of the main features of the MAE calculations is the mentioned smallness of this quantity. In the present LMTO calculations, the absolute MAE per unit cell of these systems is very small ($\sim 10^{-4}$–10^{-5} Ryd) compared with the total energy per unit cell ($\sim 10^4$ Ryd). This means that the total electronic energy obtained in self-consistent calculations must be converged with respect to the absolute value of the anisotropy energy itself. An energy convergence of at least 6×10^{-7} Ryd has been applied in all the self-consistent spin-polarized calculations, in the scalar relativistic ones, previous to the application of the force theorem, and in the fully relativistic ones, to calculate the total electronic energy. One requisite of the approximate force theorem is that the input density to the last spin-polarized scalar relativistic iteration ρ_{in} and the output density from the last spin-polarized scalar relativistic iteration ρ_{out} must be the same. This is only true in case of complete self-consistency. The spin-polarized scalar relativistic LMTO calculations have been made with a density convergence very high, at least 10^{-8} in atomic Rydbergs units. Finally, we have tested the reliability of the force theorem in these multilayers. For the same number of $\vec{k}$ points (1152) in the full Brillouin zone integration (BZ), the value of the MAE of $\mathrm{Fe}_3/\mathrm{Ge}_5$ obtained with the force theorem method and from a self-consistent calculation of the total energy in the spin-polarized fully relativistic scheme is -7.0×10^{-5} and -8.3×10^{-5} Ryd, respectively. There is, then, a relative difference of about 16%. The force theorem method is computationally more advantageous because it requires only one iteration for each orientation of the magnetic moments, but a self-consistent calculation requires, at least for the former multilayer, about 30–40 iterations. Hence, the balance between accuracy and computational effort favors the force theorem method for these multilayer systems.

In the force theorem method the number of $\vec{k}$ points within the full BZ has to be very large in order to obtain a stable (converged) value of the anisotropy energy. In the literature it is reported that for transition-metal thin film layers the force theorem MAE value is stable when sampling is done for, at least, 10^4 $\vec{k}$ points within the full BZ.[34,38–42] For these films the anisotropy energy has a value of about 10^{-3}–10^{-4} eV/atom. This is the same order of magnitude as for the present FM/SC multilayers. The dependence on the number of $\vec{k}$ points used in the force theorem type calculations of the electronic anisotropy energy and of the band energies for magnetizations parallel and perpendicular to the c axis, is shown in Fig. 2 for the $\mathrm{Fe}_3/\mathrm{Ge}_5$ and $\mathrm{Fe}_3/(\mathrm{GaAs})_5$ multilayers. The band energies have been rigidly shifted, because they are of the order of 10 Ryd and the electronic MAE is about 10^{-5} Ryd. The band energies and the electronic anisotropy energy reach stable values for about 10^3 $\vec{k}$ points. Similar results have been obtained for the other multilayers, except that for the biggest multilayers it is necessary to use about 10^4 $\vec{k}$ points.

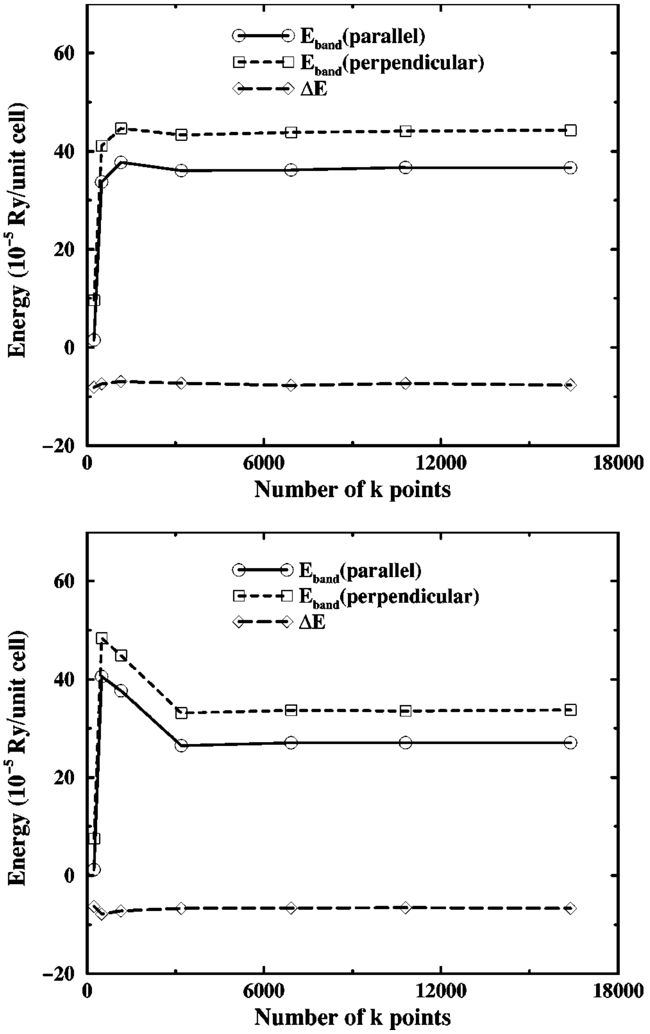

FIG. 2. Band energies for magnetizations parallel and perpendicular to the c axis, both shifted by the same quantity D, and electronic MAE per unit cell obtained with the force theorem in SPR-LMTO calculations of the $\mathrm{Fe}_3/\mathrm{Ge}_5$ (top) and $\mathrm{Fe}_3/(\mathrm{GaAs})_5$ (bottom) multilayers, as a function of the number of $\vec{k}$ points within the full BZ used in the calculations.

The so-called magnetic dipolar contribution to the MAE has been computed by means of the Ewald sum method.[57] If all the magnetic moments of the atoms are parallel to the direction $\hat{n}$, then the magnetic dipole-dipole interaction energy for this direction is given, in atomic Rydbergs units, by

$$E_d(\hat{n})=\sum_{q,q'}\frac{m_q m_{q'}}{c^2}M_{qq'}, \tag{3}$$

$$M_{qq'}=\sum_{\vec{R}}\frac{1}{|\vec{R}+\vec{q}-\vec{q'}|^3}\left(1-3\frac{(\vec{R}+\vec{q}-\vec{q'})\cdot\hat{n}}{|\vec{R}+\vec{q}-\vec{q'}|^2}\right), \tag{4}$$

where q and q′ denote the atom positions in one unit cell, m_q is the total magnetic moment in an atomic sphere around site

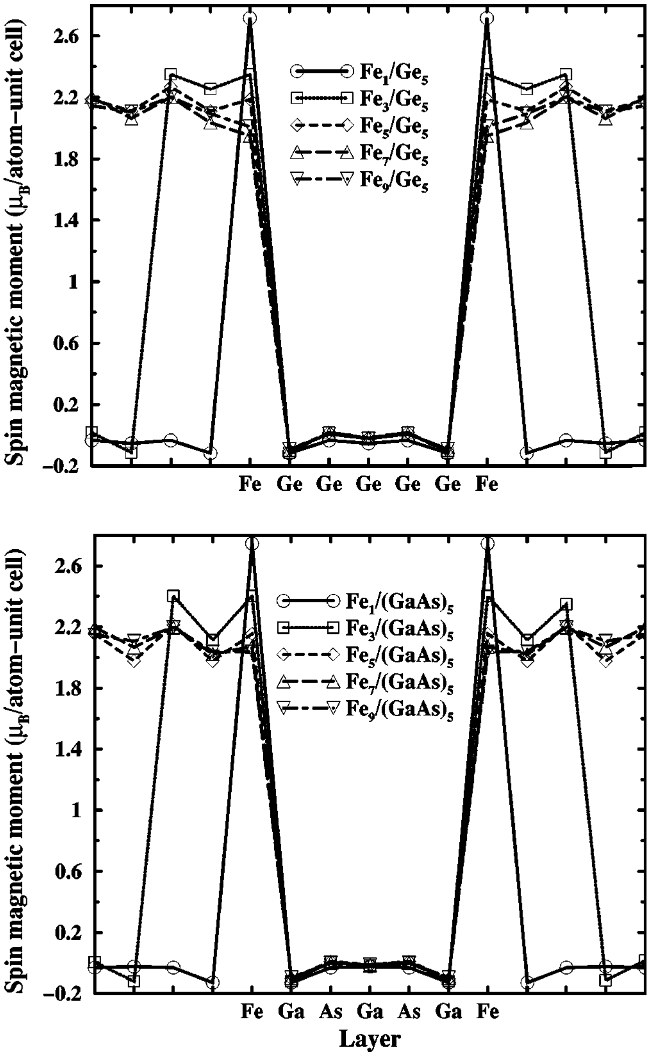

FIG. 3. Spin magnetic moment per atom and unit cell in the layers of $\mathrm{Fe}_x/\mathrm{Ge}_5$ (top) and $\mathrm{Fe}_x/(\mathrm{GaAs})_5$ (bottom) multilayers ($x = 1$, 3, 5, 7, and 9), obtained in spin-polarized scalar relativistic LMTO calculations.

q and $\vec{R}$ is a lattice site. The sum runs over all the lattice sites $\vec{R}$ except over that for which the denominator in Eq. (4) is zero. The dipolar contribution to the MAE, Eq. (1), is the difference between $E_d(\vec{M}\|\hat{c})$ and $E_d(\vec{M}\perp\hat{c})$.

IV. RESULTS AND DISCUSSION

A. Magnetization profile

The spin magnetic moments per atom and unit cell in the different layers of the investigated multilayers, obtained by spin-polarized scalar relativistic calculations, are shown in Fig. 3. The difference between the spin magnetic moments obtained in these type of calculations and the ones obtained in SPR calculations (only 1 iteration) is only about 10^{-3} μ_B or less and $\sim 10^{-2}$ μ_B for the interface Fe layers. The spin magnetic moment profile of the Fe layers depends slightly on the type of semiconductor layers, but this dependence decreases when increasing the Fe thickness of the multilayers, except for the interface Fe layers. The spin magnetic moment per atom in the Fe layers, especially in the interface Fe layers, decreases when the Fe thickness is increased, except for the last two thickest multilayers, for which, obviously, the limiting case has been reached. In *ab initio* FLAPW calculations on Fe/ZnSe superlattices with one and three Fe layers this supression of the magnetism was also observed.[18] This trend of a reduced average magnetization as a result of an increased number of Fe layers has been also experimentally observed in Fe films on ZnSe.[7] The reason of this general decrease of the magnetization in all the Fe layers is that the interfacial bonding effect, which increases the magnetism with respect to the bulk, diminishes with respect to the bulk contribution when increasing the Fe thickness. This idea is supported by several findings: the spin magnetic moment in the innermost Fe layers tends to the spin magnetic moment of bulk bcc Fe, about 2.15–2.2 μ_B, when increasing the number of Fe layers. The magnetization profile in the Fe layers in multilayers with 5, 7, and 9 Fe layers is practically the same, except in the interface Fe layers of the multilayers with 5 Fe layers. For the last two thickest multilayers the interfacial bonding effect is very small.

The reduction of the spin magnetic moment is much more pronounced for the interface Fe layers than for the other Fe layers when the Fe thickness increases and this deserves more comments. In the paper of Continenza *et al.*,[18] the decrease of the spin magnetic moment in the interface Fe layer was explained as an effect of the increase of the coordination number around the interface Fe atoms: it changes from four to six atoms, four of them Fe atoms, when passing from superlattices with one Fe layer to those with three Fe layers.[18] The theory of itinerant-electron ferromagnetism of Slater and Stoner[58,59] indicates that a reduced coordination narrows the *d* bands. This increases the density of states at the Fermi level and, in that way, the tendency towards spontaneous magnetism. This explanation could also be valid for the studied FM/SC multilayers with one and three Fe layers, because the same changes of the spin magnetic moment and of the coordination number of the interface Fe atoms are present for these. However, this idea does not explain the results for the other multilayers, because the coordination number of the interface Fe atoms does not increase when passing from multilayers with three Fe layers to multilayers with a larger Fe thickness, but the spin magnetic moment in the interface Fe layers decreases. According to the arguments based on a reduced coordination number, the spin magnetic moment should also be bigger in the interface Fe layers than in the innermost Fe layers, which is only true for the multilayers of three Fe layers, but not for the other multilayers. Finally, the spin magnetic moment in the interface Fe layers of multilayers with seven and nine Fe layers is practically the same. All this suggests that the explanation for the reduction of the magnetization in the interface Fe layers when increasing the number of Fe layers from 3 to 9 is that the hybridization is increasing with the Fe thickness, except in the two thickest multilayers, where it is very similar.

The spin magnetic moment of the semiconductor layers is quite small, but nevertheless unambigously different from

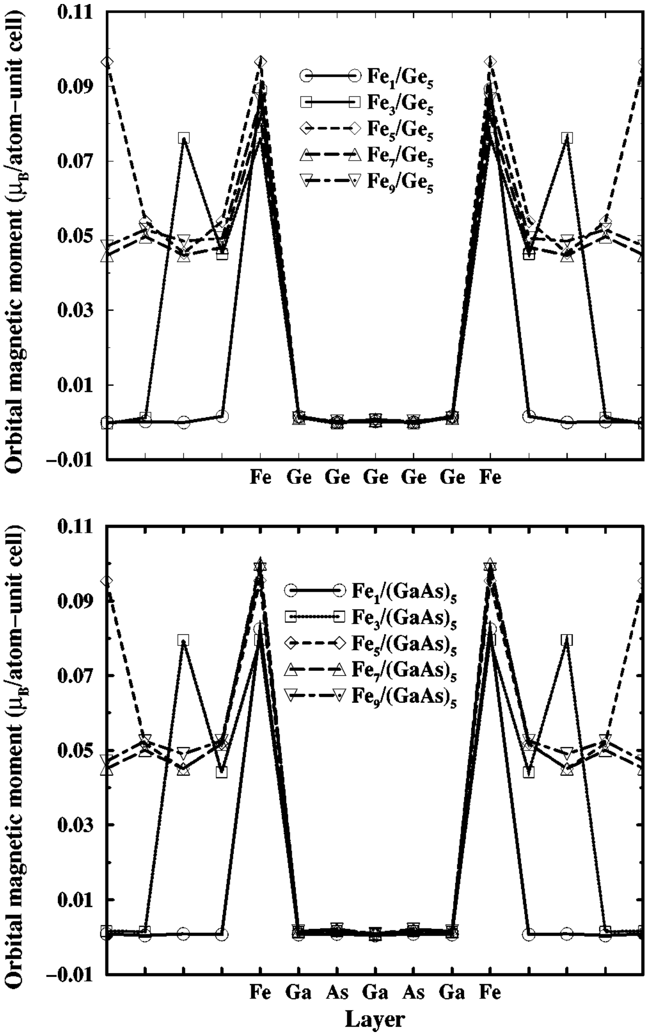

FIG. 4. Orbital magnetic moment per atom and unit cell in the layers of Fe_x/Ge_5 (top) and $Fe_x/(GaAs)_5$ (bottom) multilayers ($x = 1$, 3, 5, 7, and 9), obtained in SPR-LMTO calculations (only 1 iteration), using 16384 $\vec{k}$ points within the full BZ.

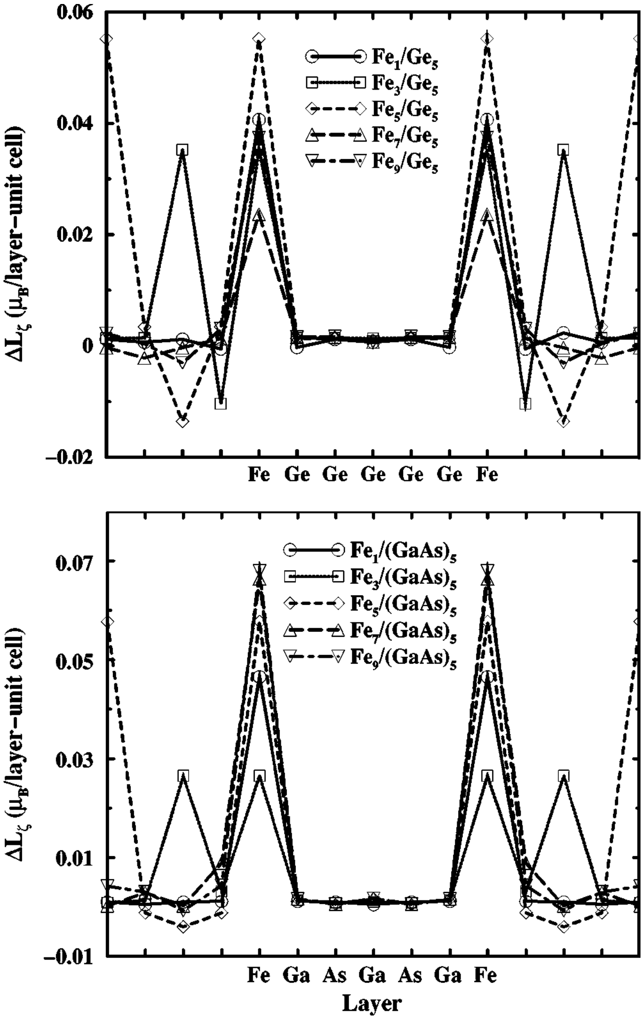

FIG. 5. Anisotropy of the orbital moment per layer and unit cell, ΔL_ζ, Eq. (5), of Fe_x/Ge_5 (top) and $Fe_x/(GaAs)_5$ (bottom) multilayers ($x = 1$, 3, 5, 7, and 9), obtained in SPR-LMTO calculations (only 1 iteration), using 16384 $\vec{k}$ points within the full BZ.

zero, and it is practically independent of the number of Fe layers. For a particular multilayer, there are some oscillations of the spin magnetic moment in the Fe layers, due to interface effects between the ferromagnet and the semiconductor part of these structures. The magnitude of these oscillations is larger near the interface Fe layers. All these properties of the spin magnetic moment profile indicate that the magnetization of these systems is mainly dominated by the Fe layers, but with an influence coming from the FM/SC interfaces.

The orbital magnetic moments per atom and unit cell in the layers, obtained in SPR calculations (only 1 iteration, as in the force theorem method) for a magnetization parallel to the c axis and using 16384 $\vec{k}$ points within the BZ, are represented in Fig. 4. The orbital magnetic moment profile of these structures also depends on the number of Fe layers, but it scarcely depends on the type of semiconductor layers. The orbital magnetic moment at the Fe layers has a value between 0.05 and 0.10 in Bohr magnetons per atom, and it is practically zero in the semiconductor layers. In the interface Fe layers it has a certain dependence on the number of Fe layers, but in the other Fe layers depends very little on that number. In all these structures, the orbital magnetic moment has the biggest value in the interface Fe layer: it is about two times bigger than for the innermost Fe layers. Its oscillations are very small in the other Fe layers. This big difference between the orbital magnetic moment in the interface Fe layer and in the other Fe layers is obviously caused by the interface between the Fe layers and the semiconductor ones. Taking into account that there is a relationship between MAE and the anisotropy of the orbital moment, these results suggest that the interface Fe layers are probably, not necessarily, playing the main role in the origin of the magnetocrystalline anisotropy energy of these multilayers. This suggestion is confirmed by the plot of the anisotropy of the orbital moment per layer of these structures, in Fig. 5. The anisotropy of the orbital moment is defined in the present work as

$$\Delta L_{\zeta}=\langle L_{\zeta}^{\downarrow}\rangle_{\parallel}-\langle L_{\zeta}^{\uparrow}\rangle_{\parallel},$$
$$-[\langle L_{\zeta}^{\downarrow}\rangle_{\perp}-\langle L_{\zeta}^{\uparrow}\rangle_{\perp}]=\Delta_{\parallel}-\Delta_{\perp}, \qquad (5)$$

instead of the usual definition as the difference between the total orbital moments for two different magnetizations. $\langle L_{\zeta}^{\uparrow(\downarrow)}\rangle_{\parallel(\perp)}$ is the expectation value of the spin up (down) sub-band orbital moment when the magnetization is parallel (perpendicular) to the c axis and the quantity Δ_{α} is equal to

$$\Delta_{\alpha}=\langle L_{\zeta}^{\downarrow}\rangle_{\alpha}-\langle L_{\zeta}^{\uparrow}\rangle_{\alpha}. \qquad (6)$$

Finally, the subscript ζ indicates that the orbital moment is induced by the spin-orbit coupling. We have used this definition of the anisotropy of the orbital moment because, as we will show in the following section, in second order perturbation theory the MAE is, according to a recent proposal,[62] proportional to the anisotropy of the orbital moment defined on this way, instead of on the usual way.

As one can see from Fig. 5, the anisotropy of the orbital moment is also larger in the interface Fe layers than in the other Fe layers and it is practically zero in the semiconductor layers. The anisotropy of the orbital moment of the two interface Fe layers per unit cell represents, together, between 80–90% of the total anisotropy of the orbital moment per unit cell. In the case of multilayers with only one Fe layer, the anisotropy of the orbital moment of this layer, the interface Fe layer, is also about 90% of the total. In Sec. IV C we will explain that this anisotropy is closely related to the magnetocrystalline anisotropy of the energy. For instance, both anisotropies increase with the number of Fe layers of the system.

B. Magnetocrystalline anisotropy energy

In Fig. 6 the computed electronic and dipolar contributions to the MAE per unit cell are shown, together with the sum of both energies for the $\mathrm{Fe}_x/\mathrm{Ge}_5$ and $\mathrm{Fe}_x/(\mathrm{GaAs})_5$ multilayers, respectively. The electronic anisotropy energy was computed by means of the force theorem and using 16384 $\vec{k}$ points within the full BZ and it is negative in all the cases. This favors an orientation of the magnetization parallel to the c axis, i.e., perpendicular with respect to the plane of the layers. The anisotropy energy is found to increase in magnitude (is more negative), in general, when increasing the number x of Fe layers. On the other hand, the dipolar MAE is always positive, which means that it favors an in-plane orientation of the magnetization. Although it also increases in magnitude with the number of Fe layers, the resulting total MAE is negative. Hence, according to our calculations, these multilayers show perpendicular magnetism. However, more theoretical work should be done increasing the number of semiconductor layers and studying the influence of the geometry and atomic arrangement at the interface.

The total electronic MAE per unit cell obtained by means of the force theorem method has been divided into contributions per atom and also per layer, in order to find the microscopic origin of this energy. This division was done by separating Eq. (2) into the band energies from the different atoms of the unit cell.[44] The results for $\mathrm{Fe}_x/\mathrm{Ge}_5$ and $\mathrm{Fe}_x/(\mathrm{GaAs})_5$ are shown in Fig. 7. This figure shows the electronic anisotropy energies per layer and unit cell obtained using the biggest number of $\vec{k}$ points, 16384, within the full BZ. We have also studied the convergence of the MAE of the invidivual layers with respect to the number of $\vec{k}$ points and we have found that there is not a clear convergence or stability of these individual anisotropy energies. Except in the case of multilayers with only one Fe layer, the electronic magnetocrystalline anisotropy energy of the interface Fe layer is the biggest one and negative, the same sign as the total one. The contributions from other layers are also important, although smaller. In addition, there are two interface Fe layers per unit cell with the same MAE, except in the multilayers with only one Fe layer. As a consequence, the total contribution from both layers altogether is much more important than the contribution from all the other layers. For similar calculations on Fe/Cu thin film layers it was also reported that the main contribution to the total MAE comes from the interface ferromagnetic layers.[44]

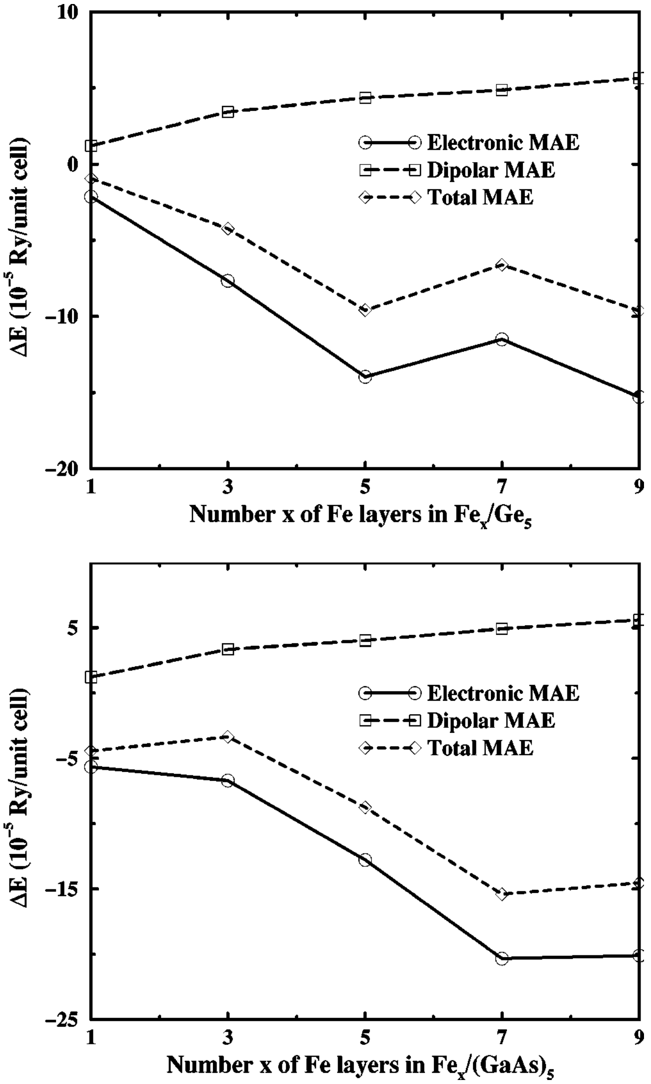

FIG. 6. Electronic MAE per unit cell, ΔE, obtained with the force theorem in SPR-LMTO calculations using 16384 $\vec{k}$ points within the full BZ, dipolar MAE and total MAE for $\mathrm{Fe}_x/\mathrm{Ge}_5$ (top) and $\mathrm{Fe}_x/(\mathrm{GaAs})_5$ (bottom) multilayers ($x=1$, 3, 5, 7, and 9).

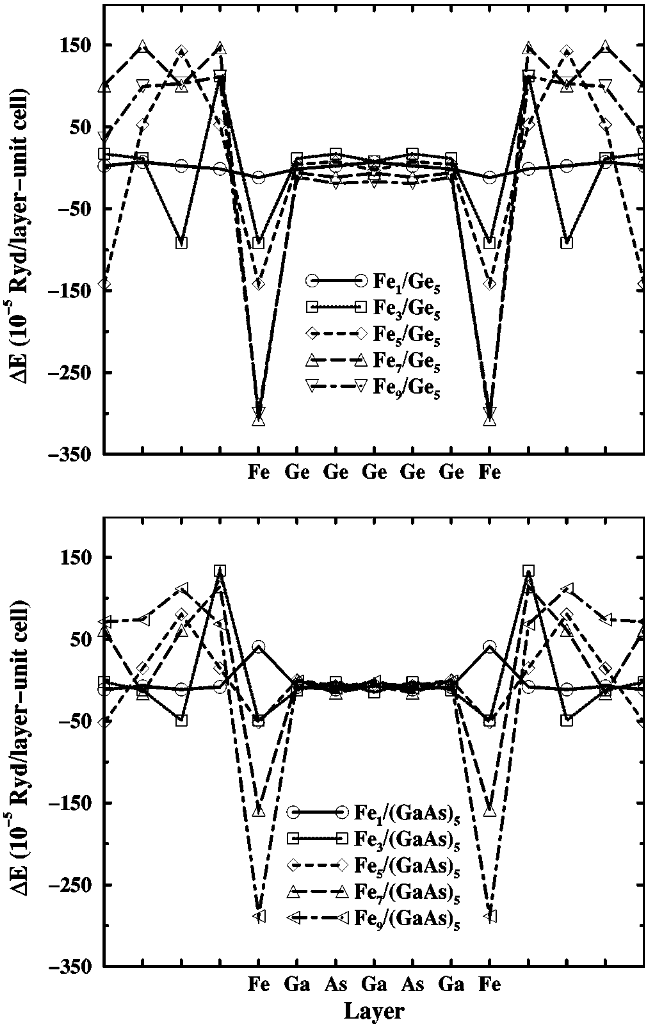

FIG. 7. Electronic MAE per layer and unit cell, ΔE, obtained with the force theorem in SPR-LMTO calculations using 16384 $\vec{k}$ points within the full BZ, for Fe$_x$/Ge$_5$ (top) and Fe$_x$/(GaAs)$_5$ (bottom) multilayers ($x = 1$, 3, 5, 7, and 9).

Finally, we have also examined the influence of the other side of the interface, the semiconductor layers in contact with the Fe layers. A comparison of the electronic MAE per layer and unit cell of Fe$_5$/(GaAs)$_5$ and Fe$_5$/(AsGa)$_5$ for 16384 $\vec{k}$ points within the full BZ, is made in Fig. 8. The electronic MAE per unit cell of these multilayers is -12.8 and -10.4×10^{-5} Ryd, respectively. According to the results shown in this figure, the anisotropy energy of the interface Fe layer in Fe$_5$/(AsGa)$_5$ is much bigger than the corresponding quantity in Fe$_5$/(GaAs)$_5$. This means that the bonding in the ferromagnetic-semiconductor interface, Fe-Ga against Fe-As bonding, plays an important role for the magnetocrystalline anisotropy energy.

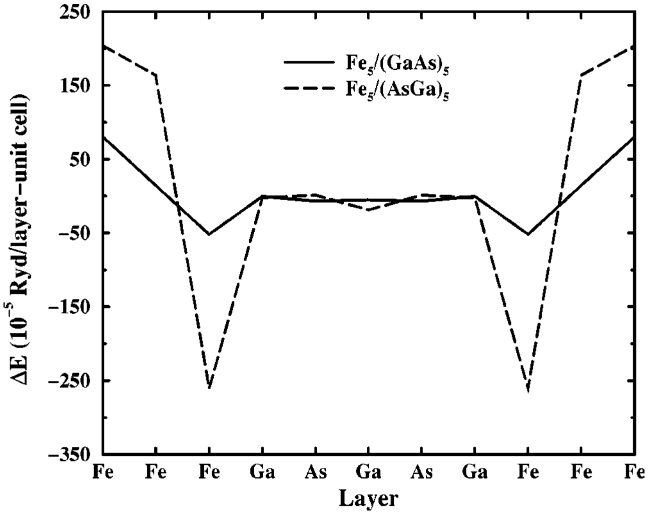

FIG. 8. Electronic MAE per layer and unit cell, ΔE, obtained with the force theorem in SPR-LMTO calculations using 16384 $\vec{k}$ points within the full BZ, for Fe$_5$/(GaAs)$_5$ and Fe$_5$/(AsGa)$_5$ multilayers.

C. Relationship between the MAE and the orbital moment: van der Laan's conjecture

Using second order perturbation theory, and considering the spin-orbit interaction as a perturbation, Bruno derived an expression which relates the MAE to the anisotropy of the orbital moment. He also showed that if the spin up sub-band is completely filled, then the change in energy due to a change in the orientation of the magnetization is proportional to the change of the total orbital moment.[60] Wang *et al.* showed that there is also a contribution due to a spin-flip term.[61] Van der Laan has extended Bruno's approach, taking also into account the spin-flip term.[62] This second term is proportional to $(\xi/\Delta E_{\mathrm{ex}})^2$, where ξ is the spin-orbit coupling parameter of the ground state of the total system and ΔE_{ex} is the energy separation of the two spin sub-bands. In $3d$ compounds ξ is between 40 and 80 meV and ΔE_{ex} is about a few eVs. Hence, this term is much smaller than the first one for these multilayers and it will not be considered.

Van der Laan's conjecture states that the second order change in the energy due to the spin-orbit coupling is equal, for a magnetization along the unit vector of the spin magnetic moment $\hat{n} = \vec{S}/S$, to

$$\delta E(\hat{n}) = -\frac{\xi}{4}[\langle L_\zeta^\downarrow\rangle_{\hat{n}} - \langle L_\zeta^\uparrow\rangle_{\hat{n}}] = -\frac{\xi}{4}[\langle L_\zeta\rangle_{\hat{n}} - 2\langle L_\zeta^\uparrow\rangle_{\hat{n}}], \tag{7}$$

where $\langle L_\zeta^{\uparrow(\downarrow)}\rangle_{\hat{n}}$ is the expectation value of the spin up (down) sub-band orbital moment when the magnetization is along the vector $\hat{n}$.[62] Then, the electronic MAE in Eq. (1) is given by

$$\begin{aligned}\Delta E &= -\frac{\xi}{4}[\langle L_\zeta^\downarrow\rangle_\parallel - \langle L_\zeta^\uparrow\rangle_\parallel] + \frac{\xi}{4}[\langle L_\zeta^\downarrow\rangle_\perp - \langle L_\zeta^\uparrow\rangle_\perp] \\ &= -\frac{\xi}{4}[\Delta_\parallel - \Delta_\perp] = -\frac{\xi}{4}\Delta L_\zeta .\end{aligned} \tag{8}$$

In Bruno's model the spin up sub-band is assumed to be filled and then $\langle L_\zeta^\uparrow\rangle_{\hat{n}} = 0$ and $\delta E(\hat{n})$ is proportional to the total orbital moment $\langle L_\zeta\rangle_{\hat{n}}$.[60] In this case the anisotropy energy is equal to

$$\Delta E = -\frac{\xi}{4}[\langle L_{\zeta}\rangle_{\parallel} - \langle L_{\zeta}\rangle_{\perp}]. \tag{9}$$

These formulas can be tested by means of first principles calculations of the MAE and orbital moments. The idea is to compare the energy ΔE calculated from first principles, by means of the force theorem, and the ones obtained using the two former perturbative formulas. This implies the additional calculation of the spin up and down orbital moments and the spin-orbit coupling parameter ξ, also in a single SPR iteration and using 16384 $\vec{k}$ points within the full BZ. It is important to clarify that this conjecture applies to the electronic MAE and the orbital moment of the whole system, and not necessarily to the electronic MAE and orbital moment of a particular atom or layer.

In the calculations of the anisotropy energy on the basis of Eqs. (8) and (9), the value of ξ_{3d} of Fe obtained in a single SPR iteration of the corresponding multilayer [0.0044 Ryd for $\mathrm{Fe}_1/\mathrm{Ge}_5$ and $\mathrm{Fe}_1/(\mathrm{GaAs})_5$, and 0.0045 Ryd for the remaining multilayers] has been used, because the Fe atoms are the main source of the magnetocrystalline anisotropy of these multilayers. This approach is justified by a detailed spatial analysis of the origin of the MAE. In Eq. (8) there are two important factors: the spin-orbit coupling parameter and the difference $\Delta_{\parallel} - \Delta_{\perp}$. For instance, in the $\mathrm{Fe}_1/(\mathrm{GaAs})_5$ multilayer there are two Fe atoms, three Ga atoms and two As atoms per unit cell and the contribution to $\Delta_{\parallel} - \Delta_{\perp}$ per atom and unit cell obtained in the SPR-LMTO calculations is 0.023, 0.001, and $0.001\mu_B$ for Fe, Ga, and As, respectively. The spin-orbit coupling parameter obtained in a single SPR-LMTO iteration for this multilayer is about 0.02 Ryd for the p valence electrons of Ga and As while for the $3d$ electrons of Fe it is 0.0044 Ryd. Hence, the Fe atoms of the unit cell contribute, according to Eq. (8), approximately 90% to the MAE per unit cell if the spin-orbit coupling parameter of Fe is used for all the layers, and about 75% if the proper values of the spin-orbit coupling parameter of Ga and As are also considered. For the other multilayer systems considered here the number of Fe atoms per unit cell and their relative individual contributions to the magnetocrystalline energy are bigger than in $\mathrm{Fe}_1/(\mathrm{GaAs})_5$ and hence, the approach is even more justified.

A comparison of the results of calculating the anisotropy energy in three different ways is shown in Fig. 9. For all the multilayers the agreement between the results based on the force theorem and the ones based on van der Laan's expression is good, especially for the $\mathrm{Fe}_x/(\mathrm{GaAs})_5$ multilayers. On the other hand, the agreement with the anisotropy energy calculated by means of Eq. (9) is worse, but the sign and the order of magnitude are the same. These results confirm van der Laan's perturbative formula[62] and also the necessity of taking into account the spin up and down sub-band orbital moments and not only the total orbital moment, to understand the relationship between the electronic MAE and the anisotropy of the orbital moment.

D. Microscopic origin of the MAE and van der Laan's conjecture

An analysis of van der Laan's formula is very useful in order to find the detailed microscopic origin of the electronic magnetocrystalline anisotropy energy of these systems. Because of the good agreement between the MAE data based on van der Laan's expression, Eq. (8), and the ones based on the force theorem (see Fig. 9), it is reasonable to extend the qualitative conclusions of this analysis to the MAE obtained by means of the force theorem. In the following, an analysis of the MAE based on van der Laan's expression and obtained in SPR-LMTO calculations for the $\mathrm{Fe}_5/(\mathrm{GaAs})_5$ multilayer, using 16384 $\vec{k}$ points within the full BZ, is performed. The qualitative conclusions drawn from this are also valid for all the other FM/SC multilayers.

In Table I we present in a layer-resolved way several quantities which are related to the spin up and down orbital moments for both magnetization directions. From Eq. (8) one can see, in particular, that the MAE is primarily deter-

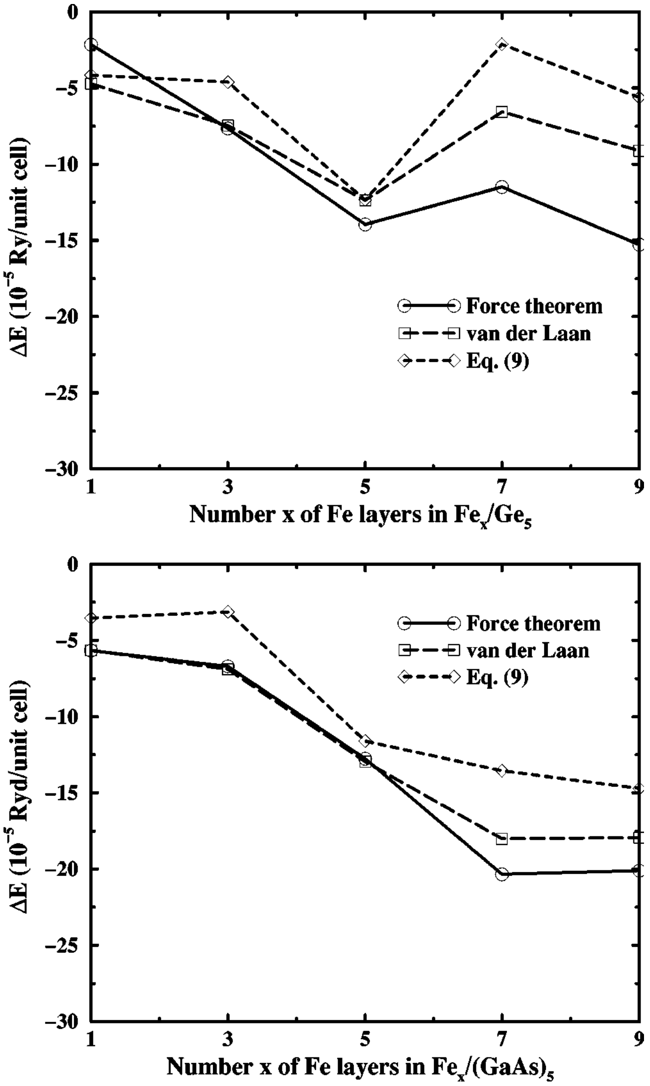

FIG. 9. Electronic magnetocrystalline anisotropy energies per unit cell, ΔE, obtained in SPR-LMTO calculations for $\mathrm{Fe}_x/\mathrm{Ge}_5$ (top) and $\mathrm{Fe}_x/(\mathrm{GaAs})_5$ (bottom) multilayers ($x=1$, 3, 5, 7, and 9), using 16384 $\vec{k}$ points within the full BZ, by means of the force theorem, van der Laan's perturbative formula, Eq. (8), and supposing that the MAE is proportional to the difference between the total orbital moments, i.e., using Eq. (9).

TABLE I. Spin up and down orbital moments, and other quantities per layer and unit cell (in μ_B units) related to van der Laan's expression, Eq. (8), for magnetizations parallel and perpendicular to the c axis. These data have been obtained in SPR-LMTO calculations for the $Fe_5/(GaAs)_5$ multilayer, using 16384 $\vec{k}$ points within the full BZ.

x	$\langle L^{\uparrow}\rangle_{\parallel}$	$\langle L^{\downarrow}\rangle_{\parallel}$	$\Delta_{\parallel}$	$\langle L^{\uparrow}\rangle_{\perp}$	$\langle L^{\downarrow}\rangle_{\perp}$	$\Delta_{\perp}$	$\Delta^{\uparrow}$	$\Delta^{\downarrow}$	$-\Delta L_{\zeta}$
Fe	−0.0630	0.2538	0.3168	−0.0537	0.2054	0.2591	−0.0093	−0.0485	−0.0577
Fe	−0.0686	0.1725	0.2411	−0.0768	0.1655	0.2423	0.0081	−0.0070	0.0012
Fe	−0.0612	0.1514	0.2126	−0.0586	0.1580	0.2167	−0.0026	0.0066	0.0040
Fe	−0.0686	0.1725	0.2411	−0.0768	0.1655	0.2423	0.0081	−0.0070	0.0012
Fe	−0.0630	0.2538	0.3168	−0.0537	0.2054	0.2591	−0.0093	−0.0485	−0.0577
Ga	−0.0076	0.0093	0.0169	−0.0071	0.0083	0.0153	−0.0006	−0.0010	−0.0016
As	−0.0164	0.0181	0.0345	−0.0167	0.0173	0.0340	0.0003	−0.0008	−0.0005
Ga	−0.0078	0.0086	0.0164	−0.0072	0.0076	0.0148	−0.0006	−0.0011	−0.0017
As	−0.0164	0.0181	0.0345	−0.0167	0.0173	0.0340	0.0003	−0.0008	−0.0005
Ga	−0.0076	0.0093	0.0169	−0.0071	0.0083	0.0153	−0.0006	−0.0010	−0.0016
Total	−0.3803	1.0674	1.4477	−0.3743	0.4830	1.3328	−0.0060	−0.1089	−0.1149

mined by the quantity $-\Delta_{\parallel}+\Delta_{\perp}$, which can be decomposed in layer contributions, in spin up and down parts and also according to the angular momentum character (s, p, or d) of the valence electrons. Table I shows that the interface Fe layer has the biggest value of $-\Delta_{\parallel}+\Delta_{\perp}$: -0.0577 in μ_B units per unit cell. Because there are two interface Fe layers per unit cell, these layers are responsible for about 99% of the MAE per unit cell. The quantity $-\Delta_{\parallel}+\Delta_{\perp}$ can be divided in spin up and down contributions, according to

$$\Delta^{\uparrow}=\langle L_{\zeta}^{\uparrow}\rangle_{\parallel}-\langle L_{\zeta}^{\uparrow}\rangle_{\perp}, \tag{10}$$

$$\Delta^{\downarrow}=\langle L_{\zeta}^{\downarrow}\rangle_{\perp}-\langle L_{\zeta}^{\downarrow}\rangle_{\parallel}. \tag{11}$$

The total spin down contribution per unit cell $\Delta^{\downarrow}$, is $-0.1089\mu_B$. This is about 95% of the MAE. On the other hand, the spin down contribution of one interface Fe layer is $-0.0485\mu_B$, which means that the spin down electrons in the interface Fe layers contribute about 84% of the total MAE.

The contribution of the $3d$ electrons of one interface Fe layer to the MAE, $-\Delta_{\parallel}+\Delta_{\perp}$, is $-0.0567\mu_B$. This is obviously the main part of the contribution of this layer, $-0.0577\mu_B$. These results confirm quantitatively that the main role in the MAE of $3d$ transition-metal layer systems is played by the $3d$ electrons. Finally, the contribution of the $3d$ electrons of an interface Fe layer can be divided, in addition, into spin up and down contributions, leading to -0.0093 and $-0.0474\mu_B$, respectively. This means that the $3d$ spin down electrons of the two interface Fe layers contribute about 82% to the electronic MAE per unit cell.

Table II contains the occupation numbers for the $3d$ spin down levels of the two inequivalent Fe atoms of the unit cell which form the interface Fe layer. The $3d$ spin down orbital

TABLE II. Occupations numbers n_{m_l} of the $3d$ spin down m_l levels for magnetizations parallel and perpendicular to the c axis and contributions (in μ_B units) to the MAE per unit cell, $\Delta^{\downarrow}_{m_l}=m_l[n^{\perp}_{m_l}-n^{\parallel}_{m_l}]$, of these levels of the two inequivalent Fe atoms of the unit cell which form the interface Fe layer of the $Fe_5/(GaAs)_5$ multilayer (see Fig. 1). These data have been obtained in SPR-LMTO calculations, using 16384 $\vec{k}$ points within the full BZ. In the last two rows, the differences between some of these quantities are shown.

	Fe_1			Fe_2		
m_l	$n^{\parallel}_{m_l}$	$n^{\perp}_{m_l}$	$\Delta^{\downarrow}_{m_l}$	$n^{\parallel}_{m_l}$	$n^{\perp}_{m_l}$	$\Delta^{\downarrow}_{m_l}$
−2	0.4127	0.4021	0.0212	0.4083	0.4260	−0.0354
−1	0.4612	0.4388	0.0224	0.4765	0.4457	0.0308
0	0.3309	0.4183	0.0000	0.3848	0.4264	0.0000
1	0.4982	0.4597	−0.0385	0.5112	0.4691	−0.0420
2	0.4548	0.4387	−0.0322	0.4544	0.4676	0.0264
Total	2.1578	2.1576	−0.0271	2.2352	2.2348	−0.0202
	$n^{\parallel}_{m_l}-n^{\parallel}_{-m_l}$	$n^{\perp}_{m_l}-n^{\perp}_{-m_l}$	$\Delta^{\downarrow}_{m_l}+\Delta^{\downarrow}_{-m_l}$	$n^{\parallel}_{m_l}-n^{\parallel}_{-m_l}$	$n^{\perp}_{m_l}-n^{\perp}_{-m_l}$	$\Delta^{\downarrow}_{m_l}+\Delta^{\downarrow}_{-m_l}$
1	0.0370	0.0209	−0.0161	0.0347	0.0234	−0.0112
2	0.0421	0.0366	−0.0110	0.0461	0.0416	−0.0090

moment is the sum over the quantum number m_l multiplied by the occupation of the corresponding level for the $3d$ spin down levels. This orbital moment is positive for both magnetization directions because the $m_l = 1$ and 2 levels are more populated than the $m_l = -1$ and -2 levels, respectively, for a given magnetization's direction (the comparison is made here between the levels with the same absolute value of m_l). The change on the total energy due to these $3d$ electrons is negative for both directions. However, the differences between the occupations of the $m_l = 1$ and -1 levels, $n_1 - n_{-1}$, and the $m_l = 2$ and -2 levels, $n_2 - n_{-2}$, are a bit larger when the magnetization is parallel to the c axis, compared with the in-plane orientation (see Table II). Therefore, and according to this table, the $3d$ spin down orbital moment of the interface Fe layer is smaller for the perpendicular magnetization, $0.2007\mu_B$, than for the parallel one, $0.2481\mu_B$. The difference between these two moments is the $3d$ spin down contribution to the MAE of one interface Fe layer and is equal to $-0.0474\mu_B$. The number of $3d$ spin down electrons in the interface Fe layer is practically the same for both directions. This means that the electronic MAE comes mainly from a *rearrangement* of the occupations of certain $3d$ spin down levels in the interface Fe layers. According to the occupation analysis, about seven electrons per unit cell of the multilayer system $\mathrm{Fe}_5/(\mathrm{GaAs})_5$ are involved in this rearrangement and are responsible for about 82% of the MAE per unit cell of this multilayer. This also applies essentially to all the remaining multilayers considered here. Finally, the contributions of the two inequivalent atoms of the interface Fe layer, Fe_1, and Fe_2, are different, -0.0271 and $-0.0203\mu_B$, respectively, because they do not have the same neighbors, as it can be noticed in Fig. 1. Both atoms have equivalent Ga neighbors, but Fe_1 has As as a neighbor in the next nearest layer while in the case of Fe_2 there is an empty sphere in its next nearest layer. This means that the atoms of the second semiconductor layer, with respect to the interface Fe layer, are also playing some role in the anisotropy energy of these structures.

V. CONCLUSIONS

We have found that the magnetization profile of the investigated FM/SC multilayers does not depend strongly on the kind of semiconductor atoms. The spin magnetic moments of the different Fe layers are similar, with small oscillations. This is also true for the orbital magnetic moment, except for the orbital moment in the interface Fe layer, which is about two times bigger than in the other Fe layers. In the semiconductor layers the spin magnetic moment is very small, but different from zero, and the orbital magnetic moment is practically zero. The magnetocrystalline anisotropy of the energy and of the orbital moment comes mainly (~ 80–$90\,\%$) from the interface Fe layers. The MAE is of the order of 1 meV/unit cell, similar to the MAE of some transition-metal thin film layers.[34,38–44] We have also obtained in our LMTO calculations a spontaneous magnetization for the FM/SC structures perpendicular to the plane of the layers. This feature increases with the number of Fe layers. The study of the MAEs per layer revealed that the interface Fe layer (there are two interface Fe layers per unit cell) is the main source for the MAE in the unit cell.

Van der Laan's conjecture about the relationship between the electronic MAE and the anisotropy of the orbital moment is very well satisfied in these systems. In this conjecture, the spin up and down sub-band orbital moments must be considered and not only the total orbital moment. The confirmation of this conjecture, as far as we know, has not been reported in any other *ab initio* calculations.

It has been explained in detail, by means of *ab initio* calculations and van der Laan's conjecture, that the main source of the magnetic anisotropy of these multilayers are the $3d$ spin down electrons of the interface Fe layers, and that the mechanism is a delicate balance between the occupations of certain $3d$ spin down levels for both magnetizations directions, in which only about seven valence electrons per unit cell play a role.

Some experimental works reported in-plane magnetic anisotropies of epitaxial Fe thin films on GaAs (001) substrate.[6,8,11] These materials are different in structure from the FM/SC materials studied in this paper. The ferromagnet-semiconductor interface is obviously very different. The present systems are superlattices with an ideal matching between the bcc Fe layers and the semiconductor ones. According to another experiment, the magnetocrystalline anisotropy energy of epitaxially grown Fe films on GaAs also favors a magnetization in the plane of the layers,[63] but it favors a magnetization perpendicular to that plane when fcc-Au layers are deposited on the Fe layers.[64] In the first case there is only one Fe interface and in the second case, there are two interfaces. The present calculations have shown that the interface, in particular the ferromagnetic-semiconductor interface, is the main source for the magnetocrystalline anisotropy of these structures and in the light on this conclusion, the former experimental results could be understood as follows. For one interface, the dipolar contribution, which favors an in-plane magnetization, overcomes the electronic contribution due to the interface, which favors a perpendicular magnetization. For two interfaces, there are two contributions which favor a perpendicular orientation and they overcome the dipolar contribution.

Further work must be done in the future. It will be interesting to know how much the MAE changes with the variation of the lattice spacing of these multilayers and with the roughness of the ferromagnetic-semiconductor interface. Another important point is to clarify whether the ferromagnet-semiconductor interface is playing the main role in the magnetic anisotropy of these structures. This can be figured out by calculating the magnetic anisotropy of two different type of systems: the same superlattices as studied here, but changing the semiconductor part, for instance, ZnSe instead of GaAs, and a superlattice composed by three type of layers: Fe, semiconductor, Ge or GaAs, and layers composed by empty spheres. In the first system there are still two Fe-semiconductor interfaces, but in the second system there is only one. Calculations of the electronic structure of SC/FM/Au systems could clarify if the origin of the perpendicular magnetic anisotropy is the number of Fe interfaces or the type of interface (ferromagnetic-metallic nonmagnetic and ferromagnetic-semiconductor). Finally, it would be interesting to study the magnetocrystalline anisotropy of FM/SC multilayers with a bigger number of semiconductor layers. Work along this line is in progress now.

ACKNOWLEDGMENTS

This work has benefited from the collaboration within the TMR (Training and Mobility of Researchers) network on *Ab-initio Calculations of Magnetic Properties of Surfaces, Interfaces and Multilayers*, funded by the European Union.

---

*Permanent address: Institute of Metal Physics, Academy of Sciences of Ukraine, 252680 Kiev, Ukraine.

[1] S. Datta and B. Das, Appl. Phys. Lett. **56**, 665 (1990).
[2] G.A. Prinz, in *Ultrathin Magnetic Structures*, edited by B. Heinrich and J.A.C. Bland (Springer, Berlin, 1994), Vol. 2, pp. 1–44.
[3] J. de Boeck and G. Borghs, Phys. World **4**, 27 (1999).
[4] G.A. Prinz and J.J. Krebs, Appl. Phys. Lett. **39**, 397 (1981).
[5] J.R. Waldrop and R.W. Grant, Appl. Phys. Lett. **34**, 630 (1979).
[6] J.J. Krebs, B.T. Jonker, and G.A. Prinz, J. Appl. Phys. **61**, 2596 (1987).
[7] J.J. Krebs, B.T. Jonker, and G.A. Prinz, J. Appl. Phys. **61**, 3744 (1987).
[8] M. Gester *et al.*, J. Appl. Phys. **80**, 347 (1996).
[9] A. Filipe, A. Schuhl, and P. Galtier, Appl. Phys. Lett. **70**, 129 (1997).
[10] P.M. Thibado *et al.*, Phys. Rev. B **53**, R10 481 (1996).
[11] E. Kneedler *et al.*, Phys. Rev. B **56**, 8163 (1997).
[12] S. Moodera, L.R. Kinder, T.M. Wong, and R. Meservey, Phys. Rev. Lett. **74**, 3273 (1995).
[13] T. Miyazaki, T. Yaoi, and S. Ishio, J. Magn. Magn. Mater. **98**, L7 (1991).
[14] T. Miyazaki, T. Yaoi, and S. Ishio, J. Magn. Magn. Mater. **126**, 430 (1993).
[15] T. Miyazaki and N. Tezuka, J. Magn. Magn. Mater. **139**, 4231 (1995).
[16] W.E. Pickett and D.A. Papaconstantopoulos, Phys. Rev. B **34**, 8372 (1986).
[17] W.E. Pickett and D.A. Papaconstantopoulos, J. Appl. Phys. **61**, 3735 (1987).
[18] A. Continenza, S. Massidda, and A.J. Freeman, Phys. Rev. B **42**, 2904 (1990).
[19] M. van Schilfgaarde and N. Newman, Phys. Rev. Lett. **65**, 2728 (1990).
[20] W.H. Butler *et al.*, J. Appl. Phys. **81**, 5518 (1997).
[21] J.M. MacLaren, W.H. Butler, and X.G. Zhang, J. Appl. Phys. **83**, 6521 (1998).
[22] J.M. MacLaren, X.G. Zhang, W.H. Butler, and X. Wang, Phys. Rev. B **59**, 5470 (1999).
[23] H. Ebert, Phys. Rev. B **38**, 9390 (1988).
[24] V.N. Antonov, A.Y. Perlov, A.P. Shpak, and A.N. Yaresko, J. Magn. Magn. Mater. **146**, 205 (1995).
[25] U. von Barth and L. Hedin, J. Phys. C **5**, 1629 (1972).
[26] J.H. van Vleck, Phys. Rev. **52**, 1178 (1937).
[27] H. Brooks, Phys. Rev. **58**, 909 (1940).
[28] G.C. Fletcher, Proc. R. Soc. London, Ser. A **67**, 505 (1954).
[29] M.S.S. Brooks, B. Johansson, O. Eriksson, and H.L. Skriver, Physica B **144**, 1 (1986).
[30] L. Fritsche, J. Noffke, and H. Eckardt, J. Phys. F: Met. Phys. **17**, 943 (1987).
[31] P. Strange, H. Ebert, J.B. Staunton, and B.L. Gyorffy, J. Phys.: Condens. Matter **1**, 3947 (1989).
[32] G.H.O. Daalderop, P.J. Kelly, and M.F.H. Schuurmans, Phys. Rev. B **41**, 11 919 (1990).
[33] G.H.O. Daalderop, P.J. Kelly, and M.F.H. Schuurmans, Phys. Rev. B **44**, 12 054 (1991).
[34] G. H. O. Daalderop, Ph.D. thesis, Technical University Delft, 1991.
[35] G.Y. Guo, W.M. Temmerman, and H. Ebert, Physica B **172**, 61 (1991).
[36] J. Trygg, B. Johansson, O. Eriksson, and J.M. Wills, Phys. Rev. Lett. **75**, 2871 (1995).
[37] S.V. Halilov *et al.*, Phys. Rev. B **57**, 9557 (1998).
[38] J.G. Gay and R. Richter, Phys. Rev. Lett. **56**, 2728 (1986).
[39] J.G. Gay and R. Richter, J. Appl. Phys. **61**, 3362 (1987).
[40] G.H.O. Daalderop, P.J. Kelly, and M.F.H. Schuurmans, Phys. Rev. B **42**, 7270 (1990).
[41] G.Y. Guo, W.M. Temmerman, and H. Ebert, J. Phys.: Condens. Matter **3**, 8205 (1991).
[42] G.Y. Guo, W.M. Temmerman, and H. Ebert, J. Magn. Magn. Mater. **104-107**, 1772 (1992).
[43] D. Wang, R. Wu, and A.J. Freeman, Phys. Rev. Lett. **70**, 869 (1993).
[44] B. Újfalussy, L. Szunyogh, and P. Weinberger, in *Properties of Complex Inorganic Solids*, edited by A. Gonis, A. Meike, and P.E.A. Turchi (Plenum Press, New York, 1997), p. 181.
[45] I.V. Solovyev, P.H. Dederichs, and I. Mertig, Phys. Rev. B **52**, 13 419 (1995).
[46] S.S.A. Razee, J.B. Staunton, and F.J. Pinski, Phys. Rev. B **56**, 8082 (1997).
[47] S.S.A. Razee *et al.*, J. Appl. Phys. **83**, 7097 (1998).
[48] M.B. Stearns, in *Magnetic Properties of 3d, 4d, and 5d Elements, Alloys and Compounds*, Landolt-Börnstein, New Series, Group III, Vol. 19, Pt. a, edited by K.-H. Hellwege and O. Madelung (Springer, Berlin, 1987).
[49] D. Weller *et al.*, Phys. Rev. Lett. **72**, 2097 (1994).
[50] H.J.G. Draaisma, F.J.A. Broeder, and W.J.M. Jonge, J. Magn. Magn. Mater. **66**, 351 (1987).
[51] F.J.A. Broeder, D. Kuiper, H.C. Donkersloot, and W. Hoving, Appl. Phys. A: Solids Surf. **49**, 507 (1989).
[52] V.V. Maykov *et al.*, Fiz. Met. Metalloved. **67**, 79 (1989).
[53] A.E. Yermakov and V.V. Maykov, Fiz. Met. Metalloved. **70**, 201 (1990).
[54] A.R. Mackintosh and O.K. Andersen, in *Electrons at the Fermi Surface*, edited by M. Springford (Cambridge University Press, Cambridge, 1980), Chap. The Electronic Structure of Transition Metals.
[55] M. Weinert, R.E. Watson, and J.W. Davenport, Phys. Rev. B **32**, 2115 (1985).
[56] P.E. Blöchl, O. Jepsen, and O.K. Andersen, Phys. Rev. B **49**, 16 223 (1994).
[57] P.P. Ewald, Ann. Phys. (Leipzig) **64**, 253 (1921).
[58] J.C. Slater, Phys. Rev. **49**, 537 (1936).

[59] E.C. Stoner, Proc. R. Soc. London, Ser. A **165**, 372 (1938).
[60] P. Bruno, Phys. Rev. B **39**, 865 (1989).
[61] D.S. Wang, R.Q. Wu, and A.J. Freeman, Phys. Rev. B **47**, 14 932 (1993).
[62] G. van der Laan, J. Phys.: Condens. Matter **10**, 3239 (1998).
[63] M. Brockmann, M. Zölfl, S. Miethaner, and G. Bayreuther, J. Magn. Magn. Mater. **198-199**, 384 (1999).
[64] G. Bayreuther (private communication).