



HAL
open science

Interface structure and magnetism of Fe₃Si/GaAs(110) multilayers: An ab initio study

Heike Herper, Peter Entel

► **To cite this version:**

Heike Herper, Peter Entel. Interface structure and magnetism of Fe₃Si/GaAs(110) multilayers: An ab initio study. *Philosophical Magazine*, 2008, 88 (18-20), pp.2699-2707. 10.1080/14786430802277657 . hal-00513924

HAL Id: hal-00513924

<https://hal.science/hal-00513924>

Submitted on 1 Sep 2010

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



Interface structure and magnetism of Fe₃Si/GaAs(110) multilayers: An *ab initio* study

Journal:	<i>Philosophical Magazine & Philosophical Magazine Letters</i>
Manuscript ID:	TPHM-08-May-0176
Journal Selection:	Philosophical Magazine
Date Submitted by the Author:	20-May-2008
Complete List of Authors:	Herper, Heike; University of Duisburg-Essen, Theoretical Physics Entel, Peter; University of Duisburg-Essen, Theoretical Physics
Keywords:	ab initio, electronic structure, Fe-based alloys, GaAs, interfaces, magnetic films, multilayer
Keywords (user supplied):	ab initio, electronic structure, Fe-based alloys
<p>Note: The following files were submitted by the author for peer review, but cannot be converted to PDF. You must view these files (e.g. movies) online.</p> <p>Herper-ICCMS.tex</p>	



RESEARCH ARTICLE

**Interface structure and magnetism of Fe₃Si/GaAs(110) multilayers:
An *ab initio* study**

H. C. Herper* and P. Entel

*Theoretical Physics, Universität Duisburg-Essen, Campus Duisburg, 47048 Duisburg, Germany**(Received 00 Month 200x; final version received 00 Month 200x)*

Ferromagnet-semiconductor (FM/SC) hybrid structures have attracted much interest in view of materials being suitable for spintronic devices. Such devices demand a high spin polarization at the FM/SC interface, as is provided by Fe₃Si. Here, we investigate the hybrid system consisting of Fe₃Si and GaAs which is of special interest due to its tiny lattice mismatch. The multilayers containing 1-3 layer thick Fe₃Si films are oriented in (110) direction. Using the (110) orientation of GaAs has the advantage that no surface reconstruction has to be considered. Free GaAs(110) surfaces show only a rippling but no reconstruction. We investigate the structural and magnetic properties of thin layers of Fe₃Si on GaAs(110) using density functional theory. Therefore we choose a multilayer geometry in order to avoid additional contributions from the surface. The ground state structure turns out to be the same independently of the number of FM layers, and the rippled GaAs(110) surface is flattened if overgrown by Fe₃Si. Moreover, we find the system being stable against diffusion effects which leads to average magnetic moments of the magnitude of bulk Fe₃Si. Concerning the magnitude of the magnetic moments our calculations suggest that Fe₃Si/GaAs(110) may be a good candidate for magnetoelectronics.

1. Introduction

The search for materials being appropriate for magnetoelectronic devices is still intensively pursued. Suitable ferromagnets should have a high spin polarization like many Heusler alloys. These systems are often half-metallic in their bulk phase, which naturally leads to a high spin polarization. Besides the 'classical' ternary A₂BC Heusler compounds with L1₂ structure, also the quasi-Heusler system Fe₃Si with DO₃ symmetry is of interest for spintronic injectors, because its spin polarization is about 43% and can be regarded as nearly half-metallic [1]. In its bulk phase, Fe₃Si has two types of Fe atoms with magnetic moments of 1.2-1.35 μ_B and 2.2-2.4 μ_B, respectively, and a Curie temperature of 840 K [1, 2]. Furthermore, it has been found that ferromagnetism can be conserved even in very thin Fe₃Si layers with a nominal thickness of two monolayers [3]. Altogether, these features make this system an interesting candidate for spintronic applications [4]. First experimental realizations of heterostructures with Fe₃Si were made on GaAs(001) and Si(111). GaAs is of special interest, because the lattice mismatch between GaAs and Fe₃Si amounts only to 0.1% which should support epitaxial growth of the multilayers. However, it is well known that GaAs(001) surfaces are highly reconstructed. The reconstruction depends on the preparation of the system, i.e., in case of As rich surfaces a β(2 × 4) reconstruction is observed [5] while for Ga rich surfaces (4 × 6) or (2 × 4) surface reconstructions are common [6]. The growth properties and the interface magnetism seem to depend on the details of the GaAs(001) surface [7, 8]. A promising alternative in which the problem of complex surface preparation and reconstruction can be avoided, is the use of (110) oriented GaAs instead. This surface does not show any reconstruction, only surface relaxation effects can be observed. Typically, the GaAs(110) surface has a

*Corresponding author. Email: heike@thp.uni-duisburg.de

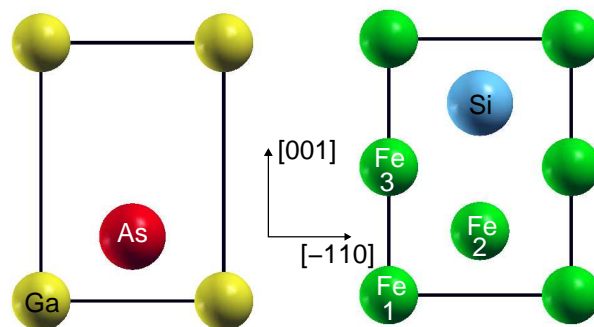


Figure 1. Schematic top view of the zinc-blende GaAs(110) (left) and Fe₃Si (right) unit cells. The numbers in the right panel refer to chemically inequivalent positions when Fe is placed on GaAs(110), for details see text.

rippled structure, which means that the Ga and As atoms on the surface layer are shifted in growth direction. From experiments with low-energy electron diffraction (LEED) techniques, it is known that the Ga atoms of the surface layer tend to move into the GaAs film layer whereas the As atoms move outwards [9, 10]. This can be related to a rotation angle of about 27-28° between the ideal and actual As-Ga bond (projection onto the (001) plane) [9]. GaAs(110) is obtained experimentally by cleaving such that the surface has the same structure as bulk GaAs and can, then be overgrown by Fe₃Si which also has its bulk composition in the (110) planes. So far, there exist some experimental results for Fe/GaAs(110) [11, 12], but not much work has been done to study the magnetic properties of Fe₃Si/GaAs(110) interfaces. In this paper, we investigate the interface structure and the magnetic configuration of thin Fe₃Si films on GaAs(110) by using multilayers instead of a single FM film on a GaAs(110) substrate. This factors out the influence of the surface on the magnetic moments and on the structure of the FM/SC system and we will be able to discuss interface effects only. The calculations are performed using density functional theory as implemented in the Vienna *Ab initio* Simulation Package (VASP) [13, 14]. Ionic relaxation has been taken into account for 1 and 3 layers of Fe₃Si to follow up the question whether the rippling of the GaAs surface survives if overgrown by Fe₃Si. Furthermore, it is known that Fe does not necessarily grow layer-wise on GaAs. Therefore, we performed calculations for (Fe₃Si)₁/GaAs(110) including diffusion at the interfaces.

2. Computational details

In order to study the interface magnetism and the structure of Fe₃Si on (110)-oriented GaAs, multilayers consisting of alternating 5 layers GaAs and 1-3 layers Fe₃Si have been investigated using periodic super-cells with 14-22 atoms. We make use of the VASP code [13, 14] with the implementation of the projector augmented wave (PAW) method [15] and the generalized gradient approximation (GGA) in the formulation of Perdew and Wang (PW91) [16] for the exchange correlation potential. The calculations have been performed with a periodicity of one lattice constant in the lateral directions using a tetragonal unit cell. A top view of the FM/SC interface layers is shown in Fig. 1. In all calculations, the experimental lattice constant of GaAs $a = 5.65 \text{ \AA}$ has been used. The theoretical lattice constant of bulk GaAs is generally overestimated by density functional theory using the GGA [17]; however, LDA is not suitable for Fe, and the use of the too large theoretical lattice constant may lead to artifacts in the magnetic moments.

In order to determine the ground state configuration of the FM on the semiconducting layer, we first kept the positions of the two subsystems fixed and placed the FM on a

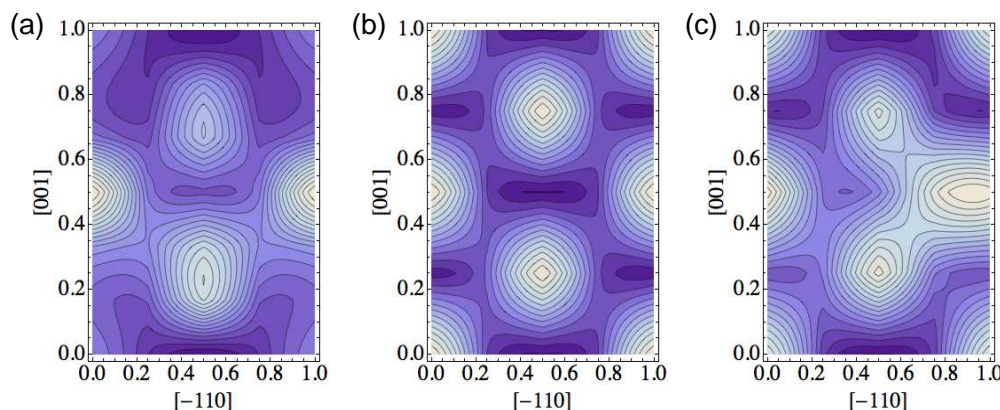


Figure 2. Constant energy surfaces of $\text{Fe}_3\text{Si}/\text{GaAs}(110)$ for 1, 2, and 3 FM layers as shown in (a), (b), and (c), respectively. The coordinates of the $[001]$ and $[-110]$ axis are the positions of the Fe atoms marked by “1” in Fig. 1. The energy increases with the brightness of the color, i.e., dark colors denote low energies. The distance of the contour lines is 0.4 eV and the minimum positions ($E = 0$ eV) are located in the middle of the $[-110]$ axis. The plot range covers the surface of one in-plane unit cell with Ga atoms sitting at the corner positions and As on the (0.5, 0.25) in-plane position.

regular grid of 6×6 positions for 1 layer and of 4×4 positions for the systems with 2 and 3 layers of $\text{Fe}_3\text{Si}/\text{GaAs}(110)$. Ionic relaxations have been performed by using a Davidson Block iteration scheme, subsequently keeping volume and cell shape fixed.

3. Results

The energies of the investigated interface structures of Fe_3Si on $\text{GaAs}(110)$ are summarized in Fig. 2. The results are plotted over the area of an in-plane unit cell with the Ga atoms sitting at the corner positions where the numbers on the axis mark the position of the Fe1 atom, cf. Fig. 1. In case of an odd number of layers, the two FM/SC interfaces are equal and we expect similar energy surfaces in both cases whereas for 2 layers of Fe_3Si , the two FM/SC interfaces are different. However, without relaxation the most stable structure is the same for all investigated systems, see Fig. 2. The atoms of the FM layer are placed in the interstitial positions of the $\text{GaAs}(110)$ layer as shown schematically in Fig. 3(a). For 2 layers of Fe_3Si , a second minimum occurs at the center of the energy surface, due to symmetry reasons, cf. Fig. 2(b). This minimum corresponds to a configuration where the Si and Fe2 positions of the interface layer are reversed and the 2nd Fe_3Si layer has the configuration shown in Fig. 3(a). The most unlikely configurations occurs for Si and Fe atoms sitting on the same positions as the Ga and As atoms in the outermost GaAs layer. These configurations have 5-7 eV higher energy than the ground state configuration and correspond to the white areas in Fig. 2. The energy contribution of the interface can be estimated from $E/N = a + b/N$ where N corresponds to the number of atoms in the unit cell and E is the total energy of the system (a and b are fit parameters). Then the slope of the straight line E/N determines the interface contribution to the energy. Here, we obtain approximately 23 eV, which is only a rough estimate because this formula is properly defined only in the limit of infinitely thick layers.

In order to determine the deviations from the ideal structure, we restrict the discussion to systems with identical interfaces, i.e., 1 and 3 layers of Fe_3Si . It turns out that the ground state structure is not much affected by relaxation. The interface is basically the same except for some relaxation effects. The structure being lowest in energy after ionic relaxation is sketched schematically in Fig. 3(b). The As atom of the interface layer is moved in $[001]$ direction by 13% from the ideal position whereas the As atoms in the layer lying below move in the opposite direction, but this effect is already extremely small (0.05%). The relaxation effects are not limited to atoms moving in the in-plane directions. We observe an additional displacement of the Ga and As atoms perpendicular to the sur-

4

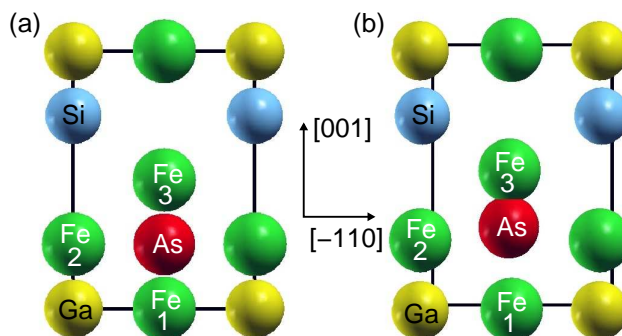


Figure 3. Schematic top view of the $\text{Fe}_3\text{Si}/\text{GaAs}(110)$ interface without ionic relaxation (a) and including relaxation (b). The relaxation mainly effects the As atom

face. In case of a free GaAs(110) surface, it is expected that the Ga atoms move inwards and the As atoms move outwards the surface, which leads to the rippled surface mentioned in the introduction. A displacement of the top GaAs layer can also be observed in the $\text{Fe}_3\text{Si}/\text{GaAs}(110)$ system. However, in our case both atoms – Ga and As – move outwards whereby the displacement of the As atom is more expressed being 2.5 times larger as compared to the displacement of the Ga atom. The Ga-As bond length is thereby enlarged by 9.4% which is not assumed to occur for a free GaAs(110) surface [18]. It should be noticed that this change cannot result from fixing the lattice constant to the experimental value, because the relaxation effect is much larger than the lattice mismatch. The change of the bond length and the displacements cause the rippling of the surface nearly to vanish. Experiments have shown that rippling is related to a rotation angle which measures the angle between the Ga-As bonds projected in the (001) plane relative to the ideal orientation of the bond. Instead of a rotation angle of $27\text{-}28^\circ$ observed in Refs. [9, 18], a rather small angle of approximately 2° results from the present calculations, which means that the rippling or buckling is destroyed if the surface is overgrown by Fe_3Si at least in case of thin FM layers separating the GaAs layers.

Besides the previously discussed relaxation effect, we observe a lateral adjustment of the interface atoms. The Ga, Fe2 and Si interface atoms are moved in the minus [-110] direction, whereas the other Fe atoms and As are shifted to the opposite direction. This seems to be an artifact of the lattice constant being fixed.

For all systems discussed so far we have neglected diffusion effects. Experiments with Fe/GaAs(110) indicate that good epitaxial growth can be expected [19]. However, we deal with very thin FM layers and we could not naively assume perfect layer by layer growth. In order to study the influence of possible interface roughness, we have systematically interchanged the positions of Ga and As with the Fe atoms of the FM layer. As, we use only a small in-plane unit cell, any interchange of atomic positions presents a large effect which may not occur experimentally. However, it can give a rough estimate of the importance of disorder in the system.

Here, we present only results for the case of 1 layer of Fe_3Si for which we expect the effects discussed above to be largest. In Fig. 4 we compare the energy of the ideal system to the energy of the systems where Fe atoms are interchanged with Ga or As. Independently from the Fe position (cf. Fig. 3(a)), replacing Ga atoms by Fe, the needed energy input is by a factor of 3 lower compared to the case in which As atoms are interchanged with Fe atoms. This may be understood from the fact that interchanging Ga and Fe creates zinc-blende Fe-As layers and it has been shown that in a zinc-blende lattice FeAs is more stable than FeGa [17]. However, none of the calculated configurations is lower in energy than the ideal structure discussed previously. From all investigated disordered structures the interchange of Fe2 with Ga requires the smallest energy. This configuration is only 51 meV/atom higher in energy compared to the ground state energy for the case without interdiffusion. The energy of 51 meV/atom corresponds to 590 K which is in the range of

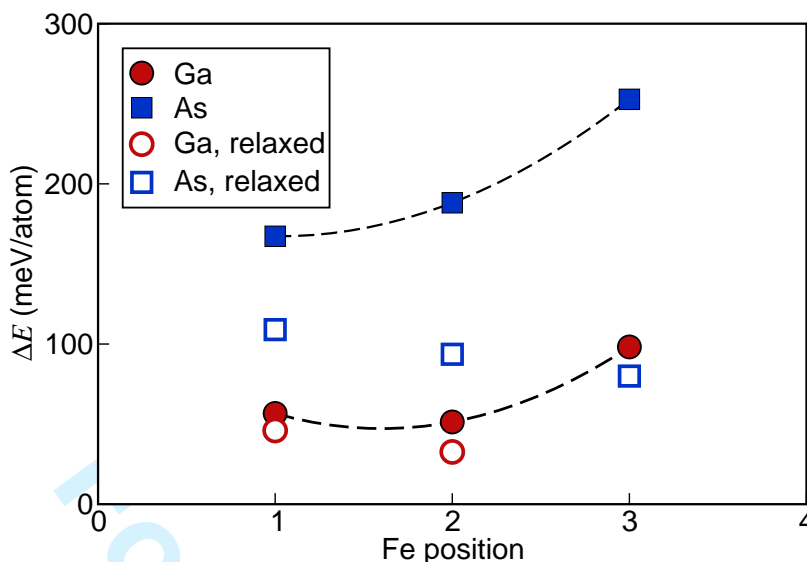


Figure 4. Increase of the total energy ΔE of $(\text{Fe}_3\text{Si})_1/\text{GaAs}(110)$ due to interchange of Ga and As atoms with Fe in the interface layers relative to the energy of the unperturbed system with ideal interfaces. The x-axis is the same as in Fig. 1. Circles mark the interchange of Ga with Fe and squares denote the results for interchange of As and Fe, respectively. Filled symbols quote results without relaxation whereas open symbols mark the energy difference for relaxed structure. The lines are only guide to the eyes.

the substrate temperatures during growth [3], thus, this configuration may eventually be stabilized thermodynamically.

Taking into account ionic relaxation does not change the picture in an essential way. The trends remain mostly the same; only the energy differences are slightly changed, see Fig. 4. The energy costs of interchanging Ga with Fe2 amounts to 32.82 meV/atom for the relaxed structures and is therefore still not favorable at $T = 0$ K. In conclusion, we expect no significant contributions from interdiffusion or roughness at low temperatures. In experiment, however, multilayers are grown at elevated temperatures which may involve interdiffusion at the interfaces to become important.

As expected, the interchange of Ga and Fe2 leads to a shift of the atomic positions. However, for most atoms this effect is only about 0.06\AA except for the Ga atom in the FM layer where it shows a significant in-plane distortion. In contrast to that, the rearrangements in the FeAs (the former GaAs interface) layer are small. The displacements in the perpendicular direction are rather small except for the As and Ga atoms. For the Ga atom in the FM layer we observe a shift of 2% outwards of the plane, i.e., in $-[110]$ direction. This seems to be correlated to a displacement in the 2nd GaAs layer in which As atoms are shifted in $[110]$ direction. Furthermore, the largest change is observed for the configuration with the interchange of As and Fe3, see Fig. 4. A detailed analysis of the structure shows that in this case Ga and As atoms move out of the interface layer of the GaAs film, i.e., the two subsystems try to separate.

As mentioned before, in the context of spintronic applications it is important to find FM materials with high spin polarization which remains unaffected if contacted with a SC material. In Fig. 5 the average magnetic moments of the Fe atoms of the ground state configurations of $(\text{Fe}_3\text{Si})_n/\text{GaAs}(110)$ ($n = 1-3$) systems are summarized. The magnetic moments show a distinct dependence on the thickness of the FM layer such that they decrease with increasing number of Fe_3Si layers. In case of a single FM layer, the average Fe spin moment corresponds to the value obtained for bulk bcc Fe $\bar{m} = 2.2 \mu_B$. Without lattice relaxation, the magnetic moments immediately drop down to $\bar{m} = 1.74 \mu_B$ or $\bar{m} = 1.46 \mu_B$ for 2 and 3 layers of Fe_3Si , respectively. If we include lattice relaxation, the magnetic moments recover, see Fig. 5. For the system with $n = 3$ we obtain a magnetic moment of $\bar{m} = 1.8 \mu_B$, i.e., 18% higher as for the non-relaxed structure. The main con-

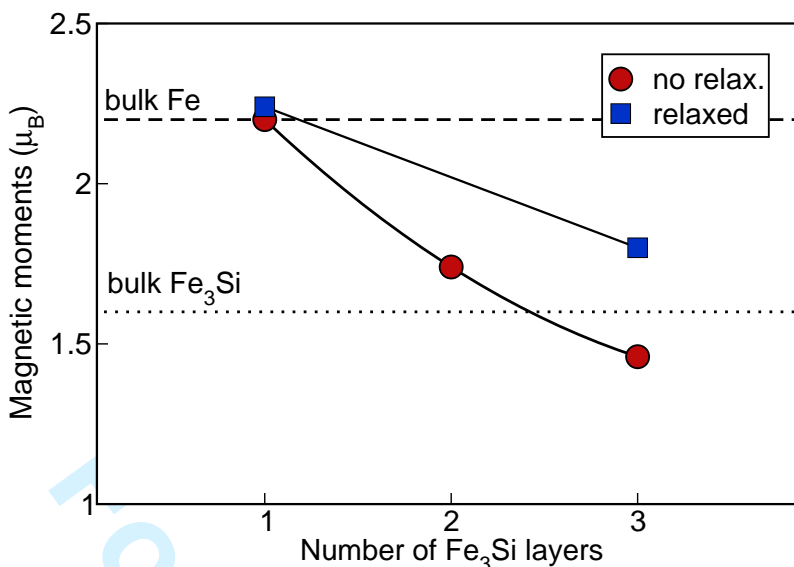


Figure 5. Average magnetic moments of the Fe atoms in $(\text{Fe}_3\text{Si})_n/\text{GaAs}(110)$ with $n = 1 - 3$ for the respective ground states. Circles denote the magnetic moments for systems without relaxation and squares give the magnetic moments after relaxation of the multilayer. The dashed and dotted lines mark the bulk values of the magnetic moments for bcc Fe and $\text{DO}_3 \text{Fe}_3\text{Si}$, respectively. The full lines are only guides to the eyes.

tributions to the enhanced magnetic moment stem from the two interface layers, whereas the moments of the central FM layer stick to the experimental values for Fe_3Si . Until now, there are no experimental values for magnetic moments in $(\text{Fe}_3\text{Si})_1/\text{GaAs}(110)$ with thin FM layers, results are only reported for the (001) orientation [3]. For the (001) direction the magnetic moments determined by a magnetic force magnetometer are close to the value of bulk Fe_3Si , cf. Fig. 5. The magnetic moments obtained from the present calculations are enhanced compared to the moments of bulk Fe_3Si , which may depend on the geometry of the system and the tiny thickness of the film. Since the magnetic moments decrease with an increasing number of FM layers, we assume that the bulk value will be approached for thick enough FM layers. This has to be verified in future investigations for larger super-cells.

If epitaxial growth is somehow distorted such that interdiffusion can take place, the magnetic structure changes drastically at least for thin FM layers which is shown here for the case $n = 1$. Keeping the atomic positions fixed, the disordered systems behave similar to the ideal system, except for the interchange of Ga and the Fe2, which has the lowest energy, see Fig. 6. For this configuration the magnetic moment amounts to $\bar{m} = 1.26 \mu_B$ only being 35% smaller as compared to the system without disorder. In contrast to the previously discussed systems with ideal interfaces, relaxation results in further decrease of the average magnetic moments having values already below the corresponding bulk value of Fe_3Si . The actual size of the magnetic moment or its reduction depends on the details of the corresponding structure, e.g., in case of Ga on Fe2 position, the magnetic moment of Fe in the zinc-blende FeAs layer amounts to $m = 0.9 \mu_B$ only. The size of the moments for atoms on the Fe1 and Fe3 positions are $\bar{m} = 1.1 \mu_B$ and $\bar{m} = 1.9 \mu_B$, respectively.

The interdiffusion effects which have been modeled in our calculations are exaggerated, when assuming the complete replacement of Ga by Fe in the interface layer. Nonetheless, we can conclude that if no epitaxial growth of Fe_3Si on $\text{GaAs}(110)$ is achieved and Fe penetrates into the GaAs layer, the moments will significantly decrease.

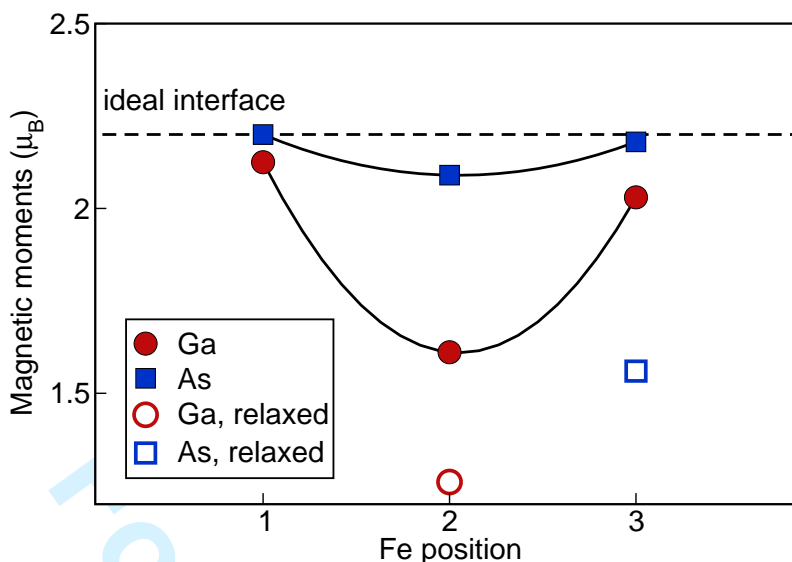


Figure 6. Average magnetic moments of the Fe atoms in $(\text{Fe}_3\text{Si})_1/\text{GaAs}(110)$ in presence of interdiffusion at the interfaces. Circles denote the magnetic moments for systems with interchange of Ga and Fe atoms and squares give the magnetic moments for systems in which As and Fe positions have been changed. The dashed line marks the average magnetic moment of the ground state configuration with ideal interfaces. The open circle and square give the corresponding magnetic moments for the configuration lowest in energy after lattice relaxation. The full line is only a guide to the eyes.

4. Conclusion

We have investigated the interface structure and the magnetic properties of $\text{Fe}_3\text{Si}/\text{GaAs}(110)$ in the limit of thin FM layers. The calculations have been carried out within *ab initio* density functional theory using the VASP code with PAW pseudopotentials and the GGA. In all calculations we used the experimental lattice constant of GaAs instead of the calculated minimum lattice constant, because the lattice constant is overestimated by density functional theory using the GGA and therefore, may cause artefacts to the magnetic structure. However, small deviations of the atoms from the ideal positions may be related to the use of the experimental value. Concerning, the general trends obtained in our calculations this can be considered of minor influence.

First, the minimum configuration of Fe_3Si system on GaAs(110) has been determined for 1-3 layer thick films of Fe_3Si assuming ideal interfaces, because GaAs(110) does not show any surface reconstruction. The most stable configuration for all 3 thicknesses was obtained for Fe and Si atoms sitting on the interstitial positions on top of the GaAs layer. The GaAs interface layers do not show the well known rippling of the (110) oriented GaAs surfaces. Therefore, the rotation angle amounts only to about 2° instead of $27-28^\circ$ for the free GaAs(110) surface. The present calculations give no evidence for interdiffusion or disorder at the interfaces at low temperatures. At higher temperatures, disorder may occur where an interchange of Ga and Fe would be favored. However, it should be kept in mind that we use a relatively small super cell in which the diffusion concentrations are extremely large. For a more detailed description, i.e., realistic concentrations larger cells have to be investigated in future work. Nonetheless, the present results point out a trend.

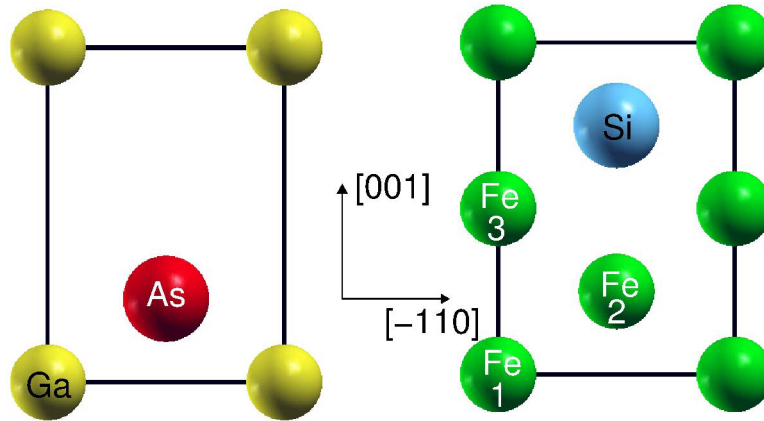
Furthermore, we investigated the magnetic structure of the FM/SC hybrid system. The average magnetic moments are larger than in bulk Fe_3Si , however they decrease with increasing thickness of the FM and seem to approach the bulk value for thicker layers. Lattice relaxation is essential to obtain the correct magnitude of the magnetic moments, because without ionic relaxation the Fe moments turn out to be underestimated by 20% in case of 3 FM layers. If the interface structure deviates from the ideal composition the magnetic moments are strongly reduced and relaxing the structure leads to even a stronger reduction of the magnetic moments.

Acknowledgements

We would like to thank M. E. Gruner for reading the manuscript. This work has been supported by the Deutsche Forschungsgemeinschaft through the SFB 491 "Spin Structure and Spin Transport in Magnetic Heterostructures".

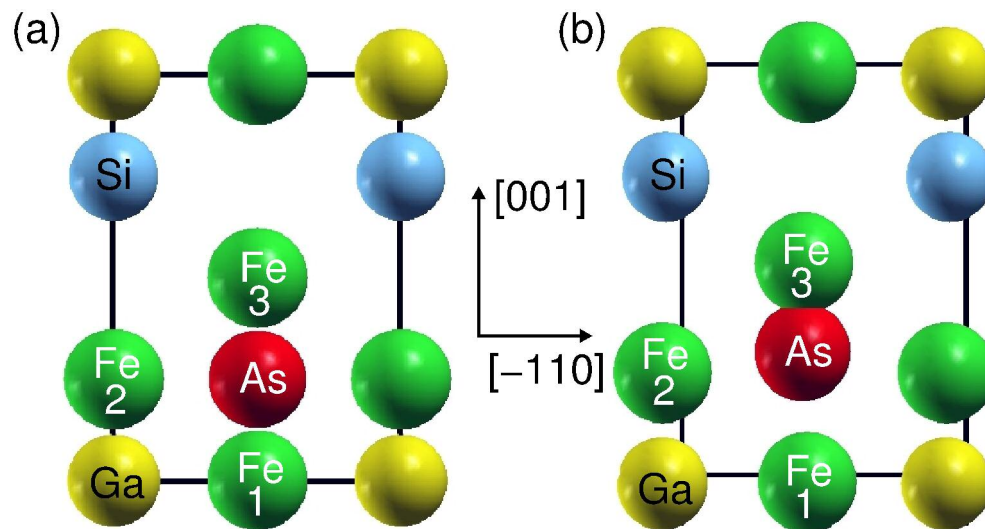
References

- [1] W.A. Hines et al., *Magnetization studies of binary and ternary alloys based on Fe₃Si*, Phys. Rev. B 13 (1976), p. 4060.
- [2] S. Yoon and J.G. Booth, *Structural and magnetic properties of Fe_{3-x}Mn_xSi alloys*, Phys. Lett; 48A (1974), p. 381.
- [3] S. Liou et al., *Magnetic properties of epitaxial single crystal ultrathin Fe₃Si films on GaAs(001)*, J. Appl. Phys. 73 (1993), p. 6766.
- [4] A. Ionescu et al., *Structural, magnetic electronic and spin transport properties of epitaxial Fe₃Si/GaAs(001)PRB*, J. Phys. D: Appl. Phys. 71 (2005), p. 094401.
- [5] V.P. LaBella et al., *Arsenic-rich GaAs(001) surface structure*, Surf. Sci. Rep. 60 (2005), p. 1.
- [6] Q. Xue et al., *Structures of the Ga-rich 4×2 and 4×6 reconstructions of the GaAs(001) surface*, Phys. Rev. Lett. 74 (1995), p. 3177.
- [7] J. Herford, H.P. Schönherr, and K. Ploog, *Epitaxial growth of Fe₃Si/GaAs(001) hybrid structures*, Appl. Phys. Lett. 83 (2003), p. 3912.
- [8] H.Wende private commun.
- [9] A.R. Lubinsky et al., *Semiconductor surface reconstruction: The rippled geometry of GaAs(110)*, Phys. Rev. Lett. 36 (1976), p. 1058.
- [10] J.E. Northrup, *Structure of GaAs(110) surface in As-rich conditions*, Phys. Rev. B 44 (1991), p. 1349.
- [11] M. Gester et al., *Continuous evolution of the in-plane magnetic anisotropies with thickness in epitaxial Fe films*, J. Appl. Phys. 80 (1996), p. 347.
- [12] R. Höllinger et al., *In-plane spin-reorientation transitions in epitaxial Fe(110)/GaAs(110) films*, J. Appl. Phys. 89 (2001), p. 7136.
- [13] G. Kresse and J. Hafner, *Norm-conserving and ultrasoft pseudopotentials for first row and transition metals*, Comput. Mater. Sci. 6 (1994), p. 15.
- [14] G. Kresse and J. Furthmüller, *Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set*, Phys. Rev. B 54 (1996), p. 11169.
- [15] P.E. Blöchl, *Projector augmented-wave method*, Phys. Rev. B 50 (1994), p. 17953.
- [16] J.P. Perdew and Y. Wang, *Accurate and simple analytic representation of the electron-gas correlation energy*, Phys. Rev. B 45 (1992), p. 13244.
- [17] S. Mirbt et al., *First-principles calculations of Fe on GaAs(100)*, Phys. Rev. B 67 (2003), p. 155421.
- [18] N. Masud, *Structure analysis of GaAs(110) surface at room temperature*, J. Phys. C: Sol. State Phys. 15 (1982), p. 3209.
- [19] M. Madami et al., *Thickness dependence of magnetic anisotropy in uncovered and Cu-covered Fe/GaAs(110) ultrathin films studied by in situ Brillouin light scattering*, J. Appl. Phys. 99 (2006), p. 08J701.



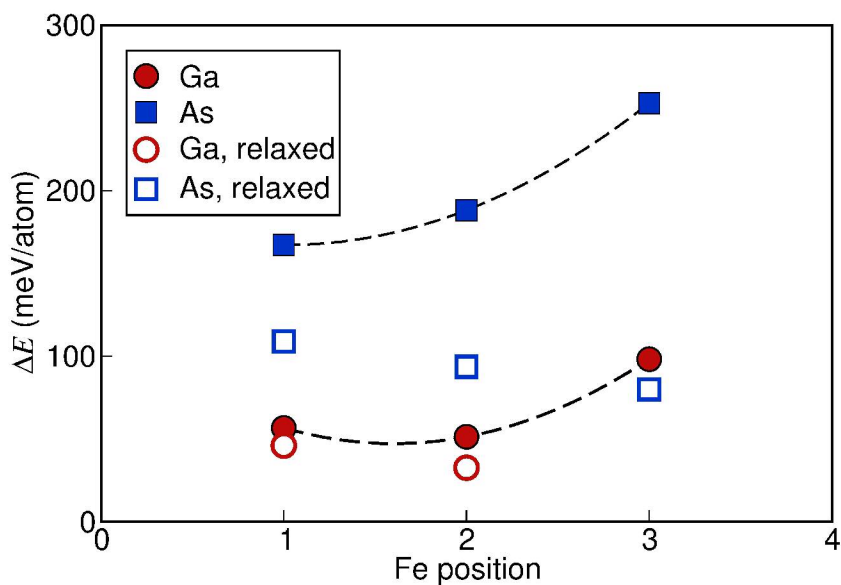
Schematic top view of the zinc-blende GaAs(110) (left) and Fe₃Si (right) unit cells. The numbers in the right panel refer to chemically inequivalent positions when Fe is placed on GaAs(110), for details see text.

408x234mm (600 x 600 DPI)



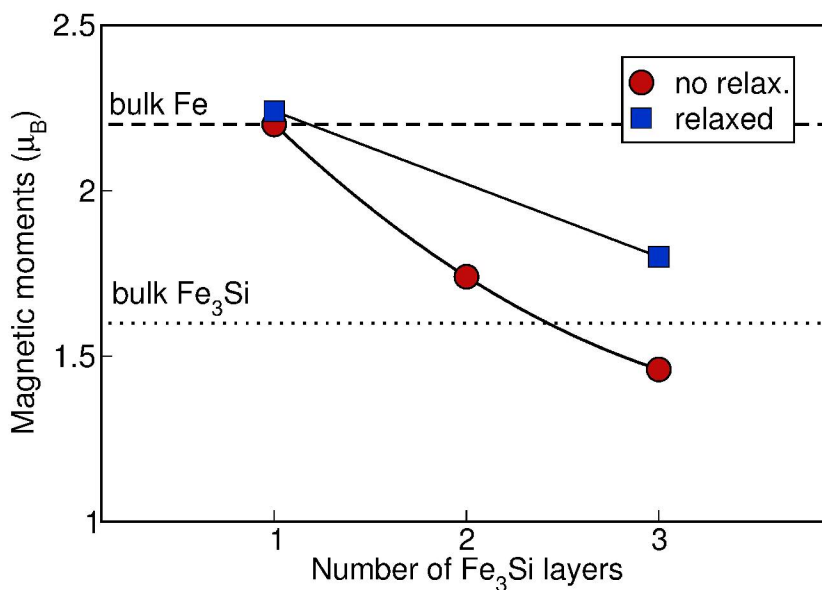
Schematic top view of the $\text{Fe}_3\text{Si}/\text{GaAs}(110)$ interface without ionic relaxation (a) and including relaxation (b). The relaxation mainly effects the As atom.

334x176mm (600 x 600 DPI)



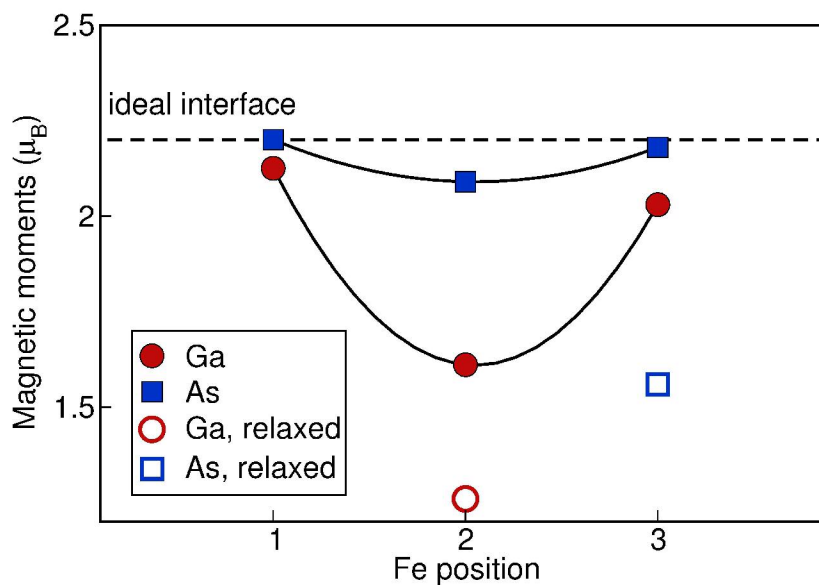
Increase of the total energy ΔE of $(\text{Fe}_3\text{Si})_1/\text{GaAs}(110)$ due to interchange of Ga and As atoms with Fe in the interface layers relative to the energy of the unperturbed system with ideal interfaces. The x-axis is the same as in Fig. \, \ref{fig:struc}. Circles mark the interchange of Ga with Fe and squares denote the results for interchange of As and Fe, respectively. Filled symbols quote results without relaxation whereas open symbols mark the energy difference for relaxed structure. The lines are only guide to the eyes.

215x279mm (600 x 600 DPI)



Average magnetic moments of the Fe atoms in $(\text{Fe}_3\text{Si})_n/\text{GaAs}(110)$ with $n = 1-3$ for the respective ground states. Circles denote the magnetic moments for systems without relaxation and squares give the magnetic moments after relaxation of the multilayer. The dashed and dotted lines mark the bulk values of the magnetic moments for bcc Fe and $\text{DO}_3 \text{Fe}_3\text{Si}$, respectively. The full lines are only guides to the eyes.

215x279mm (600 x 600 DPI)



Average magnetic moments of the Fe atoms in $(\text{Fe}_3\text{Si})_1/\text{GaAs}(110)$ in presence of interdiffusion at the interfaces. Circles denote the magnetic moments for systems with interchange of Ga and Fe atoms and squares give the magnetic moments for systems in which As and Fe positions have been changed. The dashed line marks the average magnetic moment of the ground state configuration with ideal interfaces. The open circle and square give the corresponding magnetic moments for the configuration lowest in energy after lattice relaxation. The full line is only a guide to the eyes.

215x279mm (600 x 600 DPI)