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Magnetism of cubic Mn–Ga–As compounds: an *ab initio* study

Cenk Ersan, Sergii Khmelevskyi and Peter Mohn[1]

Center for Computational Materials Science, Vienna University of Technology, Getreidemarkt 9/134, A-1060 Vienna, Austria

E-mail: phm@cms.tuwien.ac.at

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Abstract

We present calculations of the electronic and magnetic structure of the cubic phases of Mn–Ga–As and provide a systematic analysis of the magnetic moment formation of Mn and the stability of its various ordered magnetic configurations. We find that for high coordination number like for a bcc and fcc environment, the Ga/As atoms form broad metallic-like sp bands which interact with Mn. For most of these systems antiferromagnetic structures are the most stable configurations. For AsMn in the ZnS structure we find a half-metallicity both in the ferromagnetic and the [001] antiferromagnetic modification. Calculations for Mn–GaAs supercells allow us to formulate a possible mechanism to enhance the magnetic ordering temperature. Since the stability of the ferromagnetic phase is found to depend strongly on the number of excess electrons in the system, alloying with constituents with fewer electrons than As could help to stabilize the FM state and thus might increase the magnetic ordering temperature.

1. Introduction

The discovery of ferromagnetic order in diluted magnetic semiconductors made of heavily Mn doped InAs [1] and GaAs [2, 3, 5] paved the way for many semiconductor spin devices [6]. In particular the ferromagnetism of $Ga_{1-x}Mn_xAs$ adds the spin degree of freedom to the GaAs/(Al, Ga)As system which, in the last few years, has been the hallmark of interesting physics and for high speed electronic and optoelectronic devices. Thus the potential use of magnetically doped semiconductors in optoelectronic and spin-electronic devices as well as in quantum computing has been argued to have tremendous scientific and technological importance [3].

[1] Author to whom any correspondence should be addressed.

Substitution of Mn for Ga in GaAs has been shown to result in a particularly promising material and the observation of ferromagnetism at temperatures up to 100 K [5] has spurred on intensive experimental [3, 5, 10] and theoretical [11–15] activity. Typically these materials are produced by thin film growth since Mn has limited solubility in bulk GaAs. The long spin lifetime [7] and the spin coherence [8] of GaAs have already been demonstrated. Recently the feasibility of spin injection into GaAs using $Ga_{1-x}Mn_xAs$ contacts was proved [4], overcoming the intrinsic difficulty of injecting spins into semiconductors from magnetic metals [9].

In order to facilitate a technological breakthrough using magnetic semiconductors with a critical temperature above room temperature, an understanding of their magnetic properties and a correlation to the electronic structure must be achieved. Although there seems to exist a general agreement on the carrier- (hole-) mediated ferromagnetism in these systems, the detailed mechanism is still heavily debated. During the last few years quite different ideas have been put forward, including a Zener-type model [12], the competition between the double-exchange and superexchange mechanisms [11], and a double-resonance mechanism [13].

Experimental and theoretical work agree so far upon the conclusions that for $(Ga_{1-x}Mn_x)As$ the critical temperature depends on the hole concentration and that the hole concentration correlates with the concentration of Mn atoms that have substituted for Ga [10–12]. The latter is expected if Mn is assumed to be divalent in GaAs, bearing in mind that it replaces trivalent Ga. However, the correlation between the Mn and the hole concentration is not one-to-one [10], suggesting that Mn substitution is accompanied by lattice defects on the Ga and/or As sublattice. In particular, so-called As antisites, i.e. As atoms substituting on the Ga sublattice (in the literature usually denoted as As_{Ga}), are found to be the most common defects [16].

With the aim of achieving room temperature magnetic semiconductors, one could try to increase the value of the critical temperature by increasing the Mn concentration. However, growth of $(Ga_{1-x}Mn_x)As$ films with higher Mn concentration than $\sim$10% has been difficult [17]. Another way to increase the value of T_c would be via the influence on the hole concentration and possibly via the influence of defects, such as the above-mentioned As_{Ga} antisites, but in order to do this one needs to elucidate how the holes or the As_{Ga} concentration influence the magnetic properties.

First-principles calculations for ferromagnetically coupled Mn impurities yield moments of 4–5μ_B per Mn atom, whereas experimental results obtained from saturation magnetization measurements are significantly smaller ($\sim$2.5 μ_B). Bearing in mind that first-principles calculations typically reproduce the magnetic moments of any material within a few per cent, this marked disagreement cast severe doubt on the present theoretical understanding of the magnetism and its connection to the electronic structure of $(Ga_{1-x}Mn_x)As$. In most of the literature Mn is assumed to appear as Mn^{2+} which should give rise to a magnetic moment of about 5 μ_B according with $S = 5/2$. In contrast to this *ionic* picture, our present understanding relies much more on a mainly covalent description of the bonding of Mn within the host lattice. This controversy has been solved by suggesting that some of the Mn moments are coupled antiparallel with the result that a smaller average moment, as found in experiment, remains. Calculations employing the disordered local moment formalism indeed showed such a behaviour [18] upon introduction of As_{Ga} antisites. Performing frozen magnon calculations for supercells of (Ga, Mn)As [19] and for (Ga, Cr)As and (Ga, Fe)As [20], the influence of the Mn and the hole/electron concentration on the Curie temperature has been studied. In agreement with experiment, a non-monotonic dependence of the Mn concentration was found. Analogous to our results, the Curie temperature was found to increase with increasing hole concentration. These findings have also been confirmed by Sanvito *et al* [21] who suggested that at a reasonable concentration these antisites will suppress magnetism in $(Ga_{1-x}Mn_x)As$ by

introducing an antiferromagnetic component into the ferromagnetic Mn–Mn coupling which could eventually lead to a complete breakdown of long range magnetic order.

2. Scope and method of calculation

Experimentally, not too many stable phases exist between As, Ga and Mn on the Ga or As rich side of the phase diagram. Pearson's Handbook gives only MnAs in the zinc-blende (ZnS) structure and in the orthorhombic MnP structure. For Ga–Mn one finds a hexagonal disordered modification of the Mg-type structure and further, highly complex, Ga rich phases such as Ga_3Mn (Hg_4Pt structure) and Ga_5Mn (Al_6Mn structure). Since the main interest in our work is in the properties of Mn in an essentially cubic environment of Ga and As, we restricted our investigation to these partly hypothetical cubic phases, which, however, should provide the systematics of how the formation of a semiconducting gap of a half-metallic ferromagnetic phase depends on the number and type of the atomic coordinations. To this end we have performed calculations of the electronic and magnetic structures of the hypothetical alloys of Mn–Ga and Mn–As in a bcc and a fcc environment. We have thus studied the bcc phases CsCl and ABX_2 (Heusler alloy) and the fcc phases CuAu and Cu_3Au. For Mn–As we also studied the realistic ZnS structure. Finally we performed calculations for a Ga_8As_8 supercell (ZnS structure), where one Ga has been replaced by Mn in order to model the Mn doped Ga–As semiconductor for a nominal composition of $MnGa_7As_8$. Within the supercell approach, the problem of antisites (i.e. As atoms on Ga positions) will also be investigated. To simulate small concentrations of antisite atoms within the supercell we use the virtual crystal approximation, which allows us to study the stability of the magnetic order as a function of the excess electron/hole concentration. All calculations were carried out employing the augmented spherical wave (ASW) method as devised by Williams *et al* [22] which includes the possibility of calculating non-collinear magnetic order [23]. These non-collinear magnetic structures are calculated from spiral magnetic order where the direction of a magnetic moment on site i is defined by its polar and azimuthal Euler angles θ_i and ϕ_i. Keeping θ_i constant one defines a spin spiral propagation vector $\mathbf{q}$ via

$$\phi_i = \mathbf{q} \cdot \mathbf{R}_i, \tag{1}$$

where $\mathbf{R}_i$ is the position vector of site i. Spin spirals exhibit a generalized translational symmetry [23], which allows calculations in the chemical unit cell, thus avoiding computation-time-consuming supercell studies.

For all calculations a minimum number of 514 $\mathbf{k}$-points in the irreducible wedge of the Brillouin zone were used. With this choice, the self-consistency cycle was carried out until a charge self-consistency related to an interband charge transfer smaller than 10^{-6} was ensured. Within these assumptions a stability of the total energy better than 0.1 mRyd was achieved. In methods such as the ASW which rely on the ASA (atomic sphere approximation), for relatively open structures—such as the fourfold coordination in GaAs—empty spheres have to be introduced on the remaining high symmetry Wyckoff positions. Empty spheres are pseudo-atoms with charge zero, which simply provide the necessary space for the wavefunctions for describing bonds between neighbouring atoms. However, it is well known that with inclusion of these empty spheres, ASA based methods give reliable results [24]. The size of the ASA spheres was chosen such as to be proportional to the atomic volumes of the respective elemental solids. It should be kept in mind that electron counts, such as a charge transfer, of course depend on the choice of the ASA sphere size and thus represent only trends. For magnetic moments the situation is much more favourable, because for transition metals most of the 3d electron magnetic moment is localized within a radius of about 1 Bohr. The effects of exchange and correlation

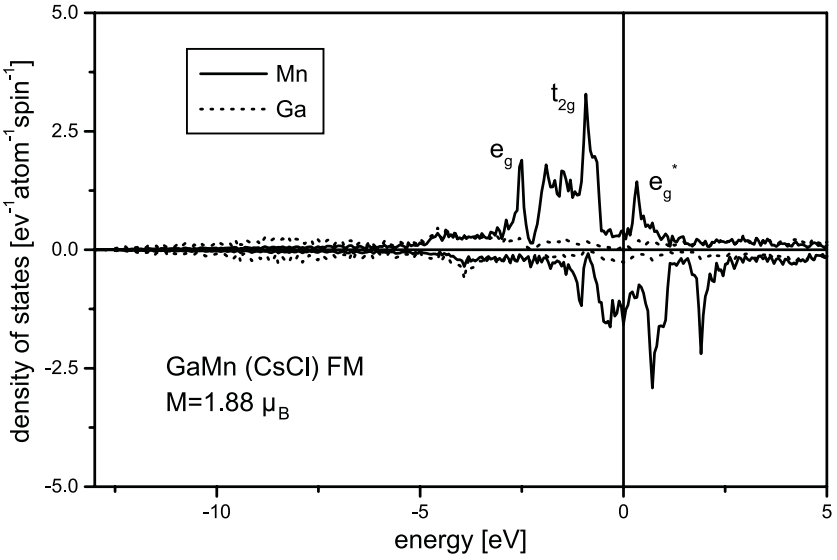

Figure 1. The density of states of ferromagnetic GaMn (CsCl) for the equilibrium volume (low spin state).

are treated within the density functional theory (DFT) [25, 26] using the LSDA (local spin density approximation) within the parametrization given by von Barth and Hedin [27].

3. Results

3.1. Body centred structures

The simplest representation of a binary alloy in a bcc structure is the CsCl phase. In this modification each Mn atom is coordinated by eight Ga/As neighbours and vice versa. Although the nominal coordination is 8, it is known that the second-neighbour shell also has a non-vanishing influence. A typical example is furnished by the aluminides of the late transition metals: FeAl [28, 29], CoAl and NiAl. In all these alloys, the crystal field produced by the first- and second-neighbour shells causes a characteristically large splitting of the transition metal d states, as is also the case for GaMn and AsMn (figure 1). In the CsCl structure GaMn (AsMn) have equilibrium lattice constants of 5.542 (5.715) Bohr, respectively. In GaMn the Mn magnetic moment is 1.88 μ_B. Increasing the lattice constant, one observes an almost discontinuous increase of the moment to a saturation value of about 3.5 μ_B (figure 2), a behaviour which is found for both GaMn and AsMn. This transition from low spin to high spin is typical for CsCl-type alloys of transition metals and sp metals such as Ga, As and Al, like for the magnetic modification of FeAl. In terms of symmetry decompositions this means that the Mn 3d band is split into e_g and t_{2g} orbitals where the e_g orbitals mediate the interaction between neighbouring Mn atoms. These states become strongly split and form the lower (bonding) and upper (antibonding) peaks of the Mn 3d band. The set of peaks in the centre of the Mn 3d band are mainly composed of states with t_{2g} symmetry. In the CsCl structure these t_{2g} states would normally describe the interaction with the eight nearest neighbours. In the case of Ga and As the corresponding sp states are, however, too low in energy to allow for a sizable overlap and thus a strong covalent bond. As a result, the t_{2g} states remain fairly localized and the resulting bonding between the Mn and the Ga sublattices turns out to be rather weak.

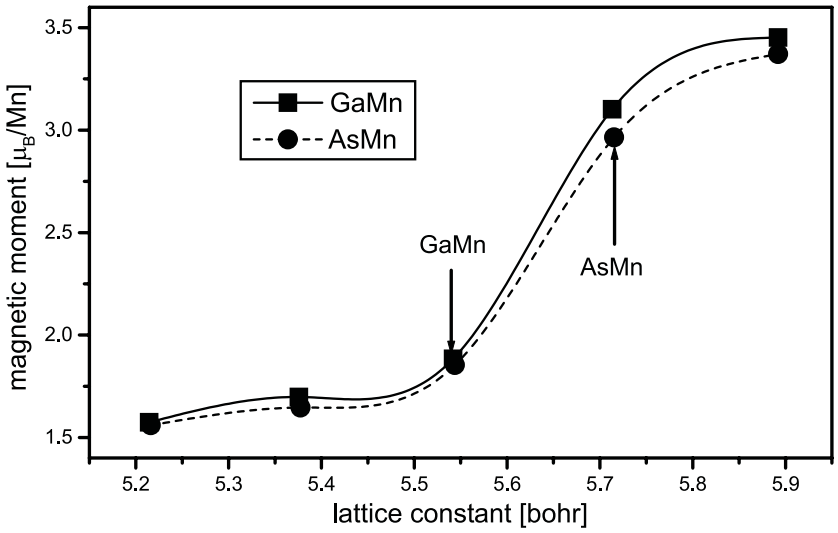

Figure 2. The volume dependence of the magnetic moment for GaMn and AsMn. The arrows denote the calculated equilibrium lattice constants.

The resulting strongly structured density of states (DOS), which is decomposed into well separated peaks, also has a major influence on the formation of the magnetic moment. In GaMn at the equilibrium volume the Fermi energy becomes pinned in the spin up band between the t_{2g} and the antibonding e_g peak. The value of the magnetic moment can thus be readily understood from the DOS: in a metallic state the d band of Mn contains about 6.4 electrons. Since in a metallic state ∼1.4 sp electrons become transferred into the d band, they add to the 5d electrons making up a total of 6.4. In the case of Mn in GaMn/AsMn the number of electrons in the spin up band is about 4 since the antibonding e_g peak can accommodate one electron but stays empty. The remaining 2.4 electrons must occupy the spin down band which results in a magnetic moment of $4 - 2.4 = 1.6\ \mu_B$. At large volume the spin up band becomes fully occupied, which causes a saturation of the magnetic moment at about $5 - 1.4 = 3.6\ \mu_B$. For AsMn the additional As electron weakens the bonding strength, so the equilibrium volume is larger than for GaMn. AsMn is found to be already in the high spin state with a Mn moment of almost 3 μ_B. Allowing antiferromagnetic ordering along the [001] direction lowers the total energy further and for both GaMn and AsMn gives a ground state with magnetic order according to the AF-I structure. The stabilization energy (i.e. the energy difference between the FM and the respective AF phase) is however small, which is typical for systems with narrow bands and weak magnetic coupling. For the AF-I structure the symmetry of the magnetic lattice is reduced from bcc to bct (body centred tetragonal), which leads to narrowing of the spin up d bands as can be seen in the density of states of GaMn (figure 3). This band narrowing also destroys the low spin state, so the magnetic moment in the AF-I modification becomes 2.51 μ_B.

Increasing the Ga/As content and retaining the bcc environment leads to an alloy of the nominal form ABX_2, the Heusler-type structure. Although this structure type contains three different constituents it allows us to study a Ga_3Mn compound, namely $Ga^{I}Ga^{II}_2Mn$, where Ga^{I} and Ga^{II} occupy different crystallographic sites. Ga^{I} has eight Ga neighbours; Ga^{II} has four Ga and four Mn neighbours. Mn is again surrounded by eight Ga/As neighbours, but since the Mn–Mn interaction is reduced as compared to the CsCl structure one, Mn forms a rather localized d band with a saturated ferromagnetic moment of about 3.7 μ_B. Varying the magnetic order

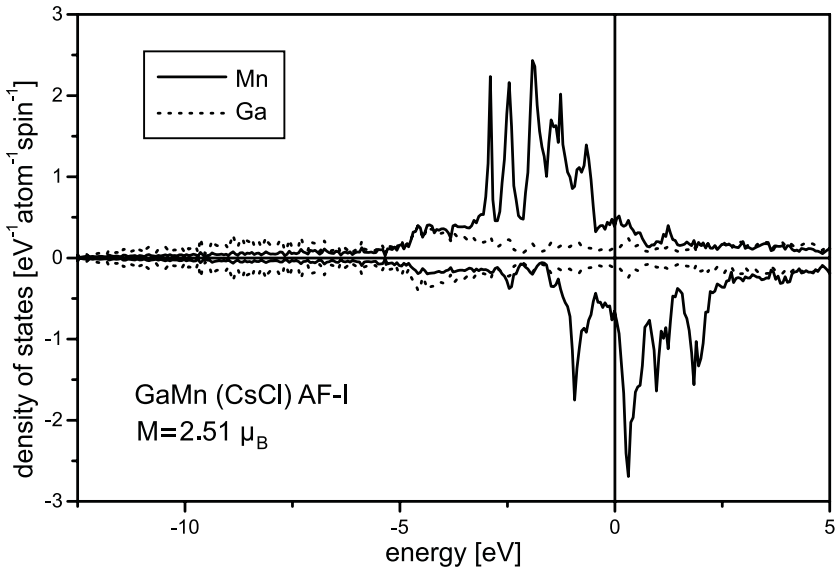

Figure 3. The density of states of AF-I GaMn.

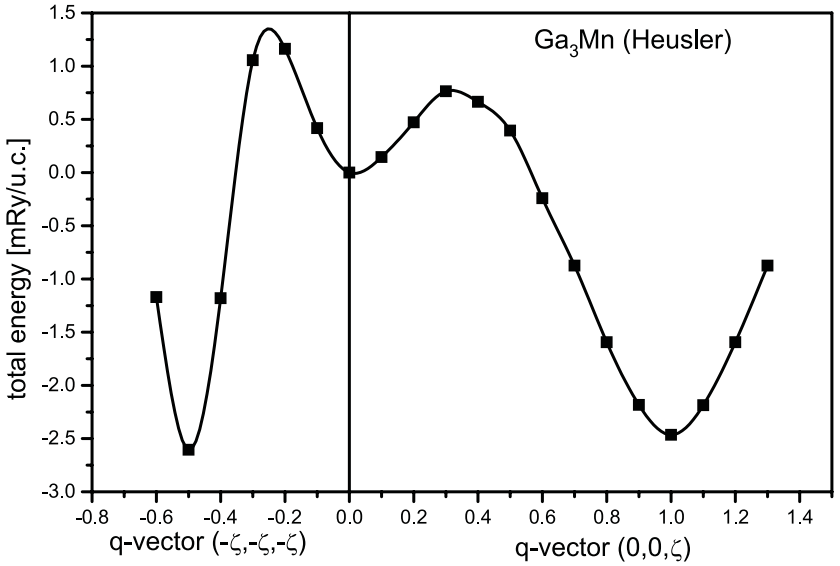

Figure 4. The total energy as a function of the spin spiral q-vector.

along the [111] and the [001] direction shows that the ground state is again antiferromagnetic (figure 4). It is also visible that the two antiferromagnetic configurations calculated are almost degenerate. This situation is not surprising because the Mn–Mn interaction is weak (the closest Mn atoms are only in the second-neighbour shell) and the [001] and the [111] magnetic order differ only slightly in the number of parallel and antiparallel spins among the Mn–Mn neighbours. For the [111] magnetic order Mn has six neighbours with parallel and six with antiparallel spin, whereas for [001] magnetic order Mn has only four neighbours with

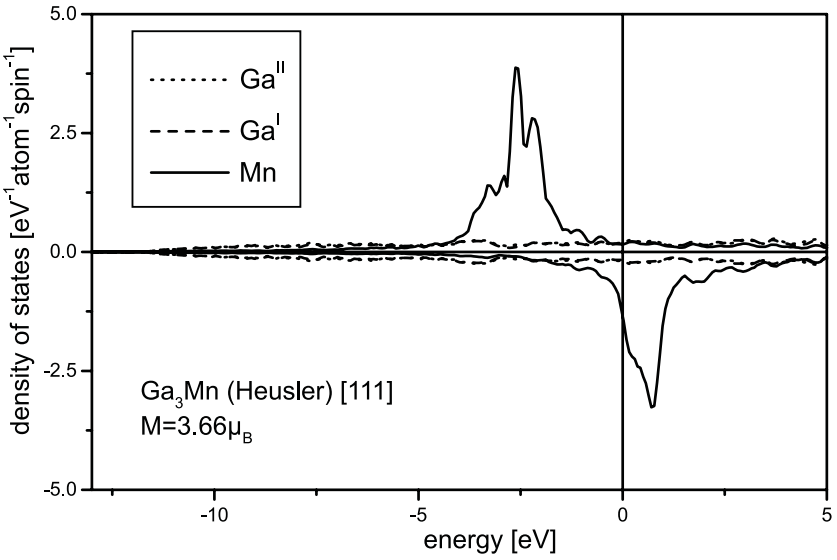

Figure 5. The density of states of Ga_3Mn (Heusler structure) for [111] magnetic order.

parallel spin. This results in a slightly more broadened Mn d-DOS in the [111] structure, since the interaction between Mn atoms with antiparallel spin is weaker than that for parallel spin (figure 5). The magnetic moment has a value as expected for Mn in a metallic state and amounts to 3.66 μ_B.

3.2. Face centred structures

The simplest fcc alloy of nominal composition GaMn is the CuAu structure. In this structure Mn and Ga/As atoms occupy adjacent planes which are stacked along the [001] direction such that actually a layered crystal structure is realized. This also has an effect on the 'chemical bonding' since each atom has four neighbours of its own kind and eight of the other. However, since this fourfold coordination is planar, a sp^3 hybridization cannot be expected. The ground state of GaMn in the CuAu structure also turns out to be antiferromagnetic along the [001] direction. The coupling between the Mn planes is mediated by the Ga/As planes and thus relatively weak. This results in a characteristically structured DOS where the in-plane Mn d orbitals overlap and form two bonding/antibonding broad peaks at the lower/upper band edge, whereas the out-of-plane orbitals continue forming a non-bonding localized peak in the centre of the d band (figure 6), a scenario which somewhat resembles the CsCl case. The equilibrium lattice constant is 6.572 Bohr and the equilibrium moment in the AF-I state is again 3.6 μ_B as in the other cases where Mn is in a metallic state.

Reducing the concentration of Mn and retaining the fcc environment leads to the Cu_3Au structure. In this structure Ga/As occupy the face centres and Mn the corners in a fcc cell, so Mn has 12 Ga/As neighbours and is thus in a rather isolated position. At an equilibrium lattice constant of 6.862 Bohr Ga_3Mn is found to be ferromagnetic with a moment of 3.6 μ_B. With this large moment, Mn is fully polarized and the band splitting becomes larger than the d bandwidth, which leads to a fairly localized magnetic moment (figure 7). Since the Mn atoms occupy the corners of a cube, the second-neighbour shell consists of six Mn atoms which are one lattice constant apart. One can easily identify that the Mn–Mn interaction again leads to

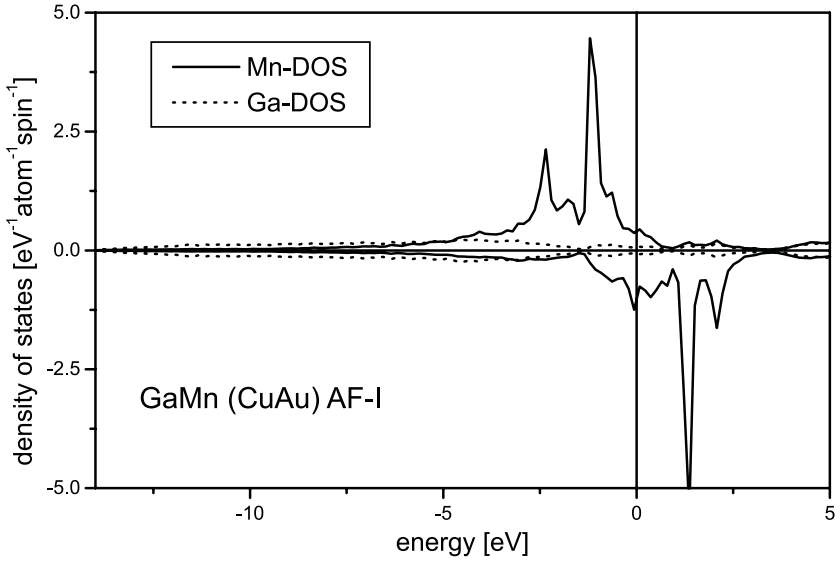

Figure 6. The density of states of GaMn (CuAu structure) for [001] magnetic order.

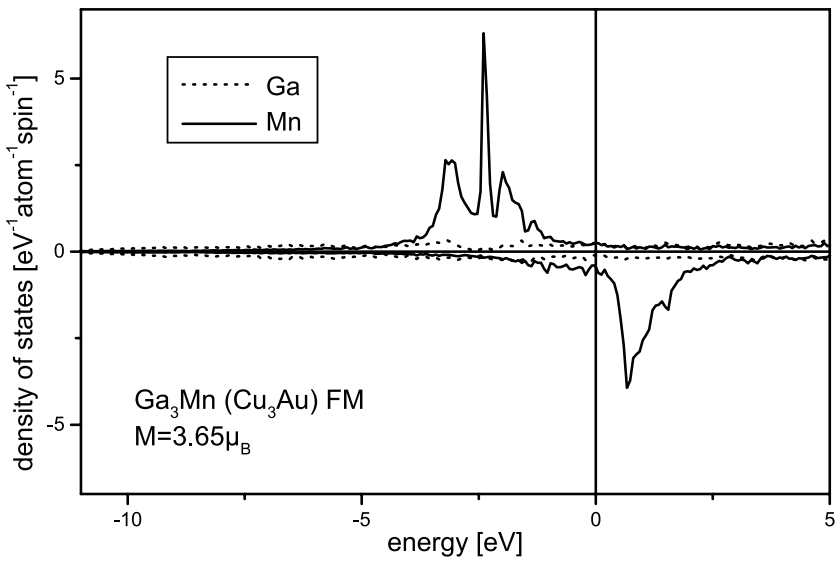

Figure 7. The density of states of Ga_3Mn (Cu_3Au structure) in the ferromagnetic ground state.

the two peaks of e_g symmetry at the lower and upper end of the d band, whereas the t_{2g} states form a narrow non-bonding peak in the centre of the d band. A variation of the spin spiral q-vector shows a metastable minimum for [111] antiferromagnetic order (figure 8), which becomes the ground state at lower volume. For the sake of brevity we have only shown our results for the Ga–Mn alloys, because those for As–Mn are very similar in their electronic and magnetic behaviour. In general we found that for all of these alloys, due to the unfavourable coordination number (strong deviation from the 8N rule), the metalloid atoms form a broad metallic s–p band which interacts only weakly with the Mn d states. As a result, the Mn d bands

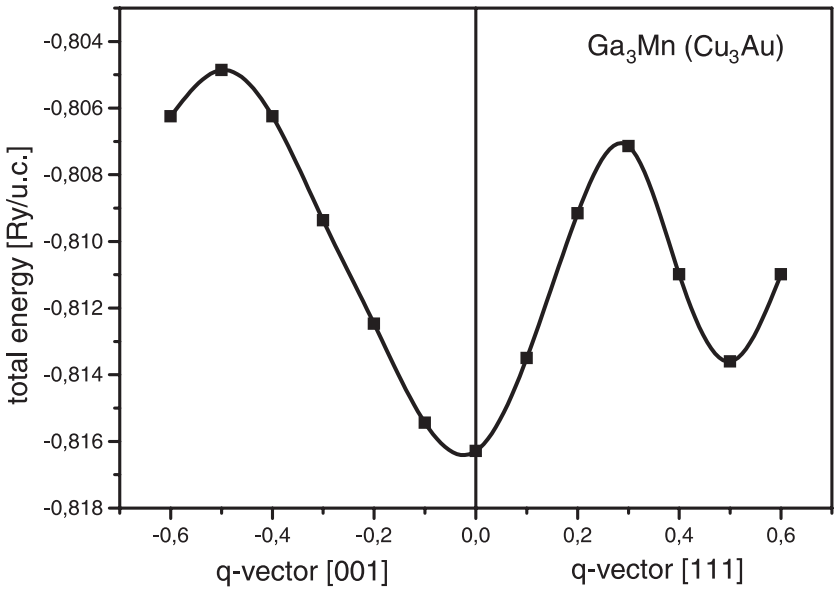

Figure 8. The total energy as a function of the spin spiral propagation vector in Ga_3Mn (Cu_3Au structure).

are relatively narrow and the magnetic moments, although not integer, are rather localized. For all structures with the exception of Ga_3Mn, the ground state is found to be antiferromagnetic. This tendency to form AF magnetic order is characteristic for Mn in such alloys. The 'half-filled' Mn d band favours AF order and, since the magnetic moment in the AF state is usually larger than for a metallic ferromagnet, the resulting gain in exchange energy can compensate easily for the loss of kinetic energy in systems where the direct Mn–Mn interaction is weak.

3.3. ZnS structure

Although the ground state of MnAs is a hexagonal NiAs-type structure, a study of the ZnS structure is justified by the fact that for the diluted semiconductors $Ga_{1-x}Mn_xAs$ the ZnS structure wold be obtained in the hypothetical limit $x = 1$. For realistic concentrations, however, Mn finds itself in a local ZnS-type environment when substituted for Ga. The ZnS (zinc-blende) structure is derived from the diamond lattice. It consists of two interpenetrating fcc lattices of Mn and Ga/As atoms which are shifted by a vector (0.25, 0.25, 0.25). Due to the tetrahedral coordination the As sp band separates into a 4s state (at about -11 eV) and p states which interact with the Mn d orbitals. The different symmetries of the As 4p and the Mn 3d states make the interaction weak, so the Mn 3d states become very narrow and look almost 'atomic-like'. The As has three p electrons, so another three electrons have to be provided by Mn to fill the As 4p state with six electrons. Assuming an atomic picture, Mn therefore supplies two 4s electrons and one 3d electron to fill this covalent state. Because Mn is now left with four 3d electrons, these have to fill the spin up band and consequently the magnetic moment becomes very large ($\sim 4\ \mu_B$). The interaction with the much less polarizable As 4p states shifts the bonding Mn 3d states to an energy of about -2.5 eV (for the spin down band), so in the spin down band a wide gap opens. This causes AsMn to form a so-called 'half-metallic ferromagnet', meaning that AsMn is metallic for spin up electrons and insulating for spin down. The density of states for the FM ground state at an equilibrium lattice constant

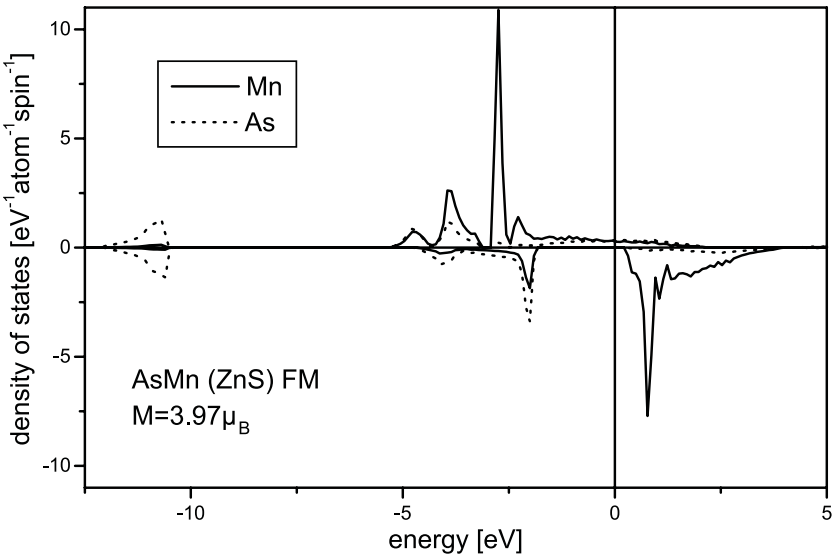

Figure 9. The density of states of AsMn (ZnS structure) in the ground state (half-metallic ferromagnet).

of 10.685 Bohr is shown in figure 9. This half-metallic state makes AsMn technologically highly interesting. If one succeeds in producing AsMn layers on e.g. a GaAs semiconductor substrate, one would be able to inject only spin up electrons into the GaAs, which would allow us to take advantage of the electron spin as an additional information bit. A stability study of AsMn for both the ZnS and the NiAs modification has been performed in [21]. If one allows antiferromagnetic order, one finds that the [111] AF structure is almost degenerate in energy (the AF modification is only about 1 mRyd/fu less stable than the FM order) and is also half-metallic with the same magnetic moment.

3.4. Mn–Ga–As supercell calculations

In order to simulate Mn diluted in a Ga–As host we performed calculations for a Ga_8As_8 supercell. Experimentally, it is claimed that, in the dilute limit, Mn occupies Ga positions, so the effective composition of our supercell reads $MnGa_7As_8$. Adding small amounts of Mn to the GaAs system, for low concentrations the usual dilute alloy mechanism can be observed. The electronic structure is of course dominated by the strong covalent GaAs orbitals, so any impurity atom has to place its states right at the Fermi energy. Normally this leads to a small, undispersed impurity peak (localized limit). In the present case, the situation is slightly different, because Mn occupies a Ga site and interacts with its four As neighbours like in MnAs (ZnS), described above. The density of states for the ferromagnetic ground state is shown in figure 10.

It is known that transition metal impurities in a semiconductor acquire an *ionic* state. It is thus assumed that Mn in a GaAs host lattice becomes Mn^{2+}, transferring two electrons to the GaAs band. Due to their delocalized (metallic) state the Mn d states hybridize with the As p states such that, because of the more mutually favourable energetic positions, the hybridization in the spin up band is much larger than that in the spin down band. For the spin up band this causes a broadening of the As p states, so the semiconducting gap closes. For the spin down band the gap remains, making Ga–MnAs a half-metallic semiconductor. However, there are Mn spin down d states below the Fermi energy which contain about 0.5 electrons (see figure 10). The resulting magnetic moment on Mn remains unsaturated at about 3.6 μ_B. Since

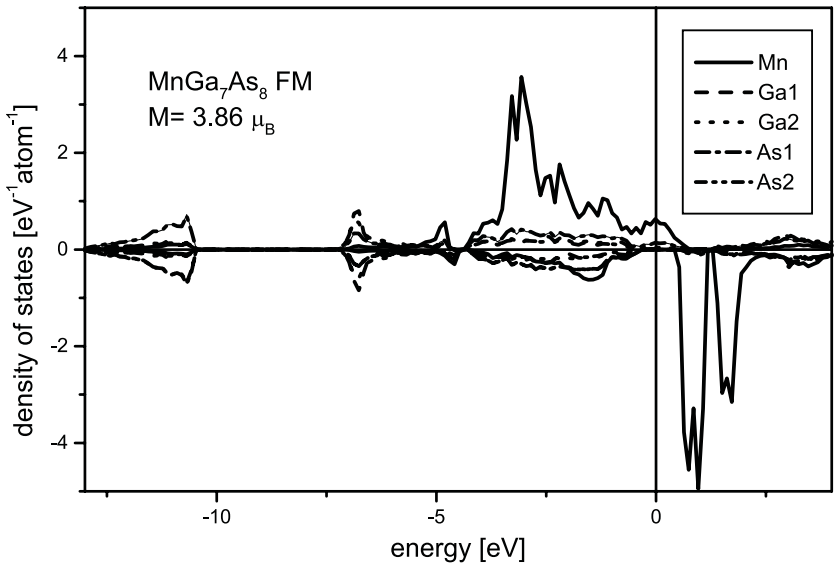

Figure 10. The density of states of $MnGa_7As_8$.

Mn supplies only two electrons, there remains one hole in the GaAs band of the host lattice. This hole allows a spin polarization of the GaAs host lattice leading to a moment of 0.4 μ_B, which couples ferromagnetically to the Mn moment. This scenario is known as hole-mediated ferromagnetism and is equivalent to the *covalent polarization model* [30]. A detailed study of transition metal impurities in a GaAs host can be found in [31].

Since the magnetic coupling is mediated by the GaAs holes [12], any change in the electron count (e.g. As antisites) must thus have an influence on the coupling constant. In lowest order that just means that there are additional sp electrons coming from As antisites present in the system. To simulate these excess As electrons, we used the *virtual crystal* (VC) approximation, replacing one Ga atom by a virtual atom having a non-integer electron number. Adding exactly one electron to the system, this means that the respective virtual atom becomes identical to Ge. The resulting density of states is shown in figure 11. The additional electron partly fills the GaAs hole and the Mn spin up d band. The magnetic moment on Mn increases to 4.1 μ_B and the filling of the GaAs hole destroys the spin polarization of the GaAs host lattice. As a result the ground state is no longer ferromagnetic but shows antiferromagnetic order along the [0, 0, 1] direction. Like donor states, the respective new states lie inside the GaAs semiconducting gap, making the whole system metallic. Increasing the excess electron number stabilizes the AF ordering even more. Plotting the energy difference between the FM modification and the respective [001] and [111] spin orderings as a function of the number of excess electrons shows that for a nominal composition of $MnGa_{6.79}As_{8.21}$ the FM state becomes unstable with respect to the [001] magnetic order (figure 12).

These results lead us to suggest a possible solution to the problem: that the ordering temperature in these diluted semiconductors has up to now been well below the ambient temperature. Since the FM order is destabilized by adding electrons and stabilized by removing electrons (see figure 12), adding excess Ga upon producing the host material could lead to an increase of T_c. Also, adding materials such as Zn could help to reduce the electron count and could increase the FM ordering temperature. This conclusion is in agreement with the discussion given in [19, 20].

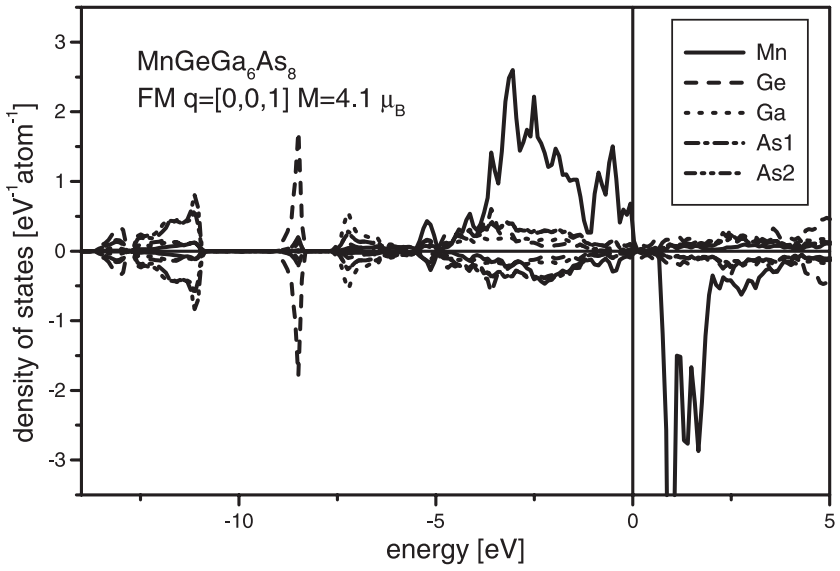

Figure 11. The density of states of $MnGeGa_6As_8$.

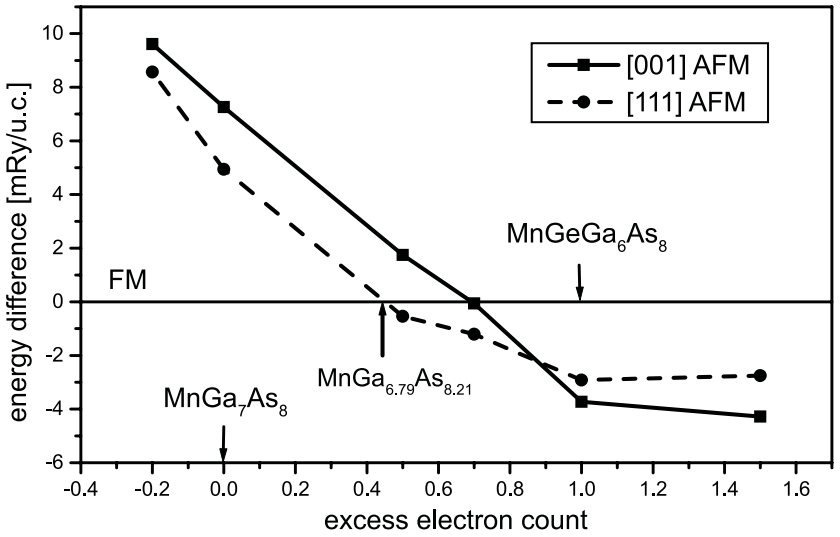

Figure 12. The energy difference between the ferromagnetic (FM) and the [001] and [111] spin orderings. Energies are plotted with respect to the FM energy (horizontal line at energy difference zero) as a function of the excess electron count per 16-atom supercell. The lowest curve is always the most stable one.

4. Conclusion

In this investigation we studied the magnetic order of Ga–Mn and As–Mn alloys. For the simple body centred (CsCl, ABX_2) and face centred (CuAu, Cu_3) modifications we found that antiferromagnetic order is the most common kind of magnetic ordering. Only for the Ga_3Mn (Cu_3) at the equilibrium volume does the ferromagnetic phase lie just below a metastable state

with [1, 1, 1] AF order. In general, we thus observed a strong tendency towards antiparallel spin ordering which is in agreement with the known properties of most Mn alloys. The degree of the localization of the Mn d band is less influenced by the varying coordination number, depending to a larger extent of the overlap with the Ga/As sp states. Because of the mutually unfavourable energetic positions, this overlap is relatively small, so in most cases the band splitting exceeds the bandwidth of the d band, which is actually a definition for localization. A case of particular interest is AsMn (ZnS), whose local coordination resembles that of Mn in the magnetic semiconductor Mn–GaAs. AsMn (ZnS) is found to be a half-metallic ferromagnet with a rather strongly localized Mn d band. This modification is of great technological interest, because if grown on a GaAs semiconductor it would allow injection of well defined spin up electrons. Finally, we performed calculations for Ga_8As_8 supercells where one Ga was replaced by Mn, leading to a nominal composition $MnGa_7As_8$. This system was also found to be a half-metallic ferromagnet with a Mn moment of 3.6 μ_B. Due to the existence of holes in the GaAs band, the GaAs host lattice becomes magnetically polarized with a rather large moment of about 0.4 μ_B. Simulating the excess As atoms (As antisites) found experimentally, which act as electron donors, we were able to show that, with increasing number of excess electrons, the stability of the ferromagnetic phase becomes progressively smaller, so for an excess of about 0.4 electrons/cell only the AF ordering can become the ground state.

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