Carrier-induced enhancement and suppression of ferromagnetism in Zn$_{1-x}$Cr$_x$Te and Ga$_{1-x}$Cr$_x$As: origin of the spinodal decomposition

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Abstract. Ferromagnetism in Zn$_{1-x}$Cr$_x$Te shows some interesting but puzzling dependence on p-type (nitrogen) and n-type (iodine) dopings that seems to contradict the current understanding of carrier-induced ferromagnetism based on the d–d double exchange mechanism. Using first-principles calculations combined with a phenomenological band coupling model to describe the magnetic interactions, we show that the formation of Cr-rich regions (spinodal decomposition) is driven mainly by the energy gain due to the magnetic interaction between Cr atoms. Thus, the previously proposed Coulomb repulsion between the magnetic Cr ions does not play a major role in the formation of Cr-rich aggregates. Similar results are predicted for Ga$_{1-x}$Cr$_x$As.

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1. Introduction

The discovery of ferromagnetism in dilute magnetic semiconductors (DMSs) has attracted much attention because it provides an opportunity to introduce both charge and spin degrees of freedom into semiconductor devices [1]–[3]. Currently, most of the efforts are devoted to search for DMSs that have Curie temperature, $T_C$, above room temperature (RT). In pursuing this goal, several DMS systems have been studied theoretically (e.g. see [3]–[7]) and experimentally, and $T_C$ above RT have been observed for several systems, e.g. Zn$_{1-x}$Cr$_x$Te [8]–[10], Ga$_{1-x}$Cr$_x$N [11], Ga$_{1-x}$Mn$_x$N [12, 13], Ce$_{1-x}$Co$_x$O$_{2-δ}$ [14]–[16] and Zn$_{1-x}$Cr$_x$O [17]. Among them, Zn$_{1-x}$Cr$_x$Te exhibits some very interesting but also puzzling results [9, 10, 18]. For example, Ozaki et al [18] reported that ferromagnetism in Zn$_{1-x}$Cr$_x$Te ($x \leq 0.09$) is suppressed (i.e. $T_C \rightarrow 0$) when nitrogen, which is a p-type dopant in ZnTe, is supplied during molecular-beam epitaxy (MBE) growth with concentrations of the order of $10^{20}$ cm$^{-3}$. However, $T_C$ can be significantly enhanced when iodine, which behaves as an n-type dopant in ZnTe, is introduced in Zn$_{1-x}$Cr$_x$Te [9, 10]. In this case, $T_C$ first increases from 30 to 300 K by adding iodine up to a concentration of $2 \times 10^{18}$ cm$^{-3}$. After that, $T_C$ starts to decrease with further increases in the iodine concentration, i.e. $T_C \approx 200$ K for iodine concentration around $1 \times 10^{19}$ cm$^{-3}$ [10]. Thus, there is a maximum in the $T_C$ curve as a function of the iodine concentration.

Although these experimental observations suggest that in Zn$_{1-x}$Cr$_x$Te, $T_C$ can be tuned by introducing carriers, the observed trends appear to contradict the current understanding of carrier-induced ferromagnetism based on magnetic interactions, namely, d–d double exchange or the p–d Zener exchange mechanism [3, 6, 19, 20]. In these conventional models for the magnetic interactions, the partial occupation of the hybridized $t_{2d}$ (or $t_{2p}$) derived states is the origin of the ferromagnetism. For example, the coupling between two ferromagnetically aligned ions introduces a set of bonding and antibonding states with a higher number of occupation on the bonding orbital, which stabilizes the ferromagnetic (FM) phase compared with the antiferromagnetic (AFM) phase. Simple electron counting suggests that when the $t_2$ level is half-occupied (i.e. with the number of holes $m_h$ per ion equal to $\frac{3}{2}$), all the bonding states are occupied, whereas all the antibonding states will be empty, which yields the largest stabilization for the FM phase, and hence, the largest $T_C$. 

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For $\text{Zn}_{1-x}\text{Cr}_x\text{Te}$, it is found that Cr substitutes the Zn sites in ZnTe. Because the Cr$^{2+}$ ion has a d$^4$ configuration, it has two electrons occupying the t$_{2g}$ level (i.e. $m_h = 1.0/\text{Cr}$). Thus, one would expect that when $m_h$ increases with p-type doping (e.g. adding nitrogen), $T_C$ should increase, whereas when $m_h$ decreases with n-type doping (e.g. adding iodine), $T_C$ should decrease. However, this expectation is exactly the opposite of experimental observations [9, 10, 18], as summarized above.

Kuroda et al [10] explained these puzzling trends by proposing that the carrier-induced formation of regions of low and high density of Cr ions (spinodal decomposition) is the origin of high $T_C$ in $\text{Zn}_{1-x}\text{Cr}_x\text{Te}$, because it is expected that Cr-rich regions could give rise to high $T_C$. They suggested that the spinodal decomposition, which has been discussed in detail by Sato et al [21]–[23] and Fukushima et al [24]–[27] in DMS systems, can be formed if the magnetic Cr ions inside ZnTe bind strongly with each other. They also suggested that the binding between the Cr ions is mainly Coulombic and can be controlled by manipulating the charge state of the Cr ions through doping.

However, this Coulomb repulsion mechanism cannot provide a consistent explanation for the formation of the Cr-rich aggregates under co-doping of iodine or nitrogen in $\text{Zn}_{1-x}\text{Cr}_x\text{Te}$. For example, iodine doping in $\text{Zn}_{1-x}\text{Cr}_x\text{Te}$ changes the nominal oxidation state of the Cr atoms from Cr$^{2+}$ in intrinsic ZnTe:Cr to Cr$^{1+}$. Because a smaller Coulomb repulsion is expected between the Cr$^{1+}$ ions than for the Cr$^{2+}$ ions, iodine doping is expected to enhance the formation of Cr-rich aggregates even for large iodine concentrations. However, experimental data show clearly that $T_C$ decreases from about 300 K (maximum $T_C$) to about 200 K when iodine concentration increases beyond the native hole concentration of ZnTe. Kuroda et al [10] reported first-principles calculations in which they show that the Cr–Cr binding is strongest when Cr is in the nominal 2+ charge state, which, again, cannot be explained only by the simple Coulomb repulsion model. Therefore, the nature of the magnetic interactions between the Cr ions in ZnTe that give rise to the spinodal decomposition, is still under debate.

In this work, using density functional theory (DFT) calculations combined with a phenomenological band coupling model (BCM) to describe the magnetic interactions [6], we will show that the enhancement and suppression of the spinodal decomposition by nitrogen or iodine co-doping and the subsequent change in the $T_C$ in $\text{Zn}_{1-x}\text{Cr}_x\text{Te}$ is mainly due to the magnetic interaction between the Cr ions, which determines the Cr–Cr binding energy and its dependence on the Cd d-level occupation. Furthermore, to show that the mechanism is general, we also performed calculations for Ga$_{1-x}$Cr$_x$As. Because Cr substituting on Ga site leads to Cr$^{3+}$ configuration, its dependence on p-type and n-type doping is expected to be opposite to that in Zn$_{1-x}$Cr$_x$Te. Indeed, for both systems, we obtain the same trends as a function of hole occupation, which demonstrate that the magnetic coupling between the Cr ions d-orbitals plays the main role in determining the spinodal decomposition, not the ionic Coulomb interaction as previously assumed [10].

2. Theoretical approach and computational details

Our spin-polarized calculations are based on the all-electron projected augmented wave (PAW) method [28, 29] and DFT within the local density approximation (LDA) as implemented in the Vienna ab initio simulation package (VASP) [30, 31]. Cutoff energies of 277 and 283 eV were used for Zn$_{1-x}$Cr$_x$Te and Ga$_{1-x}$Cr$_x$As, respectively, whereas for the Brillouin zone integration,
a \((2 \times 2 \times 2)\) \(k\)-point grid was used, while for the density of states (DOS), a dense \(k\)-point mesh of \((6 \times 6 \times 6)\) was used.

Experimental x-ray diffraction (XRD) results show that the lattice constant of \(\text{Zn}_{1-x}\text{Cr}_x\text{Te}\) follows Vegard’s law, which indicates that a majority of active Cr ions substitutes on Zn sites in the host lattice \([32]\). Thus, in this work, we considered only substitutional Cr defects in the host ZnTe and GaAs semiconductors. All calculations were performed using a 64-atom supercell with zinc-blende structure \((a_0 = 6.00 \text{ Å for ZnTe, 5.61 Å for GaAs})\), in which there are 32 cation sites for the Cr ions.

To avoid using very large supercell (about 500–1000 atoms) to describe the co-doping of Cr with nitrogen or iodine, we mimic the nitrogen and iodine co-doping by introducing holes and electrons near the valence and conduction band edges, respectively. This approach is well justified for these systems because the introduction of nitrogen and iodine generates only shallow levels slightly above the valence or below the conduction bands, respectively \([10, 33]\). For example, the ionization energy for ZnTe:N is 53 meV \([33]\). As we will show below, the Cr d-states, which play the main role in the magnetic properties, are located within the bandgap of ZnTe and GaAs, and hence, the compensation of the Cr defects level by shallow dopants can be correctly described by introducing holes or electrons. Furthermore, in this approach, the number of holes can be changed continuously by non-integer values, hence, we have a high control on the number of holes in the Cr d-states within the bandgap, which is important to check the maximum FM stability as a function of hole concentration.

3. Results and discussion

3.1. Single Cr impurity

We first study an isolated Cr ion in the host ZnTe and GaAs systems. It is known that the tetrahedral crystal field splits the Cr 3d-states into the e- and t\(_2\)-states. Our electronic structure analysis reveals that the localized spin-up e-states are occupied and located slightly below the valence band maximum (VBM) and contribute with \(2.0 \mu_B \text{Cr}^{-1}\) for both systems. The t\(_2\)-states hybridize strongly with the host anion p-states and are located within the bandgap at the Fermi level (see figure 1). The spin-up t\(_2\)-states are partially occupied in both cases and contribute with 2.0 and 1.0 \(\mu_B \text{Cr}^{-1}\) for \(\text{Zn}_{1-x}\text{Cr}_x\text{Te}\) and \(\text{Ga}_{1-x}\text{Cr}_x\text{As}\), respectively, hence, the total magnetic moments are 4.0 and 3.0 \(\mu_B \text{Cr}^{-1}\), respectively. Thus, the unoccupied t\(_2\)-states within the bandgap provide 1.0 and 2.0 holes \(\text{Cr}^{-1}\) for \(\text{Zn}_{1-x}\text{Cr}_x\text{Te}\) and \(\text{Ga}_{1-x}\text{Cr}_x\text{As}\), respectively.

3.2. Cr–Cr interactions

The interactions between Cr ions are studied by replacing two Zn/Ga nearest-neighbor atoms with two Cr atoms. The DOS of Cr in FM and AFM alignment are shown in figure 1. We can see that the coupling between the Cr ions broadens the t\(_2\)-band, as expected due to the interaction between the magnetic ions. The band width of the t\(_2\)-band is larger in the FM phase than in the AFM phase, because the direct coupling \(\Delta_{dd}^1\) between the majority spin d-state is larger than the coupling \(\Delta_{dd}^{1,2}\) between the partially occupied majority spin d-state and the unoccupied minority spin d-state, as expected from the BCM (see figure 2).
To study the magnetic interaction between the Cr ions and its relation to carrier doping for both systems, we first calculate the total energy difference between the FM and AFM phases,

$$\Delta E_{\text{tot}}^{\text{DFT}} = E_{\text{tot}}^{\text{FM}} - E_{\text{tot}}^{\text{AFM}},$$

as a function of the number of holes per Cr atom. $\Delta E_{\text{tot}}^{\text{DFT}}$ is directly related to the $T_c$, e.g. in the mean-field approximation (MFA), $T_c^{\text{MFA}} \approx - \frac{2}{3 \hbar} \frac{\Delta E_{\text{tot}}^{\text{DFT}}}{N}$, in which $N$ is the number of magnetic ions and $\hbar$ is the Boltzmann constant [34]. The calculated $\Delta E_{\text{tot}}^{\text{DFT}}$ results are shown in figure 3.

For undoped Zn$_{1-x}$Cr$_x$Te ($m_h = 1.0$) and Ga$_{1-x}$Cr$_x$As ($m_h = 2.0$) systems, $\Delta E_{\text{tot}}^{\text{DFT}}$ are negative, indicating that the FM phase is more stable, as expected from the BCM with partially occupied t$_2$-states. In both cases, $\Delta E_{\text{tot}}^{\text{DFT}}$ as a function of $m_h$ curve has the same trends: when the majority Cr t$_2$-states within the bandgap are fully occupied (i.e. $m_h = 0$) by extra electrons, the AFM phase has lower total energy than the FM phase (i.e. $\Delta E_{\text{tot}}^{\text{DFT}} > 0$) due to superexchange interactions between the majority and minority spin d-states. The stability of the AFM phase decreases with increasing number of holes; $\Delta E_{\text{tot}}^{\text{DFT}}$ changes sign at $m_h \approx 0.20$ and 0.35 for Zn$_{1-x}$Cr$_x$Te and Ga$_{1-x}$Cr$_x$As, respectively. A global minimum for $\Delta E_{\text{tot}}^{\text{DFT}}$ occurs at $m_h \approx 1.25$ for Zn$_{1-x}$Cr$_x$Te or $m_h \approx 1.0$ for Ga$_{1-x}$Cr$_x$As, which yields the maximum stability for the FM phase. Further increase in the number of holes decreases the stability of the FM phase.
Figure 2. Schematic BCM diagram based on the p–d and d–d level repulsion between the magnetic Cr ions and the host elements for the FM and AFM phases, as discussed in [6].

i.e. $\Delta E_{\text{DFT}}$ increases continuously up to $m_h = 3$. For $m_h = 3$, which is the maximum number of holes in the Cr $t_2$-states, the FM solution is only a few meV lower in energy than the AFM solution due to the FM superexchange between the spin-up d-states [35].

3.3. The BCM

To obtain a better understanding of the results summarized above, we combined our DFT results with the BCM [6]. In the BCM, the magnetic interactions are described by the p–d and d–d levels repulsion between the magnetic ions and host elements, which are schematically indicated in figure 2. Following the original derivation in [6], the relative energy difference between the FM and AFM phases for the case in which the magnetic ion d-states are located within the bandgap is given by the following equation:

$$
\Delta E^{\text{BCM}}_{\text{tot}} = \begin{cases} 
- (\Delta^1_{dd} + \Delta^{1,2}_{dd}) m_h + 3 \Delta^{1,2}_{dd}, & \text{for } 0 \leq m_h \leq \frac{3}{2}, \\
(\Delta^1_{dd} - \Delta^{1,2}_{dd}) m_h - 3 (\Delta^{1,2}_{dd} - \Delta^{1,2}_{dd}), & \text{for } \frac{3}{2} \leq m_h \leq 3,
\end{cases}
$$

where $\Delta^1_{dd}$ and $\Delta^{1,2}_{dd}$ indicate the double exchange and superexchange parameters, respectively. $m_h$ indicates the number of holes per Cr atom. The parameters $\Delta^1_{dd}$ and $\Delta^{1,2}_{dd}$ are fitted to DFT values at $m_h = 0$ and $m_h = 1.50$. The calculated results are shown in figure 3.

4 We want to point out that in [6], the number of holes is given per Cr pairs, whereas in this work, it is given per Cr atom.

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We see that the BCM results agree reasonably well with the calculated DFT values, except that in the BCM the minimum energy is at $m_h = \frac{3}{2}$, whereas the calculated DFT results show a minimum at $m_h \approx 1.25$ for Zn$_{1-x}$Cr$_x$Te and $m_h \approx 1.0$ for Ga$_{1-x}$Cr$_x$As. The reason for this difference is explained as follows. The BCM assumes that the double exchange and the superexchange parameters are independent of $m_h$. In reality, however, as $m_h$ decreases (more electrons on the $t_2$-orbital), the increased electron Coulomb repulsion delocalizes the d-orbital, thus enlarging the parameters $\Delta_{dd}$ and $\Delta_{dd}^{1,2}$. This is why the DFT minimum shifts toward smaller $m_h$ values than the conventional BCM predicts.

The BCM results in figure 3 suggest that for Zn$_{1-x}$Cr$_x$Te ($m_h = 1.0$), adding holes (e.g. through nitrogen doping) should enhance $T_C$, whereas adding electrons (e.g. through iodine doping) should suppress the $T_C$. As discussed above, this is not supported by the experimental observations [9, 10, 18]. Shifting the minimum toward $m_h \approx 1.25$ in the DFT calculation brings the trend into better agreement with experiment. However, the change in $\Delta E_{\text{DFT}}^{\text{tot}}$ in the range of $1.0 < m_h < 1.5$ is relatively small, and thus does not have a quantitative agreement with experimental observations, in which $T_C$ can change by a factor of ten through the co-doping. These analysis suggest that a homogeneous distribution of magnetic Cr ions cannot explain the variation of $T_C$ as a function of carrier density and that the effect of co-doping is to change the tendency of the spinodal decomposition through the change in Cr–Cr binding energy, as proposed by Kuroda et al [10].
3.4. Cr–Cr binding energy

In the following, we will calculate the binding energy of two Cr atoms in the host semiconductor lattice, \( E_{\text{b}}^{\text{DFT}} \), as a function of \( m_h \) and identify the origin of the carrier-induced variation of the binding energy between the magnetic Cr ions. \( E_{\text{b}}^{\text{DFT}} \) is calculated as follows:

\[
E_{\text{b}}^{\text{DFT}} = E_{\text{tot}}(\text{Cr–Cr}) + E_{\text{tot}}(\text{host}) - 2E_{\text{tot}}(\text{Cr}),
\]

where \( E_{\text{tot}}(\text{Cr–Cr}) \), \( E_{\text{tot}}(\text{Cr}) \) and \( E_{\text{tot}}(\text{host}) \) are the total energies of the host semiconductor with two, one and zero magnetic ions, respectively. An FM interaction was considered for the magnetic ions. The binding energy as a function of \( m_h \) is shown in figure 4.

We find that the DFT Cr–Cr binding energies have similar shapes for both systems. The Cr–Cr interaction is most attractive at \( m_h \approx 1.0 \), but becomes less attractive by increasing or decreasing the number of holes around \( m_h \approx 1.0 \). Thus, the formation of Cr-rich aggregates (or spinodal decomposition) is most likely for \( m_h \approx 1.0 \). The above DFT-calculated trends are similar to the findings of Kuroda et al [10] for \( \text{Zn}_{1-x}\text{Cr}_x\text{Te} \), but a closer look into the results indicates that the origin is not due to the Coulomb repulsion as suggested by them [10], because by taking into account the Coulomb interaction between the Cr ions alone, the strong binding energy should occur when the magnetic Cr ion becomes neutral, i.e. \( m_h \) goes to \(-1\). Moreover, if the Coulomb repulsion is minimum when the Cr defect level is neutral, then the binding energy minimum for ZnTe:Cr and GaAs:Cr should occur at different values of \( m_h \), e.g. \( m_h = 1 \) for ZnTe:Cr and \( m_h = 2 \) for GaAs:Cr.
We found that the calculated binding energy trends can be explained by the magnetic interactions between the Cr ions using the BCM, figure 2. In the BCM, the binding energy between two Cr ions \( E_{\text{BCM}}^b \) for the FM configuration can be calculated using the equations below:

\[
E_{\text{BCM}}^b = \begin{cases} 
-m_h \Delta_{1d}^1 - 2m_h \Delta_{1pd}^1 - 6 \Delta_{pd}^2, & \text{for } 0 \leq m_h \leq \frac{3}{2}, \\
-(3 - m_h) \Delta_{1d}^1 - 2m_h \Delta_{1pd}^1 - 6 \Delta_{pd}^2, & \text{for } \frac{3}{2} \leq m_h \leq 3,
\end{cases}
\]

along with DFT-derived parameters. The results are shown in figure 4. The binding energy as a function of \( m_h \) has a V shape, which is consistent with the DFT results. The largest binding energy from BCM occurs at \( m_h = \frac{3}{2} \), whereas DFT yields a minimum at \( m_h \approx 1.0 \). This shift of maximum binding energy position can be explained by the increased d–d coupling with reduced \( m_h \), as explained above, and the slightly reduced Coulomb repulsion between the Cr ions as \( m_h \) decreases. However, we want to emphasize that the dominant contribution to the binding between the Cr ions is the magnetic interaction, not the Coulomb interaction, which is largely screened by host electrons [36].

To compare and explain the experimental observations, we need to take into account that at normal growth conditions, ZnTe is a native p-type semiconductor with a typical hole concentration of \( \approx 10^{18} \text{ cm}^{-3} \), which is usually attributed to the formation of Zn vacancies [9, 10, 18]. This suggests that in Zn\(_{1-x}\)Cr\(_x\)Te, the initial \( m_h \) is slightly larger than 1.0 and its exact value depends on the growth conditions. For n-type (iodine) doping, \( m_h \) is reduced. From figure 4, we see that \( \Delta E_{\text{DFT}}^b \) first becomes more negative (more binding), so \( T_C \) increases due to increased spinodal decomposition. However, when \( m_h \) is reduced to less than 1.0, a further decrease of \( m_h \) (or increase of iodine doping) will make \( \Delta E_{\text{DFT}}^b \) less negative, that is, \( T_C \) will decrease. For p-type (nitrogen) doping, \( \Delta E_{\text{DFT}}^b \) always becomes more positive, and thus reduces \( T_C \). These trends (nitrogen) doping, \( \Delta E_{\text{DFT}}^b \) always becomes more positive, and thus reduces \( T_C \). These trends are consistent with the experimental observations [9, 10, 18], which have been explained based on the spinodal decomposition and supported by our results.

4. Summary

In summary, using DFT calculations combined with the BCM, we have successfully explained the puzzling behavior of the change of \( T_C \) as a function of n-type and p-type dopings in Zn\(_{1-x}\)Cr\(_x\)Te. We show that the binding energy between the magnetic Cr ions, which drives the formation of Cr-rich regions (spinodal decomposition), is mainly due to the energy gain originated from the magnetic interaction between Cr atoms. Our analysis show that the increased d–d coupling is the origin of the shift of the maximum binding energy from \( m_h = \frac{3}{2} \) to \( m_h \approx 1.0 \). Furthermore, our results point a way to enhance ferromagnetism (\( T_C \)) in other DMSs such as Ga\(_{1-x}\)Cr\(_x\)As.

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References

[1] Koshihara S, Oiwa A, Hirasawa M, Katsumoto S, Iye Y, Urano C, Takagi H and Munekata H 1997 Phys. Rev. Lett. 78 4617
[2] Ohno H 1998 Science 281 951
[3] Jungwirth T, Sinova J, Kucera J and MacDonald A H 2006 Rev. Mod. Phys. 78 809
[4] Dietl T 2002 Semicond. Sci. Technol. 17 377
[5] Katayama-Yoshida H, Sato K, Fukushima T, Toyoda M, Kizaki H, Dinh V A and Dederichs P H 2007 Phys. Status Solidi a 204 15
[6] Dalpian G M, Wei S-H, Gong X G, da Silva A J R and Fazzio A 2006 Solid State Commun. 138 353
[7] Walsh A, Da Silva J L F and Wei S-H 2008 Phys. Rev. Lett. 100 256401
[8] Saito H, Zayets V, Yamagata S and Ando K 2003 Phys. Rev. Lett. 90 207202
[9] Ozaki N, Nishizawa N, Marcel S, Kuroda S, Eryu O and Takita K 2006 Phys. Rev. Lett. 97 037201
[10] Kuroda S, Nishizawa N, Takita K, Mitome M, Bando Y, Osuch K and Dietl T 2007 Nat. Mater. 6 440
[11] Park S E, Lee H-J, Cho Y C, Jeong S-Y, Cho C R and Cho S 2002 Appl. Phys. Lett. 80 4187
[12] Reed M L, El-Masry N A, Stadelmaier H H, Ritums M K, Reed M J, Parker C A, Roberts J C and Bedair S M 2001 Appl. Phys. Lett. 79 3473
[13] Thaler G T et al 2002 Appl. Phys. Lett. 80 3964
[14] Tiwari A, Bhosle V M, Ramachandran S, Sudhakar N, Narayan J, Budak S and Gupta A 2006 Appl. Phys. Lett. 88 142511
[15] Fernandes V, Klein J J, Mattoso N, Mosca D H, Silveira E, Ribeiro E, Schreiner W H, Varalda J and de Oliveira A J A 2007 Phys. Rev. B 75 121304
[16] Vodungbo B, Zheng Y, Vidal F, Demaille D, Etgens V H and Mosca D H 2007 Appl. Phys. Lett. 90 062510
[17] Liu H, Zhang X, Li L, Wang Y X, Gao K H, Li Z Q, Zheng R K, Ringer S P, Zhang B and Zhang X X 2007 Appl. Phys. Lett. 91 072511
[18] Ozaki N, Okabayashi I, Kumeckawa T, Nishizawa N, Marcel S, Kuroda S and Takita K 2005 Appl. Phys. Lett. 87 192116
[19] Dietl T, Ohno H, Matsukura F, Cibert J and Ferrand D 2000 Science 287 1019
[20] Sato K and Katayama-Yoshida H 2002 Semicond. Sci. Technol. 17 367
[21] Sato K, Katayama-Yoshida H and Dederichs P H 2005 Japan. J. Appl. Phys. 44 L948
[22] Sato K, Fukushima T and Katayama-Yoshida H 2007 Japan. J. Appl. Phys. 46 L682
[23] Sato K and Katayama-Yoshida H 2007 Japan. J. Appl. Phys. 46 L1120
[24] Fukushima T, Sato K, Katayama-Yoshida H and Dederichs P H 2004 Japan. J. Appl. Phys. 43 L1416
[25] Fukushima T, Sato K, Katayama-Yoshida H and Dederichs P H 2006 Japan. J. Appl. Phys. 45 L416
[26] Fukushima T, Sato K, Katayama-Yoshida H and Dederichs P H 2006 Phys. Status Solidi a 203 2751
[27] Fukushima T, Sato K, Katayama-Yoshida H and Dederichs P H 2006 Physica B 376 786
[28] Blöchl P E 1994 Phys. Rev. B 50 17953
[29] Kresse G and Joubert D 1999 Phys. Rev. B 59 1758
[30] Kresse G and Hafner J 1993 Phys. Rev. B 48 13115
[31] Kresse G and Furthmüller J 1996 Phys. Rev. B 54 11169
[32] Saito H, Zayets V, Yamagata S and Ando K 2002 Phys. Rev. B 66 081201
[33] Baron T, Saminadayar K and Magnea N 1998 J. Appl. Phys. 83 1354
[34] Sato K, Dederic P H and Katayama-Yoshida H 2003 Europhys. Lett. 61 403
[35] Belhadj B, Bergqvist L, Zeller R, Dederichs P H, Sato K and Katayama-Yoshida H 2007 J. Phys.: Condens. Matter 19 436227
[36] Raebiger H, Lany S and Zunger A 2008 Nature 453 763

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