Effect of P-anion codoping on the Curie temperature of GaMnAs diluted magnetic semiconductors

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Recent measurements of GaMnAs alloy samples with a very small content of P atoms prepared by ion-implanted pulsed laser melting (II-PLM) [Phys. Rev. Lett. **101**, 087203 (2008)] have shown surprisingly low Curie temperature as compared to undoped samples. An explanation based on a possible metal-insulator transition at constant Mn doping was proposed based on a dramatic increase of the sample resistivity. However, no quantitative calculations supporting such a picture as concerns the Curie temperature were shown. We will present a parameter-free theory of the Curie temperature (T_C) which assumes that possible defects due to the II-PLM such as, e.g., space inhomogeneities, vacancies, clustering, and also conventional compensating defects will reduce the sample hole concentration. Their effect was first qualitatively modeled in the framework of the rigid-band model by adjusting the system Fermi level due to the reduction of the carrier concentration which is considered as a parameter of the theory. In addition, the effect of possible conventional compensating defects, such as, e.g., As and P antisites or P and Mn interstitials was also investigated. T_C's are calculated within the self-consistent local RPA (SCLRPA) and Monte Carlo (MC) simulations. We will demonstrate that a reasonable agreement of calculated and measured T_C can be obtained for reduced hole concentrations which are known to exist in GaMnAs samples. As concerns possible specific defects, we have shown that P and Mn interstitials are particularly effective in the reduction of the sample Curie temperature.

I. INTRODUCTION

Diluted magnetic semiconductors (DMS) rank among the physically most interesting materials. DMS are also promising technologically in spintronics due to the possibility to control both carrier concentration and magnetic properties in a single device. In the past the largest effort, both experimental and theoretical, was devoted to GaMnAs alloys.[1] One of the most important characteristics of magnetic state of DMS is their Curie temperature (T_c). While the Curie temperature is extremely difficult quantity to estimate, in particular on a parameter-free level, a relatively clear picture has emerged based on a recent development.[2–4] The Curie temperature in GaMnAs strongly depends on their technological preparation, in particular on the amount of compensating defects, i.e., the Mn atoms on interstitial positions (close either to As or Ga sublattices) and on As antisites on Ga sublattice. By careful annealing of MBE-prepared samples it is possible to prepare samples with negligible amount of Mn interstitials while the presence of As antisites is still under question. Recent first-principles calculations respecting random distribution of Mn atoms on Ga sublattice (magnetic percolation or the dilution effects) have lead to a good quantitative agreement with available experimental data for both optimally annealed samples[2–4] and samples partially compensated.[5]

Recent experiments on GaMnAs samples doped with low content of P atoms (up to about 3% atomic percent)[6] resulted in a dramatic reduction of the Curie temperature (T_C^{exp} =60 K) to approximately one half of its value in undoped sample. This is surprising result which also contradicts recent theoretical estimates of the Curie temperature for GaMnAs alloys upon P doping. While enhancement of T_c with increasing P content was predicted in Ref. 7, a weak decrease over the whole concentration range was found in Ref. 8. The effect of electron correlations was included in Ref. 7 and in both models a simplified treatment of the Curie temperature was used. It is important to note that in both papers the effect of compensated defects was neglected. Authors of above mentioned experiment have employed a different technology for P codoping, namely, the II-PLM (ion-implanted pulsed laser melting). Authors ascribe the reduction of T_c to a scenario in which holes located within an impurity band are scattered by alloy disorder on the anion sublattice assuming metal-insulator transition at a constant Mn doping (4.6% specifically). Their arguments are thus purely speculative, no attempt was made to estimate the Curie temperature of such sample.

Increased disorder upon doping, or, alternatively dramatically shorter mean-free path of holes is, however, clearly documented by an increased sheet-resistance (about ten times) as compared to the undoped case. The *sp* disorder on ideal lattice due to substitutional P atoms on As sublattice is generally weak one. As and P atoms are from the same column of the Periodic Table and thus small level disorder has to be expected, in particular for broad *sp* bands. A clear example is the *sp* alloying in Heusler alloys[9] in which the disorder results essentially in the rigid shift of the Fermi energy (which is missing for isocoric elements such as, e.g., As, Sb, and P). The resulting disorder is thus very weak and

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cannot be origin of such dramatic change of the resistivity if the driving effect is just the substitution of P atoms on a perfect As lattice with very low P doping. We think that origin of such large effect of P doping is due to the II-PLM technology. The presence of possible structural defects such as clustering, space inhomogeneities, vacancies, etc. can lead to a formation of quasilocalized states close to the top of the valence band where the Fermi level lies. The conductivity in the energy region of quasilocalized states is essentially of hopping type resulting in much larger resistivity as compared to the conventional residual resistivity. The latter seems to be the case in reasonably annealed samples prepared by the MBE technology.[10] This makes the discussion of transport properties very uncertain in the framework of conventional transport theory of residual resistivity (based on Boltzmann and/or Kubo-Greenwood approaches).

On the other hand, both the presence of compensating and/of structural defects can lead to a reduction of the effective hole concentration making thus possible to estimate the Curie temperature because it is primarily determined by carrier concentration. Unfortunately, the quantity which would allow to address such problem in detail, namely the effective hole concentration,[5] was not determined in the above mentioned experiments.

We will therefore present results of the T_c estimate in two models, namely, (i) assuming a reduction of the hole concentration by some amount and estimating corresponding exchange integrals in the framework of the rigid band model (RBM) by shifting the Fermi energy of properly chosen reference state to a new position which will accommodate corresponding number of holes (the reference state will be the case with substitutional Mn and P atoms), and (ii) assuming the presence of possible compensating defects in amount typical for GaMnAs (in this case are exchange integrals estimated for the hole concentration determined self-consistently for a given defect concentrations). We wish to verify that such strong reductions of T_c can be obtained in the framework of the theory without adjustable parameters just assuming a reasonable reduction of carrier concentration.

II. FORMALISM

The electronic structure calculations were performed using the tight-binding linear muffin-tin orbital (TB-LMTO) approach.[11] The zinc-blende lattice is simulated by inserting two empty spheres into the unit cell for a good space filling. We have employed optimized Wigner-Seitz radii (the smallest possible overlap of atomic spheres and natural atomic radii for a given structure) but results obtained by using the same Wigner-Seitz radii for all atoms and empty spheres were almost the same. The *spd* basis was employed.

It is well known that Ga 3*d*-states are too close to the valence band complex in the LSDA thus leading to a strong overbinding if the Ga 3*d* states are included as valence states. Instead, we have considered them as core states (underestimation of the binding). This approach gives a good description of both the bandwidth and the band gap (about 1.31 eV) as compared to the conventional approach.

The effect of chemical disorder was described by the coherent potential approximation (CPA) (for more details see Ref. [11]). Specifically, we have considered P- and Mn-interstitial atoms in positions close to As atoms and both As and P antisites on Ga sublattice. The CPA is particularly suitable to describe low concentration of various defects on equal footing. Low concentration of defects is usually well represented by their random distribution as contrasted with concentrated alloys where the ordering and/or segregation effects are more probable. It is well known that the CPA describes reliably the alloy carrier concentration and thus the system Fermi energy and its Fermi surface topology. These quantities are relevant for a reliable estimate of exchange integrals. We thus assume that the CPA can be employed as a reasonable starting point for the estimate of T_C. On the other hand, effects of a possible clustering, space inhomogeneities, and of a partial state localization at band edges are not included in the CPA. The problem is particularly delicate as concerns the estimate of transport properties while the effect of clustering on the Curie temperature was discussed in the past.[12,13]

The thermodynamical properties of the system are described by a classical random Heisenberg Hamiltonian making use of a two-step model,[14]

$$H_{\text{eff}} = -\sum_{i,j} J_{ij} \mathbf{e}_i \cdot \mathbf{e}_j \qquad (1)$$

and its extension into random alloys.[15,16] Here i,j are site indices, $\mathbf{e}_i$ is the unit vector pointing along the direction of the local magnetic moment at site i, and J_{ij} is the exchange integral between sites i and j. Exchange integrals J_{ij} are random quantities, which are nonzero only between sites occupied by magnetic atoms. The exchange integrals, by construction, contain the atom magnetic moments, their positive (negative) values being indicative of ferromagnetic (antiferromagnetic) coupling. It should be noted that for an evaluation of exchange integrals we assume a FM reference state. Induced moments on anion-sites are very small and their effect can be safely neglected.

As concerns the statistical part, we determine the Curie temperature corresponding to the effective Heisenberg model in Eq. (1) by making use of the mean-field approximation (MFA), the self consistent local random-phase (SCLRPA), and Monte Carlo (MC) calculations. The essential point in the statistical treatment is the magnetic percolation phenomenon or the effect of dilution. Thus, the effect of random distribution of Mn atoms has to be included properly. The virtual-crystal approximation or the MFA frequently used in model studies[1] has to be avoided. We employ the Monte Carlo sampling of Mn atoms in a simulation cell in both the SCLRPA[3] and MC treatments.[2] The SCLRPA-Curie temperatures are close to those obtained from Monte Carlo simulations[16] while the MFA is qualitatively wrong for diluted systems. Note that the SCLRPA is numerically few orders of magnitude more efficient as compared to the MC. Because the SCLRPA estimate is formulated for the ferromagnetic state, some errors can occur when superexchange interactions become possible (e.g., in the case of large compensations) when the Fermi level is sufficiently close to unoccupied minority Mn states.[15] Such interactions can induce the spin canting and thus influence the value of the Curie
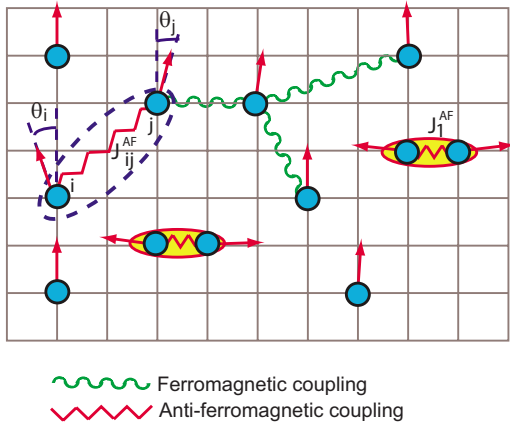
FIG. 1. (Color online) Illustration of a spin configuration with canting effects: depending on the strength of the antiferromagnetic couplings for some spins is energetically more convenient the canted (angle θ_i) configuration rather than a collinear one. For very large AF-couplings (J_1^{AF} in the figure) it may happen that some spins become almost orthogonal to the others.

temperature quantitatively. Recently it was demonstrated that the effect of spin canting (see Fig. 1 for an illustration) can be included systematically in the framework of the SCLRPA (the ground state is then calculated in order to deal with a good spin texture) leading again to a very good quantitative agreement with the Monte Carlo estimates.[17]

Finally, the presence of Mn-substitutional and Mn-interstitial atoms represents another complication which was, fortunately, recently solved by using the theory which takes into account only magnetically active atoms on Ga sublattice. A simple theory which employs effective concentrations of magnetically active atoms and the effective carrier concentration has lead to a good quantitative agreement with available experimental data for partially compensated samples.[5]

Technically, we have included 62 shells of calculated exchange integrals in the SCLRPA method while the first 25 shells were used in the Monte Carlo simulations. It was checked that the sizes of simulation cells and number of random realizations were enough the warrant accuracy few K for the Curie temperature.

III. RESULTS AND DISCUSSION

First we will consider the effect of defects on T_C in the framework of the RBM and then we will discuss some specific defects in detail.

A. Rigid band model

We shall concentrate on the sample with the lowest T_C which corresponds to P concentration of 3.1%. The reference case is thus alloy $(\mathrm{Ga}_{0.954},\mathrm{Mn}_{0.046})(\mathrm{As}_{0.969},\mathrm{P}_{0.031})$ with substitutional Mn and P atoms but without compensation defects. For a comparison we have also considered the undoped $(\mathrm{Ga}_{0.954},\mathrm{Mn}_{0.046})\mathrm{As}$ alloy for which the estimated value of the Curie temperature is 123 K in good agreement with the experimental value $T_C^{exp}=112$ K.[6] If one assumes no com-
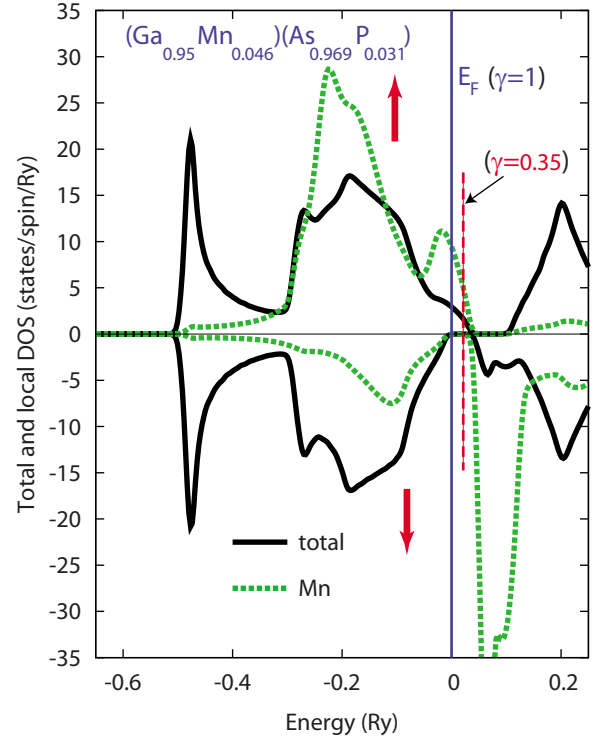

FIG. 2. (Color online) LDA calculation of the density of states for $(\mathrm{Ga}_{0.954},\mathrm{Mn}_{0.046})(\mathrm{As}_{0.969},\mathrm{P}_{0.031})$ (the Mn d states are represented with an augmented scale). The vertical continuous and dashed lines correspond to the Fermi level E_F for $n_{hole}=0.046$ (or $\gamma=n_{hole}/x_{\mathrm{Mn}}=1$) and $n_{hole}=0.016$ or $\gamma=0.35$), respectively.

pensating defects then within the accuracy of our approach are estimated T_C for above two alloys with and without P dopants the same. These results are also in agreement with previous studies.[7,8] To explain a strong reduction of T_C due to the inclusion of P dopants via II-PLM technology we will assume that various defects are present which result in a decrease of the hole concentration. We will consider the hole concentration as a parameter of the theory but for each concentration we determine the corresponding exchange integrals. To this end we have employed the RBM by assuming that the exchange integrals are determined using potentials corresponding to the reference $(\mathrm{Ga}_{0.954},\mathrm{Mn}_{0.046})(\mathrm{As}_{0.969},\mathrm{P}_{0.031})$ alloy but with the Fermi energy modified in such a way that the valence hole concentration n_{hole} is 0.046, 0.036, 0.026, and 0.016. In Fig. 2 we have plotted the density of states for the reference $(\mathrm{Ga}_{0.954},\mathrm{Mn}_{0.046})(\mathrm{As}_{0.969},\mathrm{P}_{0.031})$ alloy. It should be noted that the hole concentration 0.046 corresponds to an ideal case without any compensating defects (the Fermi energy is indicated by the continuous vertical line in Fig. 2). The corresponding compensation ratio γ is defined as $\gamma=n_{holes}/x_{\mathrm{Mn}}$, where $x_{\mathrm{Mn}}=0.046$. For the ideal, uncompensated case is $\gamma=1$ while the largest compensation $\gamma=0.35$ corresponds to $n_{hole}=0.016$ (dashed vertical line in Fig. 2) is still acceptable for compensated GaMnAs samples.[1]

In Fig. 3 we have plotted the exchange integrals (in Rydberg) for $(\mathrm{Ga}_{0.954},\mathrm{Mn}_{0.046})(\mathrm{As}_{0.969},\mathrm{P}_{0.031})$ for the densities of holes $n_{hole}=0.046$, 0.036, 0.026, and 0.016. While reducing the hole density we observe that most of the relevant cou-
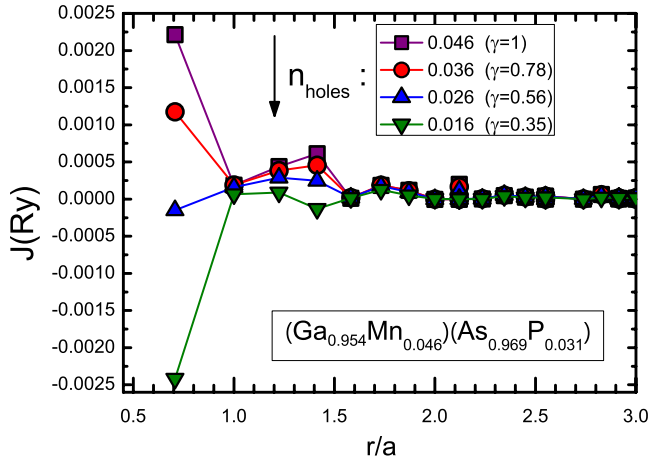
FIG. 3. (Color online) LSDA calculation of the exchange integrals (in Rydberg) for $(Ga_{0.954},Mn_{0.046})(As_{0.969},P_{0.031})$ alloy for various densities holes $n_{hole}=0.046$, 0.036, 0.026 and 0.016.

plings decrease monotonically. Note that the first coupling J_1 decreases and becomes antiferromagnetic for the two lowest hole densities. For $n_{hole}=0.026$ the coupling J_1 is relatively weak and the canting angles are expected to be small. While for $n_{hole}=0.016$ J_1 is strongly antiferromagnetic and J_4 (at the distance $r=\sqrt{2}a$) is also negative. In this last case the effect of the canting is expected to be strong.

In Fig. 4 we have plotted the Curie temperatures (in Kelvin) as a function of the hole density for $(Ga_{0.954},Mn_{0.046})(As_{0.969},P_{0.031})$ in the SCLRPA, and MC approaches. The inset corresponds to T_C (in K) in the MFA approximation.

We find a good agreement between the calculated and measured T_C for ideal sample without compensating defects ($\gamma=1$). The expected decrease of calculated T_C with reduced hole concentration is clearly observed. Both the SCLRPA and MC estimates are close each to other while the MFA
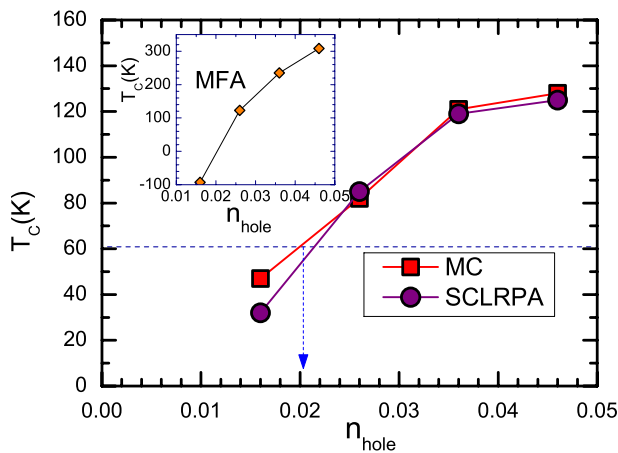

FIG. 4. (Color online) Calculated Curie temperatures (in Kelvin) as a function of the hole density for $(Ga_{0.954},Mn_{0.046})(As_{0.969},P_{0.031})$ alloys in the SCLRPA, and MC approaches. The horizontal dashed line indicates the experimental value for the P-doped sample $T_C^{exp}=60$ K (Ref. 6). Inset: critical temperature (in K) in the MFA approximation.

generally strongly overestimates T_C as a consequence of the neglect of magnetic percolation effects.[2]

In the case of the smallest hole concentration $n_{holes}=0.016$, strong superexchange coupling was found giving the first nearest-neighbors negative coupling (the AFM coupling). In this case the MFA gives the negative value (-93 K) of T_C indicating the lost of the ferromagnetic order. Note that the T_C^{MFA} is controlled here by the large antiferromagnetic coupling J_1 (if J_1 is omitted from the MFA sum a value of 52 K is obtained).

As said above spin-canted effects are expected to be strong in this case. Thus the SCLRPA calculations have been performed including the effect of spin canting[17] which lead to the Curie temperature value $T_C^{SCLRPA}=32$ K. This value is in agreement with the MC simulations ($T_C^{MC}=45$ K) in which the effect of canting is properly included.

It should be noted that AFM couplings are due to decreasing energy separation between the Fermi energy and unoccupied minority Mn-states due to reduced hole concentration (see Fig. 2) which in turn enhances the superexchange part of the exchange couplings. The superexchange contribution decreases exponentially with the separation of magnetic atoms so that only the first and/or first two couplings are actually influenced. There is thus competition between the RKKY-like and superexchange parts of the exchange interaction which are both present in the first-principle approach used here. While it is difficult to separate them out in the first-principle approach in general, in specific cases the signature of such competition can be trace down. This is, for example, the case of semi-Heusler alloys with varying carrier concentration due to the alloying on the *sp* sublattice. We refer the reader to Ref. 18 for more detailed discussion. The results indicate that the experimental $T_C^{exp}=60$ K is reached for n_{holes} about 0.02 or $\gamma\simeq0.43$ which is a reasonable value.

B. Specific defects

This part is to some extend speculative one. We wish to investigate here the effect of As and P antisites as well as of P and Mn interstitials. Due to ion implantation technology such defects could be present. The reality represents a combined effect of various defects which is difficult to describe without a detailed knowledge of their concentrations. Therefore, we will investigate the effect of each of above mentioned defects separately. Such defects concentration can exist in GaMnAs samples[1] and we will assume a fixed defect concentration of 1% in each case. In the following we consider first three kinds of alloys: (i) $(Ga_{0.944},Mn_{0.046}As_{0.01})(As_{0.969},P_{0.031})$, (ii) $(Ga_{0.944},Mn_{0.046},P_{0.01})(As_{0.969},P_{0.021})$, and (iii) $(Ga_{0.944},Mn_{0.046},As_{0.01})(As_{0.969},P_{0.021})$ with 1% of P interstitials close to As sublattice. In Fig. 5 we present the calculated exchange integrals (in Rydberg) for that set of alloys with a density of holes sets to $n_{hole}=0.026$. Except from the first coupling, we observe that the exchange integrals are very similar in the case of the presence of As and P antisites. Thus we expect similar Curie temperatures for those two kinds of defects. In the case of the presence of P-interstitials defects, the nearest-neighbor coupling J_1 is found to be
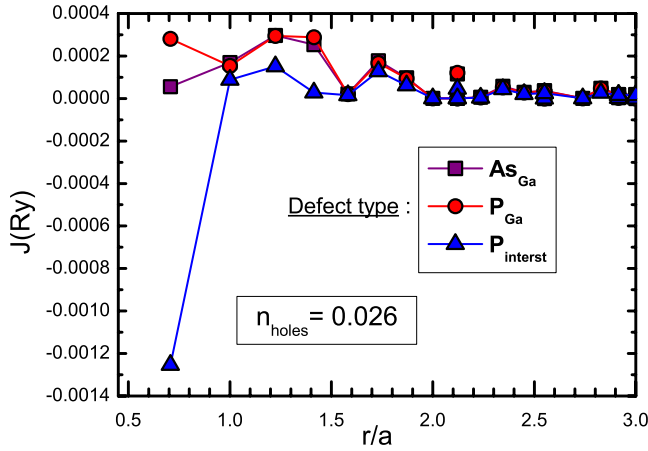
FIG. 5. (Color online) Exchange integrals (in Rydberg) as a function of the distance r (in unit of the lattice parameter (a) between two Mn spins for three types of specific defects: As_{Ga}, P_{Ga}, and $P_{interst}$. In each case the density of holes is $n_{hole}=0.026$.

strongly antiferromagnetic. Thus we expect to have a canted phase in which the set of the canted spins are almost orthogonal to the others (see the left panel of Fig. 6 for an illustration). In this case one can consider that the canted pairs are decoupled from the rest of the Mn spins. Thus in a simplified approach of the canting we have used the SCL-RPA by considering an effective Mn density (calculated for each configuration of Mn distribution) $x_{eff}=x-x_{cant}$ where x_{cant} is the density of full canted spins (see the right panel of Fig. 6 for an illustration).

In Fig. 7 we present the corresponding results for the Curie temperatures (in Kelvin). We see again a good overall agreement between SCLRPA and MC results while the MFA leads again to much larger T_C values (except from the last case where T_C^{MFA} is controlled by the strong antiferromagnetic coupling J_1). It is seen that the presence of P-interstitial atoms leads to a strong reduction of the system's Curie temperature. Moreover the agreement between the SCLRPA and MC calculation shows the confirmation of the presence of a canted phase. Both types of antisites also reduce T_C but their effect for a given concentration is weaker, and as expected we found similar critical temperatures.
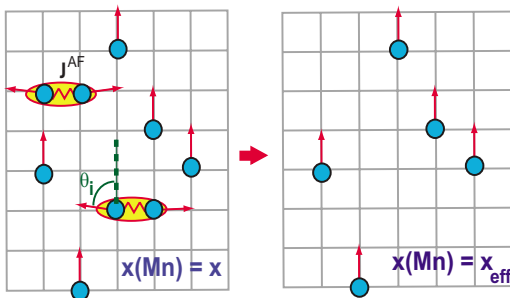

FIG. 6. (Color online) (left panel) A proportion x_{cant} of Mn spins are orthogonal (large canting $\theta_i \simeq \frac{\pi}{2}$) to the others due to a sufficiently important nearest-neighbor antiferromagnetic exchange coupling J^{AF}. (right panel) After removing all theses canted spins the effective density of Mn spins becomes $x_{eff}=x-x_{cant}$.

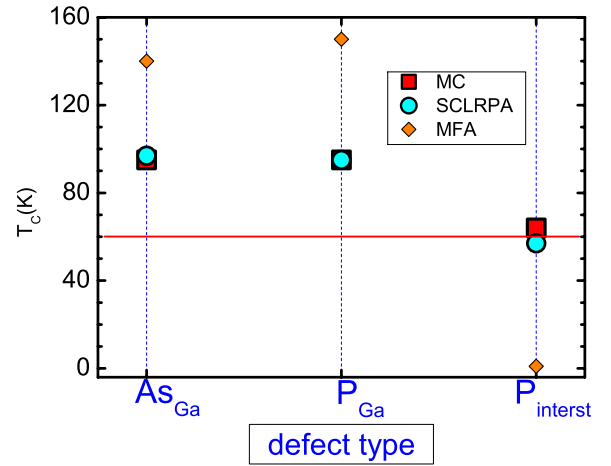FIG. 7. (Color online) Calculated Curie temperatures (in Kelvin) for (i) $(Ga_{0.944},Mn_{0.046}As_{0.01})(As_{0.969},P_{0.031})$, (ii) $(Ga_{0.944},Mn_{0.046},P_{0.01})(As_{0.969},P_{0.021})$, and (iii) $(Ga_{0.944},Mn_{0.046},As_{0.01})(As_{0.969},P_{0.021})$ with 1% of P interstitials close to As sublattice. The critical temperatures are calculated in the MFA, SCLRPA, and MC approaches. The horizontal line indicates the experimental value for the doped sample $T_C^{exp}=60$ K (Ref. 6). (The density of holes is set to $n_{hole}=0.026$.)

Finally, we have also tested the effect of Mn interstitials in the tetrahedral $T(As_4)$ position by using the model described in detail in Ref. 5. For 1% of Mn-interstitials the estimated Curie temperature is equal to 70 K (MC calculations result). This demonstrates that Mn interstitial, if present in the sample, can also reduce the Curie temperature effectively. Once again, the concentration of Mn interstitials (1%) is quite reasonable in real samples as shown, e.g., in Ref. 5. At the end we wish to point out that more specific estimates of actual defect concentrations are very difficult[6] and more experiments and corresponding theoretical estimates are needed for more detailed study.

IV. CONCLUSIONS

We have developed a simple, parameter-free theory of the Curie temperature of GaMnAs alloy codoped with P atoms by the II-PLM method. We have assumed that defects such as, e.g., clustering, space inhomogeneities, vacancies, the formation of partially localized states at the band edges, and the presence of some compensating defects will lead to a reduction of the carrier concentration which in turn will reduce the system Curie temperature compared to the undoped case. Because it is experimentally difficult to estimate the hole concentration quantitatively, we have determined T_C by assuming the carrier concentration as a parameter of the theory. The corresponding exchange integrals are, however, determined for each compensation separately assuming the rigid-band model. In this approach electronic structure of a properly chosen reference system is frozen while the Fermi energy is shifted to accommodate a reduced number of holes. The following main conclusion can be made: (i) without any compensating defects and for low P concentration is the change of T_C negligible; (ii) assuming the physically accept-

able reduction of the hole concentration and the SCLRPA we were able to obtain a fair agreement with experimentally measured Curie temperature; and (iii) the effect of specific defects such as As and Pantisites, P and Mn interstitials acting separately was also considered. Both P and Mn interstitials, if present in the sample, are very efficient in the reduction of the Curie temperature while the effect of As and P antisites is relatively weak. In the future it would be important to estimate, at least roughly, the hole concentration in the sample which will allow a more quantitative estimate of T_C.

There are clear differences between (Ga,Mn)(As,P) alloys prepared by MBE and II-LPM methods. In particular recent measurements based on samples prepared by the MBE method[19] give a small reduction of T_C and/or increase of

resistivity even for 10% of P impurities on the As sublattice. It should be noted that the present approach can be applied also to the MBE-prepared samples.

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