

Accuracy of Real Space Cluster Expansion for Total Energies of Pd-rich PdX (X=Rh, Ru) Alloys, based on Full-Potential KKR Calculations for Perfect and Impurity Systems

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Abstract. We study the accuracy and convergence of the real space cluster expansion (RSCE) for the total energies of the Pd-rich PdX (X=Ru, Rh) alloys, which are used to study the phase stability and phase equilibria of the Pd-rich PdX alloys. In the present RSCE, the X atoms of minor element are treated as impurities in Pd. The n -body interaction energies (IEs) among X impurities in Pd, being used in the expansion of the total energies of the Pd-rich PdX alloys, are determined uniquely and successively from the low body to high body, by the full-potential Korringa-Kohn-Rostoker (FPKKR) Green's function method (FPKKR) for the perfect and impurity systems (Pd-host and X_n in Pd, $n=1\sim 4$), combined with the generalized gradient approximation in the density functional theory. In the previous paper, we showed that the RSCE, in which the perturbed potentials due to the insertion of X_n impurities in Pd were redetermined self-consistently up to the first-nearest neighboring (m) host atoms around X_n impurities, reproduce fairly well (the error of ~ 0.2 mRy per atom) the FPKKR-band-calculation result of the ordered Pd₃Rh alloy in L1₂ structure, but a little wrongly (the error of ~ 0.7 mRy per atom) for the ordered Pd₃Ru alloy in L1₂ structure. In the present paper, we show that this small RSCE error for the Pd₃Ru alloy is corrected very well (from ~ 0.7 mRy to ~ 0.1 mRy per atom) by enlarging the self-consistent region for the perturbed potentials up to the 2nd- m host atoms around X_n impurities in Pd. We also clarify the correction for each value of the n -body ($n=1\sim 4$) IEs.

1 Introduction

The knowledge of interaction energies of point defects in solids is indispensable for the understanding of many basic physical processes, such as diffusion, short-range order, and phase diagrams, *etc.* We have shown that the type of phase diagrams of A-rich AX binary alloys of host (A) and impurity (X) elements, such as segregation, solid solution, and order known experimentally, may be very well discriminated by use of the sign and magnitude of the first-nearest neighboring (m) 2-body (X_2) interaction energies (IEs) in A [1]. We have also succeeded in describing the relative stabilities among different atomic structures by using the 2-body and 3-body IEs among X impurities in A; the stabilities of the ordered Al-rich AlX (X=Sc~V) alloys, the stability of AlMn quasicrystal, and the shapes of agglomerates of X impurities in the initial stage of the formation of the so-called Guinier-Preston zones of Al-rich Al_{1-c}X_c (X=Cu, Zn; $c<0.05$) alloys, such as the (001) disc in Al-rich AlCu alloys and the spherical shape in Al-rich AlZn alloys [2-5]. All of these stabilities were obtained by the present

real space cluster expansion (RSCE) [2-7]. The n -body ($n=1\sim 4$) IEs among X impurities in A were determined by the *ab-initio* calculations based on the full-potential Korringa-Kohn-Rostoker Green's function method (FPKKR) for the perfect and impurity systems (A-host and X_n impurities in A, $n=1\sim 4$), combined with the generalized gradient approximation in the density functional theory [8, 9].

We recently succeeded in quantitatively reproducing the X-concentration dependence of the observed solvus temperatures of the Pd-rich PdX (X=Ru, Rh) alloys in fcc structure [10], by the free energy calculations based on the cluster variation method (CVM) [11-13]. The internal energies in the free energies of the Pd-rich PdX (X=Ru, Rh) alloys, were calculated by use of the present RSCE from a dilute limit [2-7]. We have already studied the distance dependence of the 2-body IEs, the local lattice distortion for the 2-body IEs, existing even at 0K, and both the temperature effects for (1) the thermal vibration by the Debye-Grüneisen model and (2) the electron excitation due to the Fermi-Dirac (FD) distribution [11-13]. We very recently showed that the present RSCE

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reproduces fairly well the FPKKR-band-calculation results for total energies of the ordered Pd₃X (X=Ru, Rh) alloys in L1₂ structure (X-concentration = 25%) by including the 2-body IEs up to the 20th-*nn* pair (X₂) and the 3-body IEs up to the clusters (X₃) in two cubic cells in fcc structure [14]. We obtained the nice agreement (the error of ~ 0.2mRy per atom) for the Pd₃Rh alloy, while slightly wrong result (the error of ~ 0.7mRy per atom) for the Pd₃Ru alloy. We considered that this difference between the RSCE results for X=Ru and for X=Rh might be due to the difference of the delocalization of the perturbed potentials in the X_{*n*} impurity systems, depending on the delocalization of 4d orbitals of X impurities. It is noted that in these calculations, the perturbed potentials due to the insertion of X impurities were self-consistently redetermined up to the first-*nn* host atoms around X_{*n*} impurities in Pd, as in the usual KKR calculations for the impurity systems [9].

The purpose of the present paper is to study how the RSCE results are improved by enlarging the self-consistent (sc) region for the perturbed potentials around impurities in Pd. In Section 2, we describe the calculation procedures for the *ab-initio* calculations based on the full-potential Korringa-Kohn-Rostoker (FPKKR) method with the electron excitation effect due to the FD distribution and the present RSCE from a dilute limit. In Section 3, we show that, by enlarging the sc-region for the perturbed potentials up to the 2nd-*nn* host atoms around X impurities in Pd, the discrepancy between the RSCE and FPKKR-band-calculation results for the total energy of the ordered Pd₃X alloy in L1₂ structure is corrected very well (from ~ 0.7mRy to ~ -0.1mRy per atom) for X=Ru, while slightly (from ~ 0.2mRy to ~ 0.1mRy per atom) for X=Rh. As results, the absolute error of the RSCE becomes as small as ~ 0.1mRy per atom for both the ordered Pd₃X (X=Ru, Rh) alloys in L1₂ structure. We also clarify the correction for each value of the *n*-body IEs (*n*=1~4). Section 4 summarizes the main results of the present paper and discusses the future problems.

2 Calculation Method

2.1 Total Energies of Impurity Systems

The calculations for the total energy of X (=Ru, Rh) impurities in Pd are based on the density functional theory (DFT) in the generalized gradient approximation (GGA) [8, 9]. In order to solve the Kohn-Sham equations, we use a multiple scattering theory in the form of the KKR Green's function method for the full-potentials (FP). We use the screened version of FPKKR band calculations for Pd host, which simplifies very much the numerical calculations by introducing the short-range structural Green's functions [15, 16]. In order to simplify the total energy calculations in the GGA formalism, we use the electronic densities obtained self-consistently by the local spin density approximation in the DFT. The accuracy of the present GGA calculations are discussed in Refs.8 and 9. It was already shown in Ref. 17 that the introduction of the FD distribution into *ab-initio* Green's function

calculations is very useful to simplify the total energy calculations. Based on a contour integration in the complex energy plane we evaluate the residues at a few Matsubara frequencies, while the remaining integral is analyzed by the Sommerfeld expansion. The lattice parameter of Pd host and *T*_{FD} for the electron excitation due to the FD distribution are fixed at 7.40a.u. and 800K, respectively, in all the present calculations.

The advantage of the Green's function method is that the embedding of point defects in an otherwise ideal crystal is described correctly by introducing the host Green's function, differently from the usual supercell and cluster calculations. In order to calculate the total energies of the impurity systems, the perturbed potentials due to the insertion of impurities are usually redetermined up to the 1st-*nn* host atoms around impurities [9]. However, in the present study, we redetermine the perturbed potentials up to the 2nd-*nn* host atoms around impurities, in order to examine the delocalization of the perturbed potentials.

2.2 Real Space Cluster Expansion for Total Energies of Pd-rich PdX (X=Ru, Rh) Alloys

A characteristic feature of the present RSCE is that all the terms in the present RSCE are determined uniquely and successively from the low body to high body, by the combination of total energies in different atomic arrangements of X atoms in Pd. It is noted that the atoms of minor X element are considered as impurities in Pd. The RSCE of the total energy (per unit cell (4 atoms)) of Pd₃X alloy in L1₂ structure (Fig.1 (a)) is written as follows:

$$E_{\text{Pd}_3\text{X}}^{\text{band}} = 4E_{\text{Pd}}^{\text{band}} + \Delta E^{1\text{-body}} + \Delta E^{2\text{-body}} + \Delta E^{3\text{-body}} + \Delta E^{4\text{-body}} + \Delta E^{\text{many-body IEs beyond 4-body}} \quad (1)$$

where the first term is 4 × total energy of Pd atom in Pd (0-body), the second term the total energy change due to the insertion of a single X impurity in Pd (1-body), the 3rd~5th terms correspond to the total contributions from the *n*-body (*n*=2~4) IEs among X_{*n*} impurities in Pd (2~4-body), respectively, and the last term is the sum total of many-body IEs beyond the 4-body. Since the first (0-body) and second (1-body) energies are the quantities characteristic of Pd-host and a single X impurity in Pd, respectively, these components do not depend on the atomic arrangement of X impurities in Pd. It is noted that the atomic arrangement for X impurities in Pd, at low temperatures, are determined by the minimization of the total sum of the *n*-body IEs (*n* ≥ 2). The definition and the calculational procedure for each term in eq. (1) are described in Refs. 4 and 14.

3 Accuracy of Real Space Cluster Expansion for Total Energies of Pd₃X (X=Ru, Rh) Alloys in L1₂ structure and Delocalization of Perturbed Potentials due to X Impurities

In the previous study we found that the present RSCE reproduces fairly well (the error of $\sim 0.2\text{mRy}$ per atom) the band calculation result for the ordered Pd_3Rh alloy in $L1_2$ structure, while a little wrongly (the error of $\sim 0.7\text{mRy}$ per atom) for the Pd_3Ru alloy in $L1_2$ structure [14]. In the previous study, however, we redetermined self-consistently the perturbed potentials due to the insertion of X impurities in Pd, up to the 1st- nn host atoms around X impurities in Pd. Thus, it may be easily understood that the RSCE error becomes large for the impurity systems in which the perturbed potentials are delocalized beyond the 1st- nn host atoms around X impurities in Pd; the perturbed potentials due to the insertion of X impurities in Pd may be delocalized for $X=\text{Ru}$ than for $X=\text{Rh}$. It is noted that the nuclear charge of Ru-element is smaller than that of Rh-element so that the 4d-orbitals of X impurities in Pd is delocalized for $X=\text{Ru}$ than for $X=\text{Rh}$. In the present study, we examine the delocalization of the perturbed potentials by enlarging the sc-region for the perturbed potentials up to the 2nd- nn host atoms around impurities in Pd.

For the total energies of the ordered Pd_3X ($X=\text{Ru}, \text{Rh}$) alloys in $L1_2$ structure (Fig. 1(a)), we include the 2-body IEs up to the 20th- nn , the 3-body IEs for the X_3 clusters shown in Fig. 1(b), and the 4-body IEs for the X_4 clusters shown in Fig. 1(c), as discussed in Ref. 14. Table 1 shows the calculated results by the present RSCE (eq. (1)) from a dilute limit: the total energy of Pd-host, the total energy changes due to the insertion of a single X impurity in Pd, and the total contributions from the n -body ($n=2\sim 4$) IEs. For comparison, we also show (in the parentheses) the calculated results with the sc-region for the perturbed potentials up to the 1st- nn host atoms around impurities in Pd, being already shown in Ref. 14.

We first find, in the results by enlarging the sc-region for the perturbed potentials, the discrepancy between the RSCE and the FPKKR-band-calculation results for the Pd_3X is satisfactorily corrected (from 0.71mRy to -0.06mRy per atom) for $X=\text{Ru}$, while slightly (from 0.17mRy

to 0.05mRy per atom) for $X=\text{Rh}$ because the band-calculation result for the Pd_3Rh is reproduced very well by the RSCE even with the sc-region for the perturbation potentials up to the 1st- nn host atoms around impurities in Pd, as shown in the parenthesis.

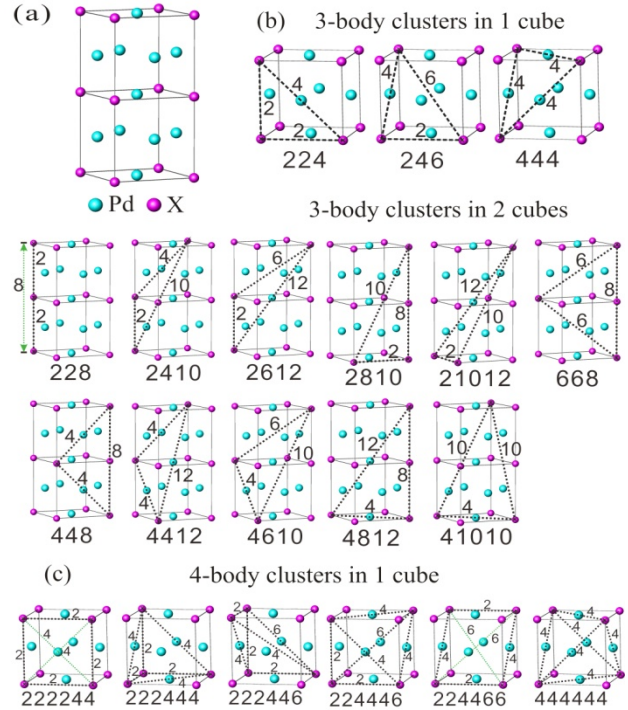


Figure 1. Atomic arrangement for X impurity clusters of the 3-body and 4-body IEs, used in the RSCE of the total energies of Pd_3X ($X=\text{Ru}, \text{Rh}$): (a) $L1_2$ structure (4 atoms in unit cell), (b) X_3 clusters for 3-body IEs, and (c) X_4 clusters for 4-body IEs. For 3-body IEs, there are the three (eleven) kinds of X_3 clusters in one cubic cell (two cubic cells) in fcc structure. For 4-body IEs, there are six kinds of X_4 clusters in one cubic cell in fcc structure. For example, the 224-cluster (the smallest X_3 -cluster for 3-body IEs) means that this cluster consists of two 2nd- nn and one 4th- nn pairs.

Table 1. Convergence of the RSCE for the total energies (in Ry) of (a) Pd_3Ru and (b) Pd_3Rh in $L1_2$ structure. The perturbed potentials due to the insertion of impurities are redetermined up to the 2nd- nn host atoms around impurities in Pd. The values in the parentheses are the calculated results in which the perturbed potentials due to the insertion of impurities are redetermined up to the 1st- nn host atoms around impurities in Pd.

	(a) Total energies of Pd_3Ru (Ry)	(b) Total energies of Pd_3Rh (Ry)
0-body [$4 \times E_{\text{band}}^{\text{Pd}}$]	-40374.470033 [4×-10093.617508]	-40374.470033 [4×-10093.617508]
up to 1-body [$\Delta E^{1\text{-body}}$]	-39344.445216 (-39344.444854) [1030.024816 (1030.025179)]	-39851.104786 (-39851.104688) [523.365247 (523.365344)]
up to 2-body [$\Delta E_{\text{int}}^{2\text{-body}}$]	-39344.425543 (-39344.423629) [0.019674 (0.021225)]	-39851.103386 (-39851.102828) [0.001400 (0.001861)]
up to 3-body [$\Delta E_{\text{int}}^{3\text{-body}}$]	-39344.432149 (-39344.4289813) [-0.006607 (-0.005352)]	-39851.104065 (-39851.103456) [-0.000679 (-0.000628)]
up to 4-body [$\Delta E_{\text{int}}^{4\text{-body}}$]	-39344.431167 (-39344.428093) [0.000983 (0.000888)]	-39851.103919 (-39851.103441) [0.000147 (0.000015)]
exact error	-39344.430939 [-0.000228 (0.002845)]	-39851.104114 [0.000195 (0.000673)]
error/atom	-0.000057 (0.000711)	0.000049 (0.000168)

The corrections for the total contributions from the n -body ($n=2\sim 4$) IEs are also very small (-0.46, -0.05, and 0.13mRy per cell) for the Pd₃Rh alloy, while somehow large (-1.55, -1.26, and 0.10mRy per cell) for the Pd₃Ru alloy. We also find that the correction for the 1-body IE is as small as -0.36(-0.10)mRy for X=Ru (Rh). It is noted that the absolute value of the 1-body IE is very large because it is the total energy change due to the replacement of one Pd-host atom with one X impurity, while the n -body IEs ($n=2\sim 4$) are small because the n -body ($n=2\sim 4$) IEs are the total energy changes due to the atomic rearrangement of X_{*n*} impurities, as discussed in Section 2.2. As results, the absolute value of the RSCE error becomes less than ~ 0.1 mRy per atom for both the ordered Pd₃X (X=Ru, Rh) alloys in L1₂ structure.

We now discuss the correction for each value of the n -body IEs ($n=2\sim 4$). Tables 2, 3 and 4 show all the values for the 2-, 3-, and 4-body IEs with the sc-regions for the perturbed potentials up to the 1st- and 2nd- nn host atoms around X (=Ru, Rh) impurities in Pd, being used in the present RSCE (eq.(1)). For the 2-body IEs, we find that a certain degree of corrections (-0.10, -0.05, -0.06mRy) appear in the 2nd- nn IEs for X=Ru, Rh and the 6th- nn IE for X=Ru, while for the other IEs the absolute values for the corrections due to enlarging the sc-region for the perturbed potentials are less than ~ 0.03 mRy. As results, the total correction from the 2-body IEs becomes as small as -1.55 and -0.46mRy for X=Ru and Rh (see Table 1).

Table 2. Calculated results (in mRy) for the 2-body IEs of (a) Ru₂ and (b) Rh₂ impurities in Pd, used for the RSCE of the total energies of Pd₃X (X=Ru, Rh) alloys. The perturbed potentials due to the insertion of impurities are redetermined up to the 2nd- nn host atoms around impurities in Pd. The values in the parentheses are the calculated results in which the perturbed potentials due to the insertion of impurities are redetermined up to the 1st- nn host atoms around impurities in Pd. The numbers of pairs per atom are also shown.

2-body	Number of pairs/atom	(a) 2-body IEs Ru ₂ in Pd (mRy)	(b) 2-body IEs Rh ₂ in Pd (mRy)
100 (2nd)	3	1.8604 (1.9641)	0.2056 (0.2580)
110 (4th)	6	2.1879 (2.2095)	0.1181 (0.1312)
111 (6th)	4	-0.2467 (-0.1860)	-0.0089 (0.0038)
200 (8th)	3	-0.0195 (-0.0353)	0.0111 (0.0095)
210 (10th)	12	0.0891 (0.0965)	0.0384 (0.0398)
211 (12th)	12	0.1012 (0.1142)	-0.0118 (-0.0092)
220 (15th)	6	-0.1198 (-0.1054)	-0.0132 (-0.0095)
221 (17th-a)	12	0.0443 (0.0617)	-0.0062 (-0.0029)
300 (17th-b)	3	-0.0398 (-0.0109)	-0.0157 (-0.0101)
310 (19th)	12	0.0028 (0.0268)	-0.0035 (0.0009)

For the 3-body IEs, as seen in Table 3, we find that the 3-body IEs for X=Rh are almost unchanged (the absolute value for the corrections $< \sim 0.002$ mRy). In contrast, the 3-body IEs for X=Ru change to a certain degree (~ -0.01 mRy) for 224-, 228-, 2410, 2810, 448-3body IEs, while the corrections for the other 3-body IEs are fairly small (the absolute values of the corrections $< \sim 0.004$ mRy). As results, the total correction from the 3-body IEs is as small as -1.26 and -0.05mRy for X=Ru and Rh (see Table 1).

For the 4-body IEs, as seen in Table 4, we find that the corrections due to enlarging the sc-region for the perturbed potentials are very small (the absolute values of the corrections $< \sim 0.004$ mRy), except for the 222244- and 444444-4body IEs for X=Ru (0.01 and -0.02mRy). It is noted that the corrections of the 222244- and 444444-4body IEs for the total energy are small because the numbers of these clusters per atom are very small (3 and 2), as listed in Table 4. As results, the total correction from the 4-body IEs becomes very small (0.10 and 0.13mRy for X=Ru and Rh; see Table 1).

Table 3. The same as Table 2 for the 3-body IEs of (a) Ru₃ and (b) Rh₃ impurities in Pd (in mRy). The numbers of X₃ clusters per atom are also shown.

3-body	Number of X ₃ clusters /atom	(a) 3-body IEs Ru ₃ in Pd (mRy)	(b) 3-body IEs Rh ₃ in Pd (mRy)
224	12	-0.1709 (-0.1609)	0.0277 (0.0269)
246	24	0.0580 (0.0604)	0.0224 (0.0231)
444	8	0.2541 (0.2540)	-0.0003 (-0.0027)
228	3	-0.3019 (-0.2886)	-0.0135 (-0.0138)
2410	24	-0.0938 (-0.0862)	-0.0019 (-0.0034)
2612	24	-0.0825 (-0.0786)	-0.0068 (-0.0062)
2810	24	-0.0731 (-0.0649)	-0.0139 (-0.0135)
21012	48	-0.0340 (-0.0316)	-0.0060 (-0.0052)
448	12	0.0308 (0.0395)	-0.0197 (-0.0205)
4412	24	0.0949 (0.0966)	-0.0031 (-0.0034)
4610	48	-0.0297 (-0.0264)	-0.0060 (-0.0055)
4812	24	-0.0113 (-0.0075)	-0.0002 (0.0002)
41010	24	0.0049 (0.0076)	0.0000 (0.0011)
668	12	-0.0438 (-0.0446)	-0.0060 (-0.0065)

Table 4. The same as Table 2 for the 4-body IEs of (a) Ru₄ and (b) Rh₄ impurities in Pd (in mRy). The numbers of X₄ clusters per atom are also shown.

4-body	Number of X ₄ clusters/atom	(a) 4-body IEs Ru ₄ in Pd (mRy)	(b) 4-body IEs Rh ₄ in Pd (mRy)
222244	3	0.1713 (0.1622)	0.0296 (0.0289)
222444	8	0.0241 (0.0215)	0.0041 (0.0028)
222446	24	0.0156 (0.0147)	0.0048 (0.0005)
224446	24	0.0097 (0.0078)	-0.0064 (-0.0076)
224466	6	-0.0767 (-0.0794)	0.0048 (0.0067)
444444	2	0.0644 (0.0828)	0.0173 (0.0179)

4 Summary and Future Problem

We examined the delocalization of the perturbed potentials due to the insertion of X (=Ru, Rh) impurities in Pd by enlarging the sc-region for the perturbed potentials. We found that the discrepancy between the RSCE and the band-calculation results for the ordered Pd₃Ru alloy in L1₂ structure is satisfactorily corrected (from ~ 0.7mRy to ~ -0.1mRy per atom) by enlarging the sc-region for the perturbed potentials from the 1st-*nn* up to the 2nd-*nn* host atoms around Ru impurities in Pd. On the other hand, the correction for the RSCE error is small (from ~ 0.2mRy to ~ 0.1mRy per atom) for the ordered Pd₃Rh alloy in L1₂ structure, because the RSCE even with the sc-region for the perturbed potentials up to the 1st-*nn* host atoms around impurities in Pd already reproduces very well the band-calculation result for the ordered Pd₃Rh alloy in L1₂ structure, as seen in Tables 1-4. We clarified how the accuracy of the present RSCE depends on the sc-region for the perturbed potentials. As results, the absolute error of the RSCE becomes as small as ~ 0.1mRy for both the Pd₃X (X=Ru, Rh) alloys in L1₂ structure. It is obvious that, according to the requested accuracy for the calculated results, we must enlarge the sc-region for the perturbed potentials around impurities in Pd. However, if we need (for example) the accuracy of 1mRy per atom, it may be enough to redetermine self-consistently the perturbed potentials due to the insertion of impurities up to the 1st-*nn* host atoms around impurities in Pd.

We are now studying quantitatively the phase stability and phase diagram of the age-hardening Al-rich AlX (X=Mg, Cu, Zn) alloys by using the free energy calculations based on the present RSCE for the internal energies and the CVM for the configurational entropy, respectively, as shown in Refs. 11-13. It is also very interesting to study the effect of another element addition on the kinetics of age-hardening behaviors of Al-rich multi-element alloys, such as Cu in Al-rich AlMgSi alloys [18, 19]. We plan to develop the calculation program for Monte Carlo simulations [20-22] which may

be useful as one of material design tools for the high quality of age-hardenable Al-rich multi-element alloys. We believe Al-rich multi-element alloys offer a good example how thermodynamical calculations can reveal quantitative insight into the underlying age hardening behavior.

As another application of the present RSCE approach for the internal energy, it may be interesting to study the morphology in the nano-scale spinodal decomposition phase [23,24], such as the magnetic network shown in Fig.5 in Ref. 24, which occur in the quenching and annealing processes in the dilute magnetic semiconductors such as (Ga, Mn) N and (Ga, Mn) As. At present we can take into account the lattice distortion effect for the chemical and magnetic IEs derived from a dilute limit [25, 26], which may be important for Mn impurities (at Ga sites) in the GaAs and GaN semiconductors because the difference between the ionic radii (2.67 and 2.38 a.u.) of Ga and Mn atoms in fcc structure is considerably large [27]. Morphological features expected by Monte Carlo simulations with such energetics will be reported in the future.

Acknowledgement

The authors are grateful for the financial support from the Ministry of the Education, Culture, Science and Technology (JSPS KAKENHI Grant Nos, 15K06422 and 16K06710). This study was partly supported by New Energy and Industrial Technology Development Organization of Japan (NEDO) Grant (P16010). One of the authors (T. Mohri) appreciates their support. This study was almost completed when T. Hoshino was at the Institute for Material Research, Tohoku University. C. Liu and T. Hoshino would like to express their sincere thanks to the crew of the Center for Computational Materials Science of the Institute for Materials Research, Tohoku University, for their continuous support of the SR16000 supercomputing facilities.

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