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Reliability of analytical potentials for point-defect simulation in GaAs

G Zollo[1], J Tarus[1,2] and R M Nieminen[3]

[1] Department of Energetics, University of Rome 'La Sapienza' and INFM, via A Scarpa 14-16, 00161 Rome, Italy
[2] Accelerator Laboratory, University of Helsinki, PO Box 43, FIN 00014, Finland
[3] COMP/Laboratory of Physics, Helsinki University of Technology, PO Box 1100, 02015 HUT, Finland

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Abstract

Molecular dynamics with analytical potentials is commonly used to obtain the distribution of defects produced by energetic particles in elemental and compound semiconductors. Collision cascades simulated by model-potential molecular dynamics are used to collect statistical data on the defect distribution but the local structure in such materials as GaAs is commonly recognized to be unreliable in comparison to tight-binding or *ab initio* total energy calculations. These two methods, however, are not practical in simulations of collision cascades because of their large computational workload. In this paper, we analyse the properties of the basic point defects in GaAs as obtained by using different model potentials and compare them to recent *ab initio* calculations based on the density-functional theory (DFT) in the local-density approximation (LDA). The aim of this work is to evaluate how close the model potential molecular dynamics predictions are to the benchmark DFT results and which model potential most accurately predicts realistic local structures of point defects.

1. Introduction

First-principles calculations are nowadays widely used for accurate and reliable prediction of point-defect properties of semiconductors. For GaAs as an example, many point-defect properties have been worked out in the last decade [1–4]. However, first-principles calculations suffer from an important limitation due to the large computational workload they require. Even with the most powerful computers, only a few hundred atoms can be handled by first-principles techniques. Sometimes, even small point-defect clusters are difficult to handle by first-principles calculation due to the large elastic interactions between the defect images and the spurious dispersion of the defect-localized electronic wavefunctions in the supercell

approach. Less accurate but more flexible techniques such as tight-binding and model-potential molecular dynamics are often used to handle larger systems. In particular, in order to deal with ion-implantation-induced defects and collision cascades, the use of classical model potentials is forced by the large size of the system under study. Many different model potentials have been proposed for GaAs [5–10] and applied to study defect production, lattice strain and erosion/growth mechanisms in GaAs [6, 11–19]. They have also been applied to model point-defect distributions in collision cascades [8]. However, even though these models can give useful results of the statistical distributions of point defects, the resulting atomic structures should be considered with care. This is because no thorough comparison with results obtained by first-principles calculations such as density-functional theory (DFT) has been reported.

In the present paper we report and discuss the atomic-scale properties of various point defects obtained with different model potentials. These include the Smith [5] and Sayed [6] potentials, and the Albe–Nordlund–Nord–Kuronen (ANNK) potential [7]. We analyse their results and compare them to the benchmark DFT results.

2. Computational methods

2.1. First-principles calculations

The first-principles results have been obtained by means of DFT [20] in the local-density approximation (LDA) [21]. The calculations are performed using the self-consistent total-energy pseudopotential (PP) method. The Perdew–Zunger [22] parametrization of the Ceperley–Alder data [23] is used for the exchange–correlation energy. Norm-conserving Hamann PPs [24] in the Kleinman–Bylander form [25] have been used for both Ga and As atoms. The valence-electron wavefunctions are expanded in a plane-wave basis set with a kinetic energy cutoff of 28 Ryd. We mainly use the $2 \times 2 \times 2$ Monkhorst–Pack (MP) [26] **k**-point Brillouin zone sampling and 64-atom supercells (SC).

The total energy calculations and consequently the optimal geometries can be affected by spurious defect–defect elastic interactions and the dispersion of the electronic gap states [27]. Thus, in order to evaluate the convergence of our calculations, several tests have been performed by using larger supercells (216-atom SCs) and different cutoff energies, to ensure that the computational parameters give converged values for isolated point defects. The *ab initio* simulations were performed for neutral point defects, namely As and Ga vacancies (V_{As} and V_{Ga}), As and Ga antisites (As_{Ga} and Ga_{As}) as well as As and Ga self-interstitials (As_i and Ga_i) for their total energies and optimal configurations.

2.2. Model-potential molecular dynamics calculations

There are several model potentials for GaAs in the literature [5–10]. From these, the one by Khor *et al* [8] does not list any parameters for Ga–Ga and As–As interactions and is thus not suitable for defect studies. The recent potential published by Conrad and Scheerschmidt [9] seems to have an endothermic heat of formation which can lead to a phase decomposition under the conditions of a collision cascade [7]. The potential by Ebbsjö *et al* [10] has been successfully used for amorphous GaAs and for GaAs surface properties, but the parameters, to the authors' knowledge, have not been published. As our aim is to find a model potential which is suitable for collision cascade studies we are left only with the Smith [5], Sayed [6] and ANNK [7] potentials[4]. The ANNK potential is the most recent one. It is fitted to a number of

[4] For the analytical form of the potentials, please refer to the original articles.

Table 1. GaAs bulk properties with different model potentials.

	ANNK	Smith	Sayed	Sayed0
Cohesive energy (eV/formula unit)	3.35	3.25	3.25	
Lattice constant (Å)	5.65	5.65	5.64	
Average nearest-neighbour (NN) distance (Å)	2.45	2.45	2.44	
Distortion (%)	0.11	0.18	0.1	
Tetrahedron volume (TV) (Å^3)	7.51	7.35	7.47	

bulk GaAs properties and thus gives an excellent ground-state description. So far this potential has only been used by its developers.

The Smith [5] and Sayed [6] potentials have been used by different groups and some criticisms have been presented against their characteristics. Sayed [5] noticed that the Smith potential has a too weak angular dependence for Ga–As interactions; he refitted this part of the potential leaving the Ga–Ga and As–As parts intact. Furthermore, Sayed set the λ_3 parameter in the potential to have non-zero values. However, it has been found that the original Sayed potential leads to unstable surface properties [11] and to a ground state other than the zincblende structure [28]. These problems seem to be fixed by setting λ_3 to zero. For consistency, we have included both versions in this study and we will refer to them in the text as Sayed and Sayed0.

We use a 64-atom simulation box for the defect studies, with periodic boundary conditions to simulate the bulk conditions. The pressure of the box is set to zero by using the Berendsen pressure control [29]. The calculations have been tested against the supercell size showing that the errors obtained for a 64-atom supercell are less than 1% with respect to the perfectly converged results.

All the different structures were heated to a temperature between 50 and 1000 K (depending on the potential and the structure) and then quenched slowly (0.015 K fs^{-1}) back to zero temperature in order to find the true ground-state geometries. In order to obtain the absolute point-defect energies, we have also calculated the ground states for elemental Ga and As as well as perfect GaAs.

3. Bulk properties

According to our first-principles calculations, the equilibrium lattice constant and the heat of formation ΔH for GaAs are 5.55 Å and 1.0 eV, compared to the experimental values being 5.65 Å and 0.75 eV [30], respectively. The obtained values are both close to previous DFT calculations, which (like ours) are affected by the well-known problem of overbinding inherent in the LDA approximation.

The performance of the different model potentials has been primarily monitored by the bulk cohesive energy of GaAs, Ga and As. In all the model potentials we used, the zincblende phase is at least stable. Moreover, the zincblende phase is the ground state except for the Sayed potential. In table 1 we report the cohesive energy and other structural parameters obtained with the different model potentials. The stable zincblende GaAs lattice obtained by analytical potentials is, however, slightly distorted. We thus also indicate the distortion as the maximum percentage deviation of the bond lengths from the average.

The lattice constants are well reproduced with all the analytical potentials, with the possible exception of the Sayed potential. Its results are slightly off the experimental values but, nevertheless, closer than the DFT–LDA predictions, affected by overbinding. The ANNK

Table 2. As and Ga bulk cohesive energy with different model potentials (eV/atom).

	ANNK	Smith	Sayed	Sayed0
As α	**2.96**	Relaxes to simple cubic		
As fcc	Not stable	2.4		
As sc	2.91	**3.32**		
As dia	2.51	2.24		
As bcc	Not stable	Not stable		
Ga α	**2.83**	2.91		
Ga fcc	Not stable	2.56		
Ga sc	2.69	**2.92**		
Ga dia	2.49	2.55		

potential reproduces the experimental cohesive energy of the GaAs zincblende lattice while both the Smith and Sayed potentials give worse results. Moreover, the weak angular forces that characterize the Smith potential cause lattice distortions when the lattice is heated above 0 K and then cooled down. This is the reason why the unit cell size decreases and the lattice constant is not unequivocally determined in the x, y and z directions.

However, the reliability of model potentials to simulate defects is primarily dependent on their capability to handle correctly different local atomic arrangements, involving different coordination numbers and As–As, Ga–Ga and As–Ga bonding. Hence it is necessary to evaluate the reliability of the different analytical potentials to reproduce the different stable As and Ga bulk phases. As can be seen in table 2, the ANNK potential is the only one that correctly predicts the As and Ga α phases as the ground states. This is because the ANNK potential has been obtained by using the bulk in the parameter fitting. On the contrary, the Smith and the Sayed potentials (which are identical for single-element interactions) give wrong results as they predict the simple cubic phase as the stablest for both Ga and As.

The DFT total energy calculations in the LDA approximation predict that the cohesive energy of the As simple cubic phase is 70 meV/atom lower than the stablest α phase. The ANNK potential, which has been built on the bulk data, reproduces the correct stable phase and also the small energy difference between the α and the simple cubic phase. It should be noted, however, that the simple cubic phase is actually distorted and that the lattice constant deviates from both the LDA and experimental results [7]. Moreover, the cohesive energy of the α phase obtained with the ANNK potential is very close to the experimental value (2.96 eV versus 2.9 eV) [31].

Having discussed the bulk properties of GaAs, Ga and As bulk solids obtained with the ANNK, Smith and Sayed potentials, we now analyse the structural properties and the formation energies of various point defects in GaAs, as obtained by using the same model potentials. Because analytical potentials cannot handle charged point defects, the simulation has been limited to neutral defects. The charge state of a defect is an equilibrium property determined by the electron chemical potential (doping, temperature) and the stoichiometry and is not a property of the collision cascades.

4. Vacancies and antisites

4.1. First-principles calculations

The results obtained by DFT for the neutral charge states of vacancies and antisites are reported in table 3. Concerning vacancies and antisites in GaAs, many results from DFT

Table 3. DFT–LDA properties of vacancies and antisites.

Defect	Formation energy (eV)	Symmetry group	Deviation from symmetry (%)	Normalized NN distance	NTV
V_{As}	3.10	T_d	0.01	0.89	0.71
V_{Ga}	3.15	T_d	0.4	0.88	0.70
As_{Ga}	2.48	T_d	0.01	1.06	1.19
Ga_{As}	2.12	$\sim T_d$	6	0.99	0.97

Table 4. Vacancy properties with different model potentials compared to DFT.

		ANNK	Smith	Sayed	Sayed0	DFT
V_{Ga}	Formation energy (eV)	2.16	0.9	0.74	0.74	3.15
	Symmetry group	T_d	$\sim T_d$	T_d	T_d	T_d
	Deviation from symmetry (%)	0	13	0	0	0.4
	Normalized NN distance	0.85	0.92–1.05	1.05	1.05	0.88
	NTV	0.61	1.09	1.09	1.14	0.7
V_{As}	Formation energy (eV)	2.46	0.5	0.34	0.34	3.10
	Symmetry group	T_d	C_{1h}; $\sim T_d$	T_d	T_d	T_d
	Deviation from symmetry (%)	0	9; 38	0	0	0.01
	Normalized NN distance	0.96	0.9–1.11	1.05	1.05	0.89
	NTV	0.86	1.11	1.13	1.14	0.71

calculations have been published in the last ten years showing some spread also for the formation energies [32–34]. Most of the those calculations, however, have been performed in 32 or 64 atom-SCs, with lower cutoff energies and poorer Brillouin-zone sampling. We are thus confident that the present results are more reliable and can be taken as benchmarks.

In order to compare these results to those obtained with different model potentials, we focus our attention on the structural properties and the formation energies. The structural properties we discuss are the symmetry, the average nearest-neighbour bond length (NN) normalized to the analogous bulk value, and the volume of the tetrahedron formed by the NNs of the specific point defect (vacancy, antisite or self-interstitial) normalized to the volume of the tetrahedron in the bulk (NTV).

As one can see, the As antisite keeps the T_d symmetry and relaxes outwards. In the other cases (both the As and Ga vacancies and the Ga antisite) the surrounding atoms relax inwards preserving the T_d symmetry, except for the Ga antisite which deviates from the T_d point group. The As antisite formation energy is close to the previously reported values of 2.5 eV [32] and 2.29 eV [33]. The neutral Ga antisite formation energy is somewhat lower than the previous results of about 2.7 eV [34]. The neutral Ga vacancy formation energy is considerably lower than previously reported (4.55 eV) [32] while the neutral As vacancy is about 0.7 eV higher than in [33]. However, all of the earlier values were obtained with a smaller SC and less accurate **k**-point sampling schemes.

4.2. Analytical potential calculations

In table 4 we report the results obtained by analytical-potential molecular dynamics with different potentials for vacancies in the two sublattices.

It appears that the ANNK potential is the only one that produces reasonably accurate results, with formation energies 2.16 and 2.46 eV for Ga and As vacancies, respectively. The other potentials give formation energies lower than 1 eV, i.e. more than 2 eV off the

Table 5. Antisites properties with different model potentials compared to DFT.

		ANNK	Smith	Sayed	Sayed0	DFT
As_{Ga}	Formation energy (eV)	5.56	1.5	1.93	2	2.48
	Symmetry group	$\sim T_d$	$\sim T_d$	C_{1h}; $\sim T_d$	C_2; $\sim T_d$	T_d
	Deviation from symmetry (%)	4.6	4.64	0; 13	0; 0.57	0.01
	Normalized NN distance	1.14	1.09	1.03; 1.17	1.06	1.06
	NTV	1.65	1.15	1.45	1.21	1.19
Ga_{As}	Formation energy (eV)	1.55	1	4.21	4.33	2.12
	Symmetry group	T_d	$\sim T_d$	C_{1h}; $\sim T_d$	T_d	$\sim T_d$
	Deviation from symmetry (%)	0	24	0.89; 16	0.64	6
	Normalized NN distance	1.00	1.02	1.01; 1.17	1.03	0.99
	NTV	0.98	1.08	1.16	1.08	0.97

DFT–LDA results that we assume as the reference. Moreover, the ANNK potential is the only one reproducing the T_d relaxation inwards as predicted by the DFT calculations; the atoms surrounding the vacancy relax outwards with all the other potentials. Concerning the As vacancy, the symmetry obtained with the Smith potential is closer to the C_{1h} than to the T_d point group. In table 4 we report the deviation of the obtained structure with respect to both these point groups.

The data obtained for the antisites are reported in table 5.

The formation energy of the Ga antisite obtained with the ANNK potential is the closest to the DFT value, while all the other potentials behave worse. In particular, the Sayed potential overshoots the DFT results by more than 2 eV. Moreover, the geometrical properties of the Ga antisite are best reproduced by the ANNK potential: all but the ANNK potential predict that the As atoms relax outwards, which is opposite to the DFT result. For the As antisite the Smith, Sayed and Sayed0 potentials give formation energies between 1.5 and 2 eV, thus reasonably close to the DFT data, while the ANNK potential gives a much higher value. The geometrical properties show that the best performance is obtained by using the Sayed0 potential: both the NN distances and the NTV data are very close to DFT results. However the Sayed0 potential predicts the C_2 symmetry even though it is still close to T_d as can be seen in table 5. The point group symmetries found with the Sayed potential are C_{1h} instead of the T_d predicted by DFT (see table 3); the deviation from the benchmark T_d symmetry has been also included in table 5. The ANNK results show that both the As–As bond length and the lattice dilation are overestimated by about 40%. Thus, except for the As antisite, the ANNK potential gives results that are the closest to the DFT data.

5. Self-interstitials

The third set of data concerns self-interstitials in GaAs, for which we have obtained the stablest DFT configurations. Also in this case we focus our attention to the formation energies and the structural properties such as the symmetry, the average nearest-neighbours bond length, the As–As bond length (for the As ⟨110⟩ dumbbell), both normalized to the Ga–As bulk bond length, and the volume of the tetrahedron formed by the NNs of the interstitial site, again normalized to the bulk value.

5.1. First-principles calculations

Interstitial modelling by DFT was first attempted in the early nineties [32–34]. Since then, due to improved computation capabilities, many properties of self-interstitials have been

Table 6. DFT–LDA properties of self-interstitials in GaAs.

Self-interstitial	As_i	Ga_i
Configuration	⟨110⟩ dumbbell	Tetrahedral
Symmetry group	C_{1h}	T_d
Deviation from symmetry (%)	0.03	0.002
Formation energy (eV)	4.07	2.98
Normalized NN distance	1.07	1.06
NTV	1.26	1.2
As–As bond length	1.01	

Table 7. As interstitial properties with different model potentials.

		ANNK	Smith	Sayed	Sayed0
As_i tetrahedral	Formation energy (eV)	6.92	5.75	—	11.85
	Normalized NN (As–As) distance	1.01	1.14	—	1.11
	NTV	1.06	0.94[a]	—	1.36
As_i⟨110⟩ dumbbell	Formation energy (eV)	7.74	4.45	3.48	8.99
	Normalized NN (As–Ga) distance	1.07	1.08	1.12	1.11
	NTV	1.37	1.22	1.58	1.38
	Normalized As–As bond length	1.21	1.2	1.01	1.12
As_i⟨100⟩ dumbbell	Formation energy (eV)	5.9	0.97	4.21	4.33
	Normalized NN (As–Ga) distance	0.95	0.98	0.95	0.95
	NTV	1.62	1.72	1.63	1.63
	Normalized As–As bond length	1.18	0.99	0.91	0.91

[a] The Ga neighbours are as close as the As neighbours.

revised [35, 36]. The recent papers, in spite of some differences concerning stable charge states of As interstitials, substantially agree in the stable configurations and their energetics. The main results obtained for self-interstitials within DFT are summarized in table 6.

The formation energies of self-interstitials are somewhat lower than those previously reported in the literature [32, 34]. However, the structural properties, also tested with larger supercells, are unambiguous. For both types of interstitials, the surrounding atoms relax outwards, as one could expect, the point groups being clearly resolved. For a more detailed discussion of self-interstitials in GaAs and their complexes, see [35].

5.2. Analytical potential calculations

Let us now discuss the results obtained with the different model potentials for self-interstitials in GaAs. It is known that primary defects in ion-implanted GaAs are vacancies and self-interstitials, either isolated or in Frenkel pairs. In table 7 we report data for As self-interstitials in three configurations: the tetrahedral, the ⟨110⟩ and the ⟨100⟩ dumbbells. These configurations are the only stable geometries in the model potential calculations. We have not evaluated the symmetry properties in these cases because the distortion inherent in the lattice for analytical potential makes the symmetry group less significant for self-interstitials.

The reported results clearly show that the only model potential that predicts the As_i⟨110⟩ dumbbell as the stablest configuration is the Sayed potential. The formation energy is, moreover, very close to the one obtained by DFT. The behaviour seems, on the whole, quite satisfactory, except for the fact that the same potential predicts the tetrahedral configuration to be unstable and the As_i⟨100⟩ metastable. According to recent DFT–LDA data [35], the

Table 8. Ga interstitial properties with different model potentials.

		ANNK	Smith	Sayed	Sayed0
Ga_i tetrahedral	Formation energy (eV)	1.1	4.9	3.5	11.46
	Normalized NN distance	1.02	1.11	**	1.11
	NTV	1.07	*	**	1.35
Ga_i hexagonal	Formation energy (eV)	2.29	2.63	3.29	7.5
	Normalized NN distance	1.06 (b)	1.04 (b)	1.09 (a)	1.04 (b)
	NTV	1.2	1.25	1.24	1.16

tetrahedral As_i is metastable while the $As_i\langle 100\rangle$ is unstable. The other potentials behave worse, especially the Smith version which predicts the $As_i\langle 100\rangle$ as the stablest configuration with the same formation energy as for vacancies and antisites. This is not realistic as only vacancies and antisites have been detected in as-grown GaAs, and As self-interstitials are unlikely to be present. Both the ANNK and the Sayed0 potentials predict the $As_i\langle 100\rangle$ dumbbell as the stablest configuration, but the Sayed0 yields too large formation energy values (more than 11 eV), while the ANNK potential gives formation energies between 5.9 and 7.74 eV. In this last case, however, the $As_i\langle 110\rangle$ has the highest formation energy. Therefore, if limited to the As self-interstitials, the Sayed potential is the model that performs the best. This indicates that while setting the value of λ_3 to zero fixes the problems with surfaces, it can make things worse for other situations.

Let us now analyse the Ga self-interstitial data obtained by using the different model potentials. The main results are summarized in table 8.

It is worth noting that the tetrahedral Ga_i calculated with the Smith potential is characterized by Ga neighbours closer than As neighbours, which makes the measure of the tetrahedron volume meaningless (denoted by * in table 8). Moreover, the calculation of the tetrahedral Ga_i with the Sayed potential results in a dumbbell $\langle 100\rangle$ configuration formed by one As and one Ga atoms (denoted by ** in table 8). For the hexagonal configuration we also report data for nearest neighbours, calculated with either five (a) or six (b) neighbours, depending on the lattice distortion around the interstitial.

All the used potentials predict as unstable all the Ga_i configurations other than the hexagonal and tetrahedral ones. According to recent DFT–LDA calculations [35] the neutral charge state of the hexagonal Ga interstitial is unstable, while the $Ga_i\langle 110\rangle$ dumbbell at the As site is metastable. The tetrahedral configuration is predicted to be the stablest configuration in the DFT–LDA calculations. This result is correctly reproduced only with the ANNK potential. However, the formation energy is 1.1 eV, which is about 1.8 eV less than the DFT result. All the other potentials predict the hexagonal configuration as the stablest, which disagrees with the DFT results.

The atomic positions indicate that for the ANNK tetrahedral configuration the distance between the interstitial and the nearest neighbours is 1.02 in units of the As–Ga bond length. This value is close enough to the DFT–LDA result, which is 1.06 (see table 6). The volume of the tetrahedron with the Ga interstitial at the centre is somewhat bigger than the DFT result but still close to it. Therefore, for Ga self-interstitials in GaAs we can conclude that definitely the ANNK potential is the one that gives results closest to the DFT values taken as the standard.

6. Conclusions

Analytical-potential molecular dynamics methods are commonly used to simulate collision cascades in condensed matter. Molecular dynamics simulations provide statistical data for

vacancy and interstitial distributions. The data collected for the structural properties of isolated defects produced in the collision cascades is usually not examined in detail, because it is recognized that the local structural properties of point defects obtained in this way are not very reliable, while statistics of the defect distribution has some validity. Various model potentials have been proposed for GaAs. We have examined how close the structures they predict are to the results obtained by DFT–LDA calculations. The aim of this work is to evaluate how useful are the structures obtained by model-potential molecular dynamics, for example, as starting configurations for further studies by more accurate methods such as tight-binding or first-principles simulations. We use the results of DFT–LDA calculations assumed as reference data. The DFT–LDA calculations, especially concerning self-interstitials, have been previously tested [35] with particular attention paid to the convergence with respect to the supercell size and **k**-point sampling.

Concerning the bulk properties, the ANNK potential gives better results than the other potentials. For point defects, we observe the general trend that the ANNK potential performs best, especially concerning vacancies and the Ga antisite. Problems arise in the case of the As antisite for which the Smith and the Sayed (in both of its versions) potentials are clearly better. Moreover, for As self-interstitials the ANNK potential predicts the stablest configuration as the $As_i\langle 100\rangle$ dumbbell which is unstable according to the DFT results. Moreover, the As–As bond length is about 20% longer than the As–Ga bond length, which indicates a large local distortion not observed in the DFT calculations where the As–As bond length is only 1% longer than the As–Ga bond length. The Smith potential and the modified Sayed potential behave quite unsatisfactorily, while the Sayed potential in its original version is the one that best reproduces the DFT result: the $As_i\langle 110\rangle$ dumbbell is correctly predicted to be the stablest configuration with its atomic positions quite close to those obtained by DFT calculations. For Ga self-interstitials, all the used model potentials predict the hexagonal configuration as a stable one, while the ANNK potential is the only one that correctly gives the tetrahedral configuration as the ground state configuration.

As a final comment, we conclude that although the ANNK potential in general performs best, it has severe limitations where the point defect imposes As–As bonds such as the As antisite or the As_i dumbbells. In these cases the ANNK potential performs badly and the Sayed potential, in its original version, is more suitable. One can attribute such a behaviour of the ANNK potential either to the effect of the As parameters or to the fitting of GaAs parameters which did not include direct As–As interactions. This specific problem represents, indeed, a severe limitation because it does not, for example, allow the simulation of dislocation cores in GaAs. If it was possible to fix this problem related specifically to the As parameters, the ANNK potential would be quite useful in predicting realistic atomic positions in the collision cascades in GaAs. The other two potentials used suffer from severe limitations which make them unsuitable for even a first approach to the local structures in collision cascades.

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