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Optimized Tersoff potential parameters for tetrahedrally bonded III-V semiconductors

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We address the issue of accurate parametrization for the Abell-Tersoff empirical potential applied to tetrahedrally bonded semiconductor materials. Empirical potential methods for structural relaxation are widely used for group IV semiconductors while, with few notable exceptions, work on III-V materials has not been extensive. In the case of the Abell-Tersoff potential parametrizations exist only for III-As and III-N, and are designed to correctly predict only a limited number of cohesive and elastic properties. In this work we show how by fitting to a larger set of cohesive and elastic properties calculated from density functional theory, we are able to obtain parameters for III-As, III-N, III-P, and III-Sb zinc blende semiconductors, which can also correctly predict important nonlinear effects in the strain.

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I. INTRODUCTION

The development of atomistic empirical potential methods for molecular dynamics (MD) and molecular statics (MS) has allowed structural simulations of low dimensional III-V semiconductor materials to become a field that has attracted a substantial amount of interest in recent years[1–10] There are three main reasons for this. First, the electronic properties of lattice mismatched epitaxial semiconductor layers are strongly affected by their structural properties.[11] Hence the reliable determination of quantities such as the elastic properties and the resulting strain is a fundamental prerequisite for implementing any accurate description of the bandstructure and the associated energy levels.[12] Second, in, e.g., epitaxial quantum dot (QD) islands the stochastic variations of the local stoichiometry are often on a nanometer scale, precluding the use of less accurate continuum models. Furthermore, the symmetry group of a spatially symmetric QD is C_{4v} but in the case of III-V semiconductors the atomistic symmetry effects lower this to C_{2v}, an effect that continuum models cannot capture.[13] Third, the use of other atomistic approaches is precluded by the volume of the average nanostructure which is normally several orders of magnitude larger than that of the largest simulation cell of a typical *ab initio* calculation.

In this paper we will show that properly parametrized empirical potentials (EPs) can capture the essential elastic and cohesive properties of a material, with the same accuracy as an *ab initio* calculation but with a substantially lower computational demand. However, it is important to understand that EPs are not universal potentials since often different parametrizations can be found that correctly predict only a specific type of structural, cohesive or vibrational property. Therefore, great care is necessary to select a parameterisation that is appropriate for the particular case study.

In this work we make use of the empirical form of the Abel-Tersoff potentials (ATPs),[14–17] which have emerged as the preferred choice for atomistic modeling of the group IV and III-V semiconductors. We will thus present a comprehensive collection of highly optimised parameter sets for zinc blende III-V semiconductor materials to enable the use of the ATP for atomistic studies through MD and MS of realistically sized nanostructure such as quantum wells, wires and dots. By fitting to the cohesive energy, lattice constant, the three elastic constants, the internal sublattice displacement and, in some cases non linear effects, we obtained parametrizations for III-P and III-Sb, which to our knowledge were previously not available, while we have significantly improved the accuracy of the prediction of the elastic properties compared to previous parameterisations of III-As and III-N.

II. THE FUNCTIONAL FORM

The ATP was formulised to preserve the intuitive nature of the exponential Morse-like pair bonding and to enhance this nature with the inclusion of a many-body term to account for local neighbours (both in terms of the distance from the atom under consideration and the subtended bonding angle). The potential was originally proposed as a tradeoff between accuracy and timing when performing a simulation to describe the material properties of solid silicon and was designed to reproduce cohesion in a large range of coordination and bonding topologies. This represents a substantial improvement compared to the Stillinger-Weber potential,[18] because of the better description of the chemistry of the bonds, and also the Keating-Valence force field[19] method, because of the possibility of treating nontetrahedral systems and the ability to provide a better description of the anharmonic region of the energy vs bond length curve. The original form of the Tersoff potential[17] is shown below with a couple of modifications to nomenclature for compatibility with other authors:

$$E=\frac{1}{2}\sum_{j\neq i} f_c(r_{ij})[V_R(r_{ij})-b_{ij}V_A(r_{ij})] \tag{1}$$

which expresses the fact that the total energy is the difference between the attractive (V_A) and repulsive (V_R) components which are a function of the interatomic separation r_ij. The pairwise terms V_A and V_R are classical pairwise attractive and repulsive terms, whereas b_{ij} is a many body term that scales the attractive part to the repulsive one, the functional form of which will be given later. The pairwise terms are written as

$$V_R = \frac{D_e}{S-1} e^{-\beta\sqrt{2S}(r_{ij}-r_e)}, \tag{2}$$

$$V_A = \frac{SD_e}{S-1} e^{-\beta\sqrt{2/S}(r_{ij}-r_e)}. \tag{3}$$

These last expressions use different parameters (D_e, S, β, r_e) from the ones used in the original paper by Tersoff,[17] but are identical in substance. To restrict the calculation to just a certain number of nearest neighbours of the atom i under observation, a spherical cut off function f_c is introduced:

$$f_c(r) = \begin{cases} 1, & r_{ij} < D - D_{\text{cut}}, \\ \frac{1}{2}[1 - \sin[\pi(r_{ij} - D)/2D_{\text{cut}}]], & |r_{ij} - D| \leqslant D_{\text{cut}}, \\ 0, & r_{ij} > D + D_{\text{cut}} \end{cases} \tag{4}$$

so that the parameters D and D_{cut} determine the position of the cut off and the half width of the region in which the function changes smoothly from 0 to 1.

The many body term b_{ij}, which depends on the parameters γ and n, can be expressed as

$$b_{ij} = [1 + (\gamma\zeta_{ij})^n]^{-1/2n} \tag{5}$$

which is intentionally designed to have a $-1/2$ power dependence in respect of the number ζ_{ij}. In fact ζ_{ij} provides a weighted measure of the number of other bonds, labeled k, competing with the bond ij and models the coordination number Z of the open-lattice semiconductor material.[14] The pseudocoordination number ζ_{ij} is a function of the local environment. In fact it is expressed in terms of the cutoff function f_c, a function $g(\theta)$ which takes in account the angular dependence, an exponential function ω_{ijk} that tunes the radial dependence and a set of atom type dependent parameters $(\gamma, n, c, d, h, \lambda)$:

$$\zeta_{ij} = \sum_{k \neq i,j} f_c(r_{ik}) g(\theta_{ijk}) \omega_{ijk} \tag{6}$$

where $g(\theta)$ is expressed by

$$g(\theta_{ijk}) = 1 + \left(\frac{c}{d}\right)^2 - \frac{c^2}{d^2 + (h - \cos\theta_{jki})^2} \tag{7}$$

with θ_{ijk} the angle between bonds ij and ik. It has been demonstrated that the mathematical expression of Eq. (7) is not an arbitrary choice. In fact the expression for $g(\theta)$ is functionally equivalent to that derived from an approximation to tight binding theory that expands the electronic density of states to the second moment.[20] The role of the exponential factor in the expression for ζ_{ij} was discussed by Sayed *et al.*[2] and shown to reduce the otherwise unrealistic influence of distant neighbors on immediate bonds:

$$\omega_{ijk} = \exp[\lambda^3(r_{ij} - r_{ik})^3]. \tag{8}$$

For completeness, and to avoid confusion we will briefly give the expressions that link the parameters in the original form,[17] where the pairwise terms are expressed in terms of A, B, λ_{ij}, and μ_{ij}, and the one given above which depends instead on D_e, S, β, and r_e:

$$A = \frac{D_e}{S-1} e^{\beta\sqrt{2S} r_e}, \quad B = \frac{SD_e}{S-1} e^{\beta\sqrt{2/S} r_e}, \tag{9a}$$

$$\lambda_{ij} = \beta\sqrt{2S}, \quad \mu_{ij} = \beta\sqrt{2/S}. \tag{9b}$$

III. CALCULATION OF MATERIALS PROPERTIES

The evaluation of the materials properties chosen to parameterise the potential follows standard procedures.[6] The equilibrium lattice constant a and cohesive energy E_{coh} are easily estimated from the energy vs bond length relationship at the energy minimum. To evaluate the bulk modulus B we use

$$B = \left. \frac{1}{\Omega} \frac{d^2E}{dv^2} \right|_{E=E_{\text{coh}}}, \tag{10}$$

where Ω is the atomic volume and v is defined through the uniform deformation

$$R^1 = v^{1/3} R. \tag{11}$$

To obtain instead the shear constant C', defined through

$$C' = \left. \frac{1}{\Omega} \frac{d^2E}{d\varepsilon^2} \right|_{E=E_{\text{coh}}} \tag{12}$$

a nonuniform deformation is used:

$$R_x^1 = R_x(1 + \varepsilon),$$

$$R_y^1 = R_y/(1 + \varepsilon),$$

$$R_z^1 = R_z. \tag{13}$$

It is worth pointing out also that C' and B, for the zinc blende crystal, are related to the elastic constants (c_{11} and c_{12}) through

$$c_{11} = B + \frac{4}{3} C',$$

$$c_{12} = B - \frac{2}{3} C'. \tag{14}$$

The third elastic constant c_{44}

$$c_{44} = \left. \frac{1}{\Omega} \frac{d^2E_{\text{coh}}}{d\gamma^2} \right|_{E=E_{\text{coh}}} \tag{15}$$

is related to shear deformation in the plane:

TABLE I. Predicted elastic and cohesive properties for III-As and III-N using the parameters of Sayed *et al.* (Ref. 2), Nordlund *et al.* (Ref. 41), Moon *et al.* (Ref. 7), and Goumri-Said *et al.* (Ref. 8). In brackets we compare with experimental/DFT calculated values: all from Ref. 54, apart from ζ of GaAs and InAs (Ref. 59), E_{coh} (Ref. 22) and the lattice constant a (Ref. 60). The elastic constants c_{11} and c_{12} are obtained from the values of B and C'.

	Ga-As (Sayed)	In-As (Nordlund)	Al-As (Sayed)	Ga-N (Moon)	Al-N (Goumri-Said)
E_{coh} (eV/atom)	−3.25	−3.57	−3.78	−5.55	−5.76
	(−3.25)	(−3.10)	(−3.78)	(−4.45)	(−5.76)
a (Å)	5.655	6.059	5.661	4.450	4.371
	(5.653)	(6.058)	(5.662)	(4.500)	(4.380)
B (Mbar)	0.748	0.581	0.781	2.366	2.483
	(0.757)	(0.617)	(0.747)	(2.060)	(2.030)
C' (Mbar)	0.328	0.191	0.316	17×10^{-5}	0.544
	(0.364)	(0.229)	(0.288)	(0.825)	(0.698)
c_{11} (Mbar)	1.182	0.835	1.203	2.366	3.207
	(1.242)	(0.922)	(1.131)	(3.159)	(2.961)
c_{12} (Mbar)	0.530	0.453	0.570	2.366	2.119
	(0.514)	(0.465)	(0.555)	(1.510)	(1.564)
c_{44} (Mbar)	0.687	0.395	0.671	34×10^{-5}	1.409
	(0.634)	(0.444)	(0.547)	(1.976)	(2.004)
ζ	0.536	0.651	0.554	1.000	0.704
	(0.455)	(0.598)	(0.592)	(0.477)	(0.550)

$$R'_x = R_x + \gamma R_y,$$

$$R'_y = R_y,$$

$$R'_z = R_z, \tag{16}$$

however, when performing this calculation one has to take into account the internal displacements which move the interpenetrating fcc sublattices in the diamond structure along the z axis, and therefore minimise the energy for every given γ, with respect to this internal displacement. The condition of minimum energy is characterized by the Kleinman's internal displacement parameter ζ,[21] which defines the distance between the two sublattices as being $\zeta\gamma a/4$ of the lattice constant.

This parameter has a deep meaning. If one concentrates on a single tetrahedron with e.g., a cation in the origin of the coordinate system, a positive shear distortion tends to pull apart two cations along the $[110]$ direction, while pulling together the other two cations in the $[1\bar{1}0]$ direction. Because of these movements the anion at the center of the tetrahedron is subject to radial and angular forces, which resist bond length and bond angles change, respectively, and the displacement that minimises the total energy is a result of a subtle balance between the two.[22] Hence correctly reproducing this effect is an indication that the angular and radial functions in the functional form of the potential are correctly balanced.

IV. REVIEW OF PREVIOUS WORK

In this section we will briefly summarize the previous efforts of several authors who used the ATP as a tool to study materials properties. Though by far the ATP has been used primarily for the study of group IV semiconductors,[9,23–42,42–44] in this paper we will focus the discussion on the III–V semiconductor materials with the zinc blende crystal structure, omitting also the reported studies of II–VI materials[45,46] or metals.[47] Instead we will briefly discuss some application studies that are of general validity.

A. III-arsenides

The ATP for III–V semiconductor materials is a straight extension of the original ATP for Si and Ge when used for the Si-Ge alloy. Smith[1] provided the first parametrization of the Tersoff potential for a III–V semiconductor and followed a recipe for parametrization based on fitting to elastic properties and cohesive energies. Sayed and co-workers[2] improved on Smith[1] by better representing the level of angular dependence and also parametrized AlAs. Murdick *et al.*[48] compared the Stillinger-Weber potential[49] to the ATP and concluded that the ATP provides the best agreement with experimental behaviour when considering thin-film GaAs. A parametrization for InAs was found by Ashu *et al.*[3] and later on improved by Migliorato *et al.*[6] while Nakamura *et al.*[4] proposed the addition of a long range ionic term to allow simulations of epitaxial deposition. Nordlund *et al.*[41] used the ATP to simulate ion implantation damage and recovery at

TABLE II. Parameters for III-V zinc blende semiconductors.

	Ga-As	In-As	Al-As	Ga-P	In-P	Al-P
D_e	1.78044	1.76845	2.3347	2.20178	2.17758	6.02242
S	6.96025	1.32755	1.54131	1.59411	1.5811	1.66971
β	1.5665	1.49877	1.44845	1.62365	1.52761	1.45727
R_e	2.4324	2.56931	2.36843	2.28675	2.45854	1.97527
D	3.5	3.7	3.7	3.1	3.3	3.3
D_{cut}	0.1	0.1	0.1	0.1	0.1	0.1
c	2.16345	2.10031	1.05025	1.26417	1.2179	1.0377
d	0.750147	0.827636	0.850097	0.799535	0.831026	0.699934
$-h$	0.448899	0.442115	0.458041	0.433247	0.461576	0.475714
n	3.55586	2.35072	8.36992	5.42195	5.3449	0.643958
γ	0.257183	0.139688	0.359702	0.339811	0.338811	0.180382
λ	0.244341	0.140874	1.38402	1.81771	1.89106	3.09086

	Ga-N	In-N	Al-N	Ga-Sb	In-Sb	Al-Sb
D_e	2.39175	2.20268	3.96453	2.10427	1.89293	2.78722
S	2.51918	1.69411	2.1498	1.43393	3.02624	2.67111
β	1.9793	1.89216	1.70088	1.4777	1.43782	1.73871
R_e	1.93373	2.11896	1.80623	2.4991	2.72026	2.52233
D	2.5	2.65	2.335	3.5	3.7	3.5
D_{cut}	0.1	0.1	0.15	0.1	0.1	0.1
c	2.59473	1.07074	2.33154	1.20875	5.32122	3.44865
d	0.891376	0.725308	0.831225	0.839761	1.39907	1.20819
$-h$	0.505871	0.533599	0.638531	0.427706	0.489527	0.210583
n	6.15189	9.74096	2.66213	4.60221	1.8926	122.43
γ	0.24139	0.30813	0.19987	0.363018	0.304347	0.604408
λ	1.80993	1.59607	1.99072	0.968688	2.47677	0.955563

various semiconductor interfaces including Si/Ge, AlAs/GaAs, and InAs/GaAs. Migliorato *et al.*[50,51] used the ATP to simulate $\text{In}_x\text{Ga}_{1-x}\text{As}$ alloys and applied it to the study of self-assembled QDs. Albe *et al.*[52] proposed a modification to the potential in order to better describe thermodynamic properties of GaAs while recently Hammerschmidt [53] found ATP parametrizations of InAs and GaAs that correctly reproduce a number of surface energies, together with the elastic properties, including the Kleinman parameter, and applied these improved potentials to the study of uncapped epitaxial islands.

In Table I we show the predictions of the elastic properties using the parameters of Sayed *et al.*[2] for GaAs and AlAs and Nordlund *et al.*[41] for InAs. In brackets we show the experimental values for E_{coh} and lc, and calculated density functional theory (DFT) within the local density approximation (LDA) values.[54] One source of discrepancy is clearly the fact that the parameterisations were obtained by fitting to the experimental values of the elastic constants, which differ slightly from the DFT-LDA values. The results clearly show that the Kleinman parameter is always poorly reproduced. Furthermore the E_{coh} of InAs is not in agreement with the experimental value of −3.1 eV/atom.

B. III-nitrides

Benkabou *et al.*[5] parametrized for the first time cubic III-N materials. The ATP along with the III-N parameter sets has been used for bulk GaN studies,[55–57] cubic aluminium nitride (*c*-AlN),[5,8] GaN nanotubes,[58] and as a basis for improved parameter sets.[7] In Table I we show the predictions of the elastic properties of GaN using the parameters of Moon *et al.*[7] With this parametrization only the lattice constant and c_{11} are in fair agreement with the experimental and DFT-LDA values. The other two elastic constants are predicted to be very small, while the Kleinman parameter is calculated as 1.0, which indicates that when under shear the four bonds in the tetrahedron would all have the same length. This is a clear indication that the potential is fully and incorrectly biased towards the radial forces. This is an identical problem to the one encountered in GaAs when using the parameters of Smith,[1] an issue observed and resolved by Sayed *et al.*[2] by correctly incorporating the exponential function in the expression for ζ_{ij}. We tested the parametrization for InN of Benkabou *et al.*[5] and could not replicate their results. We also tested the parametrization for AlN of Goumri-Said *et al.*[8] and once again found that only the cohesive energy and lattice constant are in good agreement with the experimental

TABLE III. Predicted elastic and cohesive properties for III-V zinc blende semiconductors using the parameters of Table II. In brackets we compare with experimental/DFT calculated values: all from Ref.54 apart from ζ of GaAs and InAs (Ref. 59), E_{coh} (Ref. 22), the lattice constant a (Ref. 60) and E_{coh} of AlSb which we could not find. However, total energy values in Ref. 61 indicate that it is not very different from that of GaAs. The elastic constants c_{11} and c_{12} are obtained from the values of B and C'.

	Ga-As	In-As	Al-As	Ga-P	In-P	Al-P
E_{coh} (eV/atom)	−3.25	−3.10	−3.78	−3.56	−3.48	−4.26
	(−3.25)	(−3.10)	(−3.78)	(−3.56)	(−3.48)	(−4.26)
a (Å)	5.653	6.058	5.662	5.450	5.869	5.463
	(5.653)	(6.058)	(5.662)	(5.451)	(5.869)	(5.463)
B (Mbar)	0.754	0.614	0.748	0.919	0.739	0.885
	(0.757)	(0.617)	(0.747)	(0.921)	(0.736)	(0.886)
C' (Mbar)	0.365	0.232	0.288	0.443	0.267	0.329
	(0.364)	(0.229)	(0.288)	(0.440)	(0.269)	(0.329)
c_{11} (Mbar)	1.240	0.923	1.131	1.509	1.095	1.323
	(1.242)	(0.922)	(1.131)	(1.507)	(1.095)	(1.325)
c_{12} (Mbar)	0.510	0.459	0.556	0.624	0.561	0.665
	(0.514)	(0.465)	(0.555)	(0.628)	(0.556)	(0.667)
c_{44} (Mbar)	0.637	0.446	0.546	0.763	0.524	0.628
	(0.634)	(0.444)	(0.547)	(0.763)	(0.526)	(0.627)
ζ	0.478	0.593	0.590	0.521	0.610	0.615
	(0.455)	(0.598)	(0.592)	(0.516)	(0.615)	(0.604)
	Ga-N	In-N	Al-N	Ga-Sb	In-Sb	Al-Sb
E_{coh} (eV/atom)	−4.45	−3.86	−5.76	−2.96	−2.80	−3.25
	(−4.45)	(−3.86)	(−5.76)	(−2.96)	(−2.80)	(−3.25)
a (Å)	4.501	4.981	4.380	6.096	6.479	6.135
	(4.500)	(4.980)	(4.380)	(6.096)	(6.479)	(6.135)
B (Mbar)	2.064	1.481	2.032	0.566	0.477	0.855
	(2.060)	(1.476)	(2.030)	(0.567)	(0.476)	(0.855)
C' (Mbar)	0.824	0.419	0.697	0.272	0.182	0.414
	(0.825)	(0.424)	(0.698)	(0.270)	(0.183)	(0.414)
c_{11} (Mbar)	3.162	2.040	2.961	0.929	0.719	1.407
	(3.159)	(2.040)	(2.961)	(0.927)	(0.720)	(1.407)
c_{12} (Mbar)	1.514	1.201	1.567	0.385	0.356	0.579
	(1.510)	(1.190)	(1.565)	(0.378)	(0.354)	(0.579)
c_{44} (Mbar)	1.972	1.136	2.004	0.462	0.341	0.399
	(1.976)	(1.141)	(2.004)	(0.462)	(0.341)	(0.399)
ζ	0.464	0.620	0.562	0.532	0.599	0.598
	(0.477)	(0.639)	(0.550)	(0.530)	(0.603)	(0.601)

values, though this parametrization does not suffer from the "stiffness" problem of that of Moon *et al.*[7] for GaN.

V. RESULTS AND DISCUSSION

In order to obtain reliable parameterisation of the Tersoff potential we developed a variant to the common simplex algorithm, which we call "granular radial search." This approach relies on generating random parameter sets within a predetermined 12-dimensional sphere and a steepest descent algorithm that allows the gradual reduction of the search resolution, till convergence is achieved. On a 3 GHz Desktop machine, independent on any starting point, we can typically obtain a very accurate set that reproduces a maximum of ten physical quantities, in a maximum of 8 h. Details of the algorithm will be given elsewhere.

In Table II we present the obtained parameterisation for various commonly used III–V zinc blende semiconductors. It is worth noting that the values of the parameters are consistently within 1 order of magnitude, apart from the exponent n of AlSb. In general this is to be expected as the cohesive and elastic behaviour of all the materials presented is not particularly dissimilar.

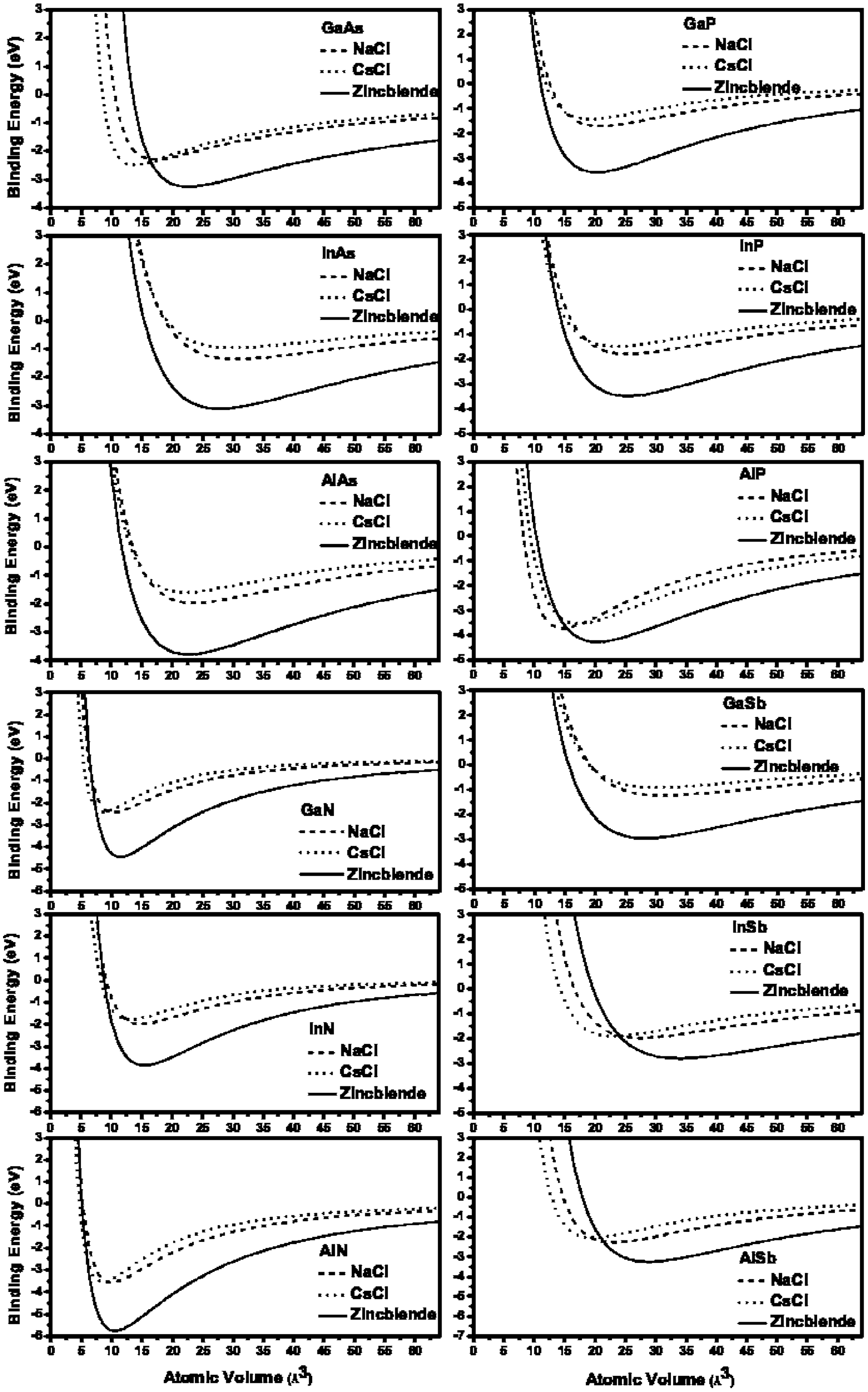

FIG. 1. Phase diagrams for III-As, III-N, III-P, and III-Sb semiconductors with the zinc blende (solid line), simple cubic (dash), and face centered cubic (dot). Correctly the zinc blende is the lowest energy structure.

The predicted elastic and cohesive properties using the parameters of Table II, are presented in Table III, with the experimental and calculated values in brackets for comparison. All of the predicted values are in excellent agreement with the experimental and calculated data, with the exception of the Kleinman parameter ζ, for which the quality of the

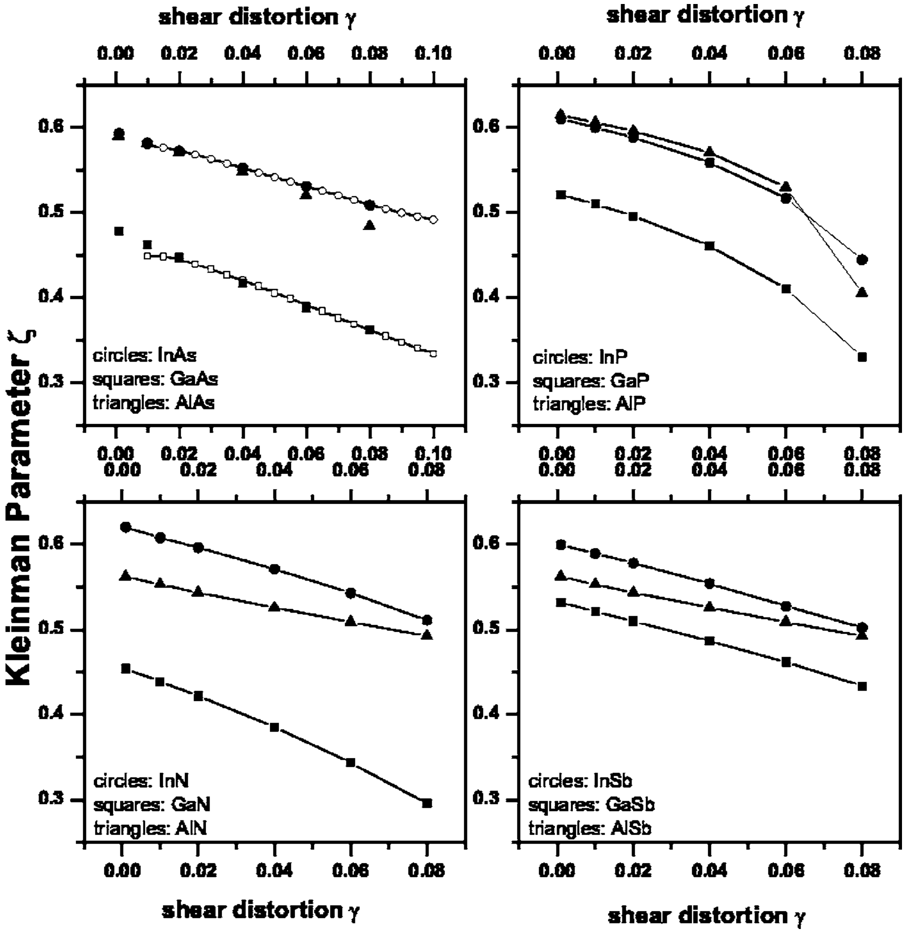

FIG. 2. Dependence of the sublattice internal displacement parameter ζ on shear strain for III-As, III-N, III-P, and III-Sb semiconductors. Ga (squares), In (circles), and Al (triangles) compounds are shown. For GaAs and InAs theoretical data (Ref. 59) (hollow symbols) is also shown for comparison.

agreement varies from material to material, though it is never more than 5% different.

In Fig 1, we show the calculated phase diagrams for the different materials studied. We compare the energy vs unit cell volume of the zinc blende phase to that of the rocksalt (NaCl) and cesium cloride (CeCl) crystals. Correctly, in all 12 cases the zinc blende is the lowest energy structure, which is a prerequisite to implementing MS or MD simulations.[15] In calculating the energy vs unit cell volume dependence we have omitted the cutoff function specified in Eq. (4), while always ensuring that every atom is bonded by the correct number of nearest neighbours in the different crystals. This is why the often abrupt effect of the cut off function for cell dimensions larger than the cutoff radius is not visible. Furthermore we are deliberately neglecting the energy vs unit cell volume of the wurtzite phase. The Tersoff potential only includes the first nearest neighbors in the calculation and in this approximation the wurtzite and zinc blende phases, though they have different volumes, have exactly the same energy. Furthermore, in Fig. 2, we show the dependence of the Kleinman parameter ζ upon shear strain. These values are calculated in a very similar way to what follows from Eq. (15), the only difference being that the strain tensor is 1 and $\gamma/2$ for the ε_{ii} and ε_{ij} components, respectively. In the case of InAs and GaAs we also show the DFT-LDA calculated data, reproduced from Ref. 59 It is clear that the linear decay is correctly reproduced by our parametrizations, a clear indication of the correct balance of radial and angular forces in the potential. For all the semiconductor materials parametrized this behavior is very similar, though at present no DFT-LDA data is available to compare directly. It is worth mentioning a set of parameters that reproduces correctly the small strain value of ζ does not necessarily reproduce the large strain decay correctly. On occasion we had to dismiss sets that would predict either negative or very large values of ζ for large values of γ, or unrealistic nonlinear decays. Therefore the sets we present have been obtained with the prerequisite of an acceptable linear decay.

VI. CONCLUSIONS

We have obtained accurate Tersoff potential parameterisations for zinc blende III-As, III-N, III-P, and III-Sb semiconductors. This parameter sets are able to correctly reproduce DFT-LDA calculated values of the elastic properties and also one important nonlinear effect in the strain, therefore capturing the essence of the balance of radial and angular forces in the functional form of the potential.

This allows the use of the Tersoff potential for implementation of molecular dynamics and molecular statics simulations, applied to problems such as structural relaxation of environments where the atoms are fully bonded (i.e., excluding point defects and surfaces). Particularly in nanostructured semiconductors, these problems rely on accurately predicting the elastic and cohesive behaviour of the materials. Therefore if the calculations are limited to properties that are directly linked to the ones used in the parametrization procedure (note that we have not tested for, e.g., melting, coefficient of linear expansion or phonons), these simulations can rival the accuracy of DFT, but with a substantial saving in computing time.

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