

## Empirical bond-order potential for semiconductors

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An empirical bond-order potential for semiconductors is developed. The total energy is expressed as the sum of contributions of individual bonds weighted by a bond-order term. For the bond-order term the tight binding second moment approximation is used. The application to silicon in its diamond structure gives results comparable to those obtained with the Tersoff potential. A parameter set for GaAs is proposed yielding elastic constants and surface and defect properties in good agreement with experimental and quantum mechanical results. Because of its generality and small number of fitting parameters, the potential is easy to apply to a wide range of semiconducting materials. [S0163-1829(98)01031-5]

### I. INTRODUCTION

Empirical potentials in molecular dynamics (MD) or molecular statics simulations have become an increasingly powerful means of understanding and predicting material properties. In spite of the recent dramatic growth of computer capacities and the usage of first-principles calculations, empirical potentials provide most valuable insights into systems beyond the scope of quantum mechanical methods. This includes the study of grain boundaries, extended defects, or the dynamics of crystal growth. In addition, hybrid methods use empirical potentials for regions that are expected to remain in configurations to which these potentials are fitted.

For semiconductors, the most successful approaches to develop empirical potentials are those of Stillinger and Weber<sup>1</sup> and Tersoff.<sup>2</sup> Originally, the former potential was proposed for silicon and has been fitted to a number of chemical elements, including the group IV semiconductors and their binaries and III-V compounds.<sup>3-10</sup> One of the disadvantages in applying this approach to III-V compounds is that the homonuclear interactions cannot be fitted so straightforwardly as it is possible for the group IV elements and their binaries. Thus, for a great number of potentials these interactions are not fitted or they are absent. This reduces their applicability considerably.

The approach of Tersoff is essentially different with the atomic interactions depending on the environment of bonds or atoms. Following Abell,<sup>11</sup> Tersoff expressed the total energy  $V$  of a given structure as

$$V = \sum_{i \neq j} A e^{-\lambda r_{ij}} - B b_{ij} e^{-\mu r_{ij}}, \quad (1)$$

where  $r_{ij}$  is the distance between atoms  $i$  and  $j$ ;  $A$ ,  $B$ ,  $\lambda$ , and  $\mu$  are parameters; and  $b_{ij}$  is the bond-order term, which accounts for an effective coordination. As it is the case for the Stillinger-Weber (SW) potential, the Tersoff potential was fitted to the group IV semiconductors and to a number of III-V compounds.<sup>12-15</sup> No preference of one of these approaches over another seems to be justified *a priori*. The Tersoff potential, however, seems to be more successful if other chemical elements are included. Brenner<sup>16</sup> has given a parametrization for C-H interactions yielding a good overall

description for diamond, fullerenes, and hydrocarbons. Murty and Atwater<sup>17</sup> proposed a parameter set for Si-H interactions agreeing well with experiments for hydrogen absorbed on Si(001) surfaces and small Si-H molecules.

The main difficulty in fitting empirical parameters to systems containing more than one atomic species is that one does not know on which atomic species the bond-order term should depend. For Si-C and Si-Ge interactions, it is assumed to depend on the central atom  $i$  and it is weighted by a factor that distinguishes homonuclear and heteronuclear interactions. In the potentials of Smith<sup>13</sup> and Ashu *et al.*<sup>14</sup> for GaAs and  $\text{In}_x\text{Ga}_{1-x}\text{As}$ , the bond-order term depends solely on the central atom. In the Si-H and C-H potentials the angular terms depend complexly on two or three atoms involved. Beardmore and Smith<sup>18</sup> have combined these potentials to model Si-H-C interactions. Since there is not only one way to combine these interactions, different combination rules imply different results. In the approach of Albe *et al.*<sup>15</sup> for BN, the parameters of the bond-order term depend on the atomic species  $i$  and  $j$ . Khor and Das Sarma<sup>19</sup> have proposed a universal potential similar to the potential and applied it to several III-V compounds. Although the homonuclear interactions are fitted to some physical properties, Khor and Das Sarma omitted the angular dependence of these interactions. In addition, the bond-order term is not smooth if the coordination changes, making it impossible to be used in MD simulations. The aim of this paper is to show that an empirical bond-order term derived from the second moment approximation of the tight binding model can be used to establish a general empirical potential at the level of the Tersoff potential.

### II. SECOND MOMENT APPROXIMATION

Several authors<sup>20-24</sup> have proposed to use the moments of the electronic density as one way to derive physically motivated semiempirical potentials for different materials ranging from silicon to metals and transition metals. Carlsson<sup>22</sup> has pointed out that both metallic and covalent systems may be described on this basis. It is now well established that the empirical potentials of Finnis and Sinclair,<sup>21</sup> Daw and Baskes,<sup>25</sup> and Tersoff can, in some respect, be regarded as certain approximations of such a moment expansion. The

TABLE I. On-site energies in eV used for the present potential.

Element	$E_s$	$E_p$
Si	0.0	8.295
Ga	-2.657	3.669
As	-8.343	1.041

usefulness of the SW potential lies in the fact that in the covalent limit the bond energies are independent of each other and hence additive. On the other hand, the success of Tersoff's approach is based on the fact that for a wide range of materials the ratio of the bond energy to an effective coordination number is proportional to the equilibrium bond length.

In this paper we use the tight binding second moment approximation to write the bond order explicitly in terms of elements of the tight binding Hamiltonian matrix. Using physically motivated matrix elements, the remaining two-body parameters are fitted to elastic constants, equilibrium bond lengths, and cohesive energies. We show that, despite the relatively small number of adjustable parameters, this formalism leads to a potential comparable to the Tersoff potential for Si. A second parameter set is given for GaAs to demonstrate the applicability to III-V compounds.

The total binding energy can be written as (see, e.g., Ref. 26)

$$V = \sum_{i,j} V_{ij}^{rep} + V_{ij}^{\text{bond}}. \quad (2)$$

Here the first term is the ionic repulsion. The second term is the attractive bond energy. According to Pettifor,<sup>27</sup> the latter term may be written as

$$V_{ij}^{\text{bond}} = 2 \sum_{\alpha,\beta} H_{i\alpha,j\beta} \Theta_{j\beta,i\alpha}. \quad (3)$$

$\mathbf{H}$  is the bond integral matrix of Slater and Koster<sup>28</sup> and  $\Theta$  is the corresponding bond-order matrix. Here we restrict ourselves to systems with  $s$  and  $p$  electrons, only, so that the diagonal elements of  $\mathbf{H}$  are the on-site energies  $E_s$  and  $E_p$  (Table I); the nondiagonal elements are the hopping integrals  $ss\sigma$ ,  $sp\sigma$ ,  $ps\sigma$ ,  $pp\sigma$ , and  $pp\pi$ . Under certain conditions for the matrix elements (see, e.g., Ref. 27) and the neglect of  $\pi$  bonding, Eq. (3) becomes

$$V_{ij}^{\text{bond}} = -2h_{\sigma ij} \Theta_{i\sigma,j\sigma}, \quad (4)$$

with  $h_{\sigma ij} = -ss\sigma_{ij} + pp\sigma_{ij}$ . Using the abbreviations  $E_{sp} = E_p - E_s$ ,  $p_\sigma = pp\sigma/|ss\sigma|$ , and  $E_\sigma = (E_s + p_\sigma E_p)/(1 + p_\sigma)$ , we write the first term of the expansion following Alinaghian *et al.*:<sup>29</sup>

$$\Theta_{i\sigma,j\sigma} \propto \left( 1 + \frac{1}{h_{\sigma ij}^2} (\Delta^2 + \Sigma^2) \right)^{-1/2}, \quad (5)$$

with

TABLE II. Hopping elements in eV used for the present potential. Note that for Ga-As, Ga-Ga, and As-As the parameters are the same and  $pp\pi = 0$  for all interactions.

Element	$ss\sigma$	$sp\sigma$	$pp\sigma$
Si	-1.820	1.960	3.060
Ga, As	-1.613	2.204	3.028

$$\Delta^2 = \frac{1}{2(1+p_{\sigma ii})} \left( \frac{1}{4} \Delta E^2 + \frac{p_{\sigma ii}}{1+p_{\sigma ii}} E_{spi}^2 \right) + \frac{1}{2(1+p_{\sigma jj})} \left( \frac{1}{4} \Delta E^2 + \frac{p_{\sigma jj}}{1+p_{\sigma jj}} E_{spj}^2 \right), \quad (6)$$

$$\Delta E = E_{\sigma i} - E_{\sigma j}, \quad (7)$$

and

$$\Sigma^2 = \frac{1}{2} \sum_{k \neq i,j} h_{\sigma ik}^2 g_\sigma(\theta_{jik}) + \frac{1}{2} \sum_{l \neq i,j} h_{\sigma jl}^2 g_\sigma(\theta_{ijl}). \quad (8)$$

The angular terms depend on the hopping elements (Table II)

$$g_\sigma(\theta_{jik}) = a + b \cos(\theta_{jik}) + c \cos(2\theta_{jik}), \quad (9)$$

$$a = 1 - b - c, \quad (10)$$

$$b = \frac{4c}{p_{\sigma ik}}, \quad (11)$$

$$c = \frac{p_{\sigma ik}^2}{2(1+p_{\sigma ik})^2}. \quad (12)$$

In Eq. (5) the proportionality factor depends on band filling. Here we assume it to be constant. Note that some matrix elements depend on only one atomic species, whereas other elements depend on both species of a specific bond. The advantage of using Eq. (5) as the bond-order term of an empirical potential is therefore evident. First, it is clear which atomic species the angular terms depend on. Second, the parameters are the elements of the bond integral matrix; thus it is not necessary to fit angular terms, which is probably the most difficult part of a fitting procedure. As it was pointed out earlier, numerically the angular part of the Tersoff potential for Si is almost identical to expression (9) for appropriate matrix elements.<sup>29</sup>

### III. FIT OF THE POTENTIAL

In order to use expression (5) as the bond-order term in an empirical potential, we rewrite the potential energy as

$$V = \sum_{i < j} f_c(r_{ij}) (A e^{-\lambda r_{ij}} - B b_{ij} e^{-\mu r_{ij}}), \quad (13)$$

with

$$b_{ij} = 2h_{\sigma ij} \Theta_{i\sigma,j\sigma} \quad (14)$$

and  $f_c$  being a cutoff function. In contrast to the Tersoff potential, the sum in Eq. (13) is over bonds rather than atoms. Since the environment of both atoms  $i$  and  $j$  is taken

TABLE III. Two-body parameters.

Elements	A (eV)	B (eV)	$\lambda$ ( $\text{\AA}^{-1}$ )	$\mu$ ( $\text{\AA}^{-1}$ )
Si-Si	1845.8640	75.03	2.60	1.66
Ga-As	1310.8480	42.5446	2.58	1.54
Ga-Ga	795.54034	87.245595	2.26	1.71
As-As	2002.1275	7.9773487	3.05	1.01

into account, the bond order shows the symmetry  $b_{ij}=b_{ji}$ . Since the elements of the Hamiltonian matrix depend on the interatomic distance, the bond order is also a function of this distance. We assume that this radial dependence can be transferred into the factor  $Be^{-\mu r_{ij}}$  so that only the equilibrium values of the matrix elements have to be considered in Eq. (14).

The parameters of the potential energy function (13) can be divided into three groups. The parameters of the cutoff function, for which we assume the same functional form and cutoff distance as in the Tersoff potential, are fixed between the first and the next neighbor shell of atoms. The second group consists of parameters  $E_s$ ,  $E_p$ ,  $ss\sigma$ ,  $sp\sigma$ ,  $sp\pi$ , and  $pp\pi$  entering the angular term. These parameters are taken from tight binding models of the system under consideration and they are no longer free. The third group, which we call the two-body parameters since they do not appear in the angular term, are  $A$ ,  $B$ ,  $\lambda$ , and  $\mu$ . Only these parameters are used in the fitting procedure.

First, the potential (13) is tested for silicon by fitting the two-body parameters (Table III). Because of its technological importance, silicon is one of the most extensively studied systems with an enormous data base of bulk, surface, and defect properties available. Therefore, silicon has always been a test system for first-principles methods, tight binding calculations, and empirical potentials.

For the matrix elements and the on-site energies we use the tight binding parameters of Goodwin *et al.*<sup>50</sup> As mentioned above,  $\pi$  bonding is neglected by setting  $pp\pi$  equal to zero. The functional form of Eq. (13) is flexible enough to be fitted, simultaneously, to the cohesive energy, equilibrium bond length, and the elastic constants of Si in the diamond structure. In addition, the potential is tested for some well known surface and defect properties. We obtain a dimer length of 2.37  $\text{\AA}$  and an energy gain of 1.62 eV per dimer for the Si(001)- $2\times 1$  reconstruction. The elastic constants and defect energies are summarized in Tables IV and V. The potential was also tested for the high-density  $\beta$ -tin, simple cubic, bcc, and fcc Si structures. Our results given in Table

TABLE IV. Elastic constants of Si and GaAs, present potential, and experimental data. All values are given in Mbar. Experimental data are from Refs. 44 and 45.

Structure	Source	$C_{11}$	$C_{12}$	$C_{44}$
Si	present work	1.7	0.62	0.61
Si	experiment	1.67	0.65	0.80
GaAs	present work	1.06	0.39	0.36
GaAs	experiment	1.18	0.54	0.59

TABLE V. Defect formation energies of Si interstitials: the tetrahedral ( $E_T$ ), the hexagonal ( $E_H$ ), the  $\langle 110 \rangle$  split ( $E_{\langle 110 \rangle}$ ), and the extended configuration ( $E_{Ie}$ ), and the vacancy formation energy ( $E_{vac}$ ). The values (all in eV) obtained via the Tersoff potential ( $T3$ ), a tight binding model (TB, Ref. 46), and the local density approximation (LDA, Refs. 47 and 48) are given for comparison.

Source	$E_T$	$E_H$	$E_{\langle 110 \rangle}$	$E_{Ie}$	$E_{vac}$
present work	4.03	4.80	4.63	3.81	4.04
T3	4.09	5.22	4.64	4.50	3.70
TB	4.12	5.93			
LDA		3.30			3.75

VI are in good agreement with the results of the Tersoff potential and in reasonable agreement with *ab initio* calculations.<sup>31,32</sup>

In order to establish a parameter set for GaAs, we use the on-site energies and hopping integrals of Goringe *et al.*<sup>33</sup> Since our approach does not distinguish the Ga-As bonds from As-Ga ones, the same value for  $sp\sigma$  is used (which is, in fact, the geometric mean of the As-As and the Ga-Ga values). The overall agreement for the bulk modulus and elastic constants is quite good. However, we were not able to find a parameter set that leads to a negative Cauchy pressure if the error for the elastic constants is restricted to below 10%. The parameters for the As-As interactions are fitted to the bulk modulus and the cohesive energy of arsenic in the A7 structure by neglecting interactions between different layers. The potential function for arsenic exhibits a minimum of the potential energy for the A7 structure. Its use for MD simulations at a finite temperature would require  $\pi$  bonding to stabilize the layers.

We have not fitted the Ga-Ga interactions to the rather complicated orthorhombic structure but followed the approach of Ito *et al.*<sup>34</sup> and fitted these parameters to Ga in the fcc structure. For both the Ga-Ga and the As-As interactions

TABLE VI. Volume and energy differences  $\Delta E$  of several structures of Si and GaAs with the present potential compared with LDA results. For Si, the results are also compared with those obtained with the Tersoff potential ( $T3$ ).  $\Delta E$  is measured with respect to the zinc blende structure and is given in eV/atom for Si and in eV/molecule for GaAs.  $V_0$  is the volume per atom for Si and the volume per molecule for GaAs in the diamond and zinc blende structure, respectively. See the text for references.

Model	Structure	$V/V_0$			$\Delta E$		
		LDA	Present work	T3	LDA	Present work	T3
Si	$\beta$ -Sn	0.76	0.76	0.77	0.27	0.30	0.33
	sc	0.79	0.81	0.82	0.35	0.29	0.32
	bcc	0.73	0.73	0.73	0.53	0.43	0.56
	fcc	0.72	0.73	0.72	0.57	1.36	1.13
GaAs	cinnabar	0.83	0.89		0.35	0.25	
	NaCl	0.80	0.79		0.54	0.50	
	CsCl	0.77	0.67		1.00	0.78	
	SOD	1.24	1.30		0.40	0.20	
	ATO	1.33	1.40		0.42	0.20	
	ATV	1.03	1.09		0.29	0.15	

there is a large number of parameter sets yielding the correct bulk moduli, cohesive energies, and bond lengths. For both types of interactions we have chosen sets that led to reasonable bond lengths of the dimers of the reconstructed GaAs(001) surfaces. With the present potential, all different phases of GaAs(001) surface reconstructions are stable in a MD simulation at room temperature. Of course, it is not useful to draw conclusions about the relative stability of the different phases of the surface reconstruction since charge effects are not included in this potential. The parameter set was tested for some point defects in GaAs. Seong and Lewis<sup>35</sup> have shown in their tight binding calculations that the Ga vacancy exhibits, irrespectively of the charge state, an inward relaxation of about 0.32 Å. Our parameter set yields an inward relaxation of 0.4 Å. For the Ga antisite, we obtain two minima: one corresponding to the “broken bond” geometry and the second showing a “bond” between the Ga<sub>As</sub> and the neighboring Ga. For the geometry of the As antisite, which is also independent of the state of charge, we obtain an outward relaxation by less than 1%, in good agreement with the results of Seong and Lewis.<sup>35</sup> The formation energies of these point defects are in the range 1–3 eV depending on the atomic chemical potential chosen. These are reasonable values for the neutral defects. In contrast to the geometries of the defects investigated here, the charge state of the defect and the electron chemical potential strongly influence their formation energies (ranging, e.g. from 2 to 5 eV for the antisite defects). These effects are beyond the present model.

As a further test for the As-As interactions we investigated the geometries of the split As antisite and the (110) split As interstitial as it was recently proposed by Landman *et al.*<sup>36</sup> We found that all bond lengths differ by less than 5% from those obtained by the *ab initio* calculations of Landman *et al.* The binding energy of 0.8 eV of the split antisite relative to the isolated split interstitial and the isolated As antisite is somewhat lower than the *ab initio* value of 1.1 eV.

Finally, the GaAs potential is tested for other crystal structures. We have investigated GaAs in the high-density phases CsCl and NaCl and in the recently described cinnabar phase as well as in the theoretical low-density phases

sodalite (SOD), ALPO<sub>4</sub>-25 (ATV), and ALPO<sub>4</sub>-31 (ATO). In analogy with zeolite nets, the latter phases were proposed as expanded volume phases and investigated via *ab initio* methods by Demkov *et al.*<sup>37</sup> Our potential gives the correct ordering of the high-density phases with respect to their energy as compared to *ab initio* results<sup>38–40</sup> and at least a good estimation of the low-density structures, with the maximum error in energy being 0.22 eV per molecule. The results are summarized in Table VI.

#### IV. CONCLUSIONS

We used the tight binding second moment approximation to describe the bond-order term in an empirical potential. Using quantum mechanically motivated hopping integrals and on-site energies and fitting the two-body parameters to lattice constants and elastic properties yield an empirical potential for Si and GaAs. Since the number of adjustable parameters is relatively small and the most complicated part of the fitting, i.e., fitting the angular terms, is avoided, the potential can readily be applied to a wide range of materials. In addition, this potential allows one to directly include information from tight binding calculations since, at least in their real space representations, bond orders and bond energies are the physical quantities that are dealt with. We emphasize that the parameter sets presented here were fitted only to properties of the diamond (zinc blende) structure. However, it should be possible to find parameter sets that can describe different phases simultaneously or to fit the parameters to another specific phase of interest.

Since it is assumed to be negligible for the systems considered here, our approach has omitted  $\pi$  bonding for the sake of simplicity. However, the inclusion of  $\pi$  bonding for appropriate systems is possible at no extra cost and will be considered in a subsequent paper.<sup>41</sup> Several authors have proposed to use environment-dependent hopping integrals in the moments expansion<sup>42</sup> as well as in conventional tight binding models<sup>43</sup> instead of fixed values in order to take into account that hybridization may change with coordination. Such an approach can most easily be implemented in the present potential and is under development.

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