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Structure descriptor for surface passivation in the simulation of atomistic models

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Abstract Surface passivation is an essential step for atomistic simulations. There can be many possible surface passivation results for a given device model, such as semiconductor devices that consist of Si, GaAs, or other materials because the bonding directions of the surface atoms may not be unique. Based on the structure analysis of the given model, a generation method with structure descriptor (SDG) is proposed for surface passivation. Compared with other existing solutions, the SDG method not only provides trimmer results, but also reduces the torsion angle energy of the model, which is preferred in the simulation of atomistic models. The efficiency of this method was validated through test results from several applications.

Keywords computer aided design, structure analysis, torsion angle, universal force field, surface passivation, atomistic model

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1 Introduction

Integrated circuits (IC) are the foundation of modern technologies, which may consist of tens of thousands of transistors on one chip. Drift diffusion [1,2] and effective mass [3] are traditional methods employed to simulate and analyze the performance of semiconductor devices. Traditional methods can handle models on the scale of 10 nm to 100 μm or even larger. However, in the semiconductor industry, the feature size of devices is already approaching the sub-10 nm scale. These methods would fail at such small scales, as quantum effects such as nonlocal and hot-carrier effects [4] begin to play important roles at these dimensions. Quantum mechanics based simulation methods, such as density functional theory combined with non-equilibrium Green's functions (DFT_NEGF) [5, 6] are introduced to simulate devices at the 10 nm scale, so that quantum effects can be treated properly. Quantum simulation methods can aid the design of new devices. For this kind of simulation, an atomistic model is needed, as depicted in Figure 1. Surface passivation is an important step while creating atomistic models. In this work, a novel method will be introduced to facilitate this step.

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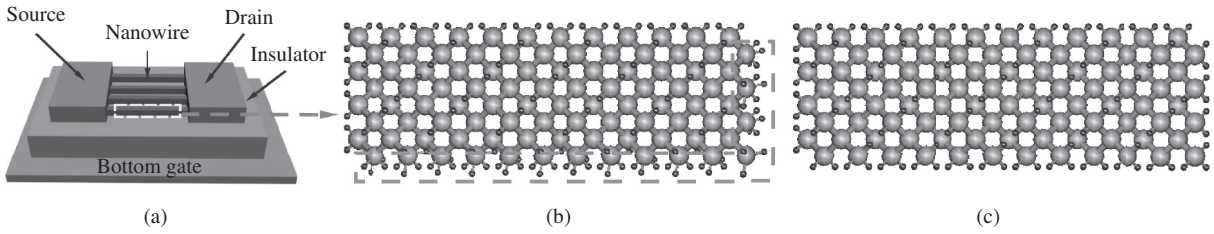


Figure 1 (a) A transistor composed of parallel Si nanowires. Source, drain and bottom gate are the three terminals of the transistor. The enlarged molecular model of the dashed area is shown in (b) and (c), which show different surface passivation results of a Si nanowire. In (b) and (c), The larger spheres are Si atoms; while the smaller spheres are H atoms. (b) Side view of the result based on the bonds status of atoms. H atoms in the dashed area are not so trim as others. (c) The result from the SDG method.

Surface passivation has been widely discussed in the simulation of atomistic models [7–9]. In these applications, each atom on the surface would normally be terminated with enough hydrogen (H) atoms to maintain charge balance, to stabilize the structure. For example, one of the common semiconductor materials, silicon (Si), need four single bonds on each atom to keep its charge balance. These four bonds point to the vertices of a tetrahedron. If two or three of the bonds are fixed, the remainder of the structure is determined. However, if only one bond is fixed, there are not enough constraints to determine the other three. Si atoms at an edge or corner are in this situation. H atoms can be added randomly to fit these unfilled positions, as depicted in Figure 1(b). It is clear that the H atoms in the dashed rectangular area are not passivated in the same pattern as others. General surface passivation methods [10] cannot solved this problem easily.

In this work, a method based on the generation of structural descriptors (SDG) is proposed that can generate better-organized results using structural descriptors (SDs), as depicted in Figure 1(c). The SDs are generated from the original model, which can represent the structure features of the given model. Based on the SDs, the surface passivation can be easily finished. The advantages of this method include:

- Generate trimmer results for surface passivation of different materials with SDs.
- SDs can be generated based on the given structure, no additional model information is required.
- The proposed method can be easily extended to other materials with crystalline structures.

2 Related work

Surface passivation is an essential step in building atomistic models for quantum simulations. A widely-used practice is to add and bond adequate H atoms to any unsaturated surface atoms in device models. The bonding status of atoms (BSA) is used to generate a surface passivation result [8], which has been widely implement in research efforts [11, 12] and commercial software [13, 14]. It is based on the bonding status of each atom in the model and identifies empty bonding directions for passivation. However, the passivation results are not unique for atoms along the edge or at the corner of the model. So this method often generates inelegant results, as shown in Figure 1(b).

Beyond the above solutions, researchers have also explored the surface of atomistic models by experimental observation [15]. In [16], the status of Si-H bonds on small diameter silicon nanowires were captured with scanning tunneling microscopy. An efficient computation method is also proposed to find the possible structure of Si-H bonds [17]. However, most of the previous methods can only provide a guess of the possible structure for the passivation of a device during simulations. Those methods cannot be fully automated and require various degrees of human involvement.

In research involving atomistic models, information of structure is widely used in the model classification or searching applications [18]. However, few studies have introduced information of structure to generate or manipulate these models. In this paper, a method based on the geometric analysis of the given model is proposed to treat the surface passivation of atomistic models.

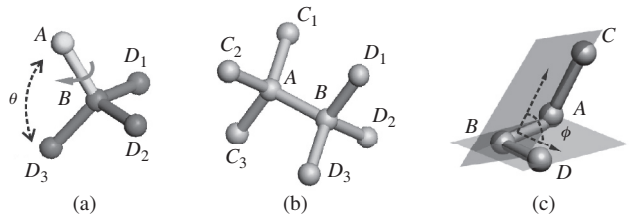


Figure 2 (a) Possible bonding directions based on the bonding status of Si atoms; (b) possible bonding directions based on existing bonds; (c) definition of torsion angle ϕ, it is the angle between the plane defined by atoms ABC and the plane defined by atoms ABD, which share the same bond, AB.

3 Structure descriptor

3.1 Motivation

As shown in Figure 1(b), if the bonding status of atoms is used as the only constraint for surface passivation, the result is not unique for atoms with only one bond. Taking Si atom B in Figure 2(a) as an example, it has only one fixed bond (AB). The remaining possible bonding directions of BD_1, BD_2 and BD_3 are free. In this case, the angles among AB and other three bonds satisfying $\theta \approx 109^\circ$ is the only constraint, which leaves the freedom to bond with new atoms at different directions. For example, in Figure 2(a), BD_1, BD_2 and BD_3 can rotate around the bond AB to generate infinite possible passivation results.

Nevertheless, those Si atoms with four bonds can provide enough information to generate a unique passivation result. In this work, structure information is extracted from a given model to constrain these possible bonding directions. The orientation of bonds and the atoms of their two ends are introduced to generate SDs, which can be used to fix the bonding directions of these atoms with only one bond. As depicted in Figure 2(b), if both ends of a bond have specified bonding directions, all torsion angles are fixed. The passivation result should be trimmer than that obtained from the BSA method. The torsion angle (ϕ) is the angle defined by four connected atoms, as shown in Figure 2(c), which is important for geometry optimization of models.

3.2 Definition

An SD is a collection of three components: the orientation of the bond and the bonding directions of both atoms in the bond. It can be presented as $SD = \{\boldsymbol{O}, V_S, V_E\}$, where $\boldsymbol{O}$ is the orientation of the bond, which is AB in Figure 2(b). V_S is a set of vectors representing the uncounted bonding directions of the start atom, $V_S = \{\boldsymbol{V}_{AC_1}, \boldsymbol{V}_{AC_2}, \boldsymbol{V}_{AC_3}\}$ in Figure 2(b) and V_E is a set of the uncounted bonding directions of the end atom, $V_E = \{\boldsymbol{V}_{BD_1}, \boldsymbol{V}_{BD_2}, \boldsymbol{V}_{BD_3}\}$ in Figure 2(b).

Based on this data structure, the bonding directions of the two atoms from the same bond are fixed. If one atom with only one bond is found, it can be terminated similarly to those atoms with two or three bonds. With the help of the SDs, the final surface passivation results should be in the same pattern as other atoms. Since there is no additional freedom for these atoms, the results from the SDG method is trimmer than that obtained from the BSA method.

The models input may exhibit floating point errors, which may lead to a variance in the calculated directions for the same type of bond. This variance could cause the generation of multiple SDs. To solve this problem, a tolerance (ϵ) is introduced to reduce this error. Directions calculated within the acceptable range are considered to be the same. Taking the Si-bar model in Figure 4 as an example, there are 12 different SDs with no tolerance. By introducing ϵ, the number of different SDs is reduced to 4.

3.3 Potential energy interpretation

The models generated from these SDs not only have a more consistent surface, but also have less torsion angle energy. In the execution of atomistic model simulations, force fields are commonly used to do

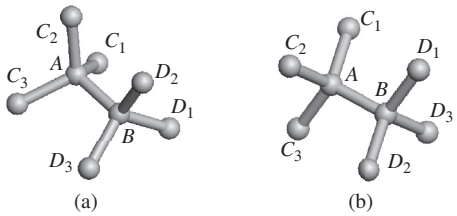


Figure 3 (a) One set of the torsion angles generated by BSA method for atom B; (b) torsion angles generated by SDG method.

geometry optimization [19, 20]. Taking the universal force field (UFF) as an example, the potential energy of a model is defined as follows:

$$E = E_R + E_\theta + E_\phi + E_w + E_{\text{vdw}} + E_{\text{el}}. \tag{1}$$

Here, E_R is the bond stretch interaction energy among atoms. E_θ is the angle bending term. E_ϕ is the torsional term for any two connected bonds. E_w is the inversion term. E_{vdw} is the van der Waals forces for non-bonded interaction energy. E_{el} is the electrostatic interactions. Although different force fields have different definitions of the potential energy [20,21], they still share some general energy components, such as E_R, E_θ and E_ϕ.

For the geometry optimization of a well-bonded and charge-balanced model, the first four terms in (1) are critical to the potential energy, while E_{vdw} and E_{el} are less important. Among the first four terms, different bonding directions are related only to E_ϕ. So only E_ϕ need to be considered for the difference of termination directions. The computation of the torsion angle energy (E_ϕ) is

$$E_\phi(M) = \sum_{i=1,\ldots,n} w(\phi_i), \tag{2}$$

$$w(\phi_i) = \frac{1}{2} V_\phi [1 - \cos n\phi_0 \cos n\phi_i], \tag{3}$$

where Eq. (3) is used to calculate the torsion angle energy. In (3), V_ϕ, n and ϕ_0 are dictated by the bonding status of the atom. i is the ith torsion angle in the given model, M. As an example, for Si atoms, $V_\phi = 1.225$ kcal/mol, $n = 3$ and $\phi_0 = 180^\circ$ [19]. The only unknown variable for Si atoms is the torsion angle, ϕ_i. For different passivation results, as depicted in Figure 3 (a) and (b), their torsion angles are axisymmetric. We only need to calculate one set of them, as the rest of the sets have the same torsion angles. Among the torsion angles in Figure 3(a), only $\phi_{C_1ABD_1}$, $\phi_{C_1ABD_2}$ and $\phi_{C_1ABD_3}$ need to be calculated. Following the definition of torsion angle mentioned above, $\phi_{C_1ABD_1} = 0^\circ$, $\phi_{C_1ABD_2} = 120^\circ$, and $\phi_{C_1ABD_3} = -120^\circ$. Similarly, for the torsion angles in Figure 3(b), $\phi_{C_1ABD_1} = 180^\circ$, $\phi_{C_1ABD_2} = 60^\circ$, and $\phi_{C_1ABD_3} = -60^\circ$. With these torsion angles, the E_ϕ can be calculated by (2) and (3).

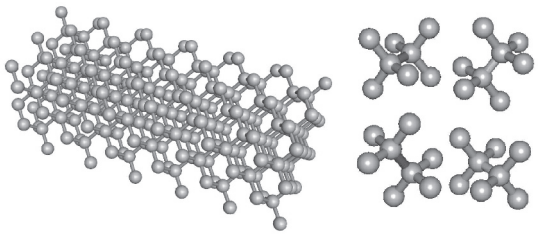
For a model from the BSA method, the torsion energy of the bond AB is

$$E_\phi(M_{\text{BSA}}) = 3 \times (w(0^\circ) + w(120^\circ) + w(-120^\circ)) = 9V_\phi. \tag{4}$$

For a model from the SDG method, the torsion energy of the bond AB is

$$E_\phi(M_{\text{SDG}}) = 3 \times (w(180^\circ) + w(60^\circ) + w(-60^\circ)) = 0. \tag{5}$$

From (4) and (5), it can be seen that the resulting energy from the SDG method is smaller than that from the BSA method. Since the torsion angle energy is always larger than 0, the torsion angle generated by the SDG method gives the lowest torsion angle energy for Si nanowire models. Based on this, the SDG method also shows another advantage - it requires fewer iterations for geometry optimization. Several simulation samples with UFF computational results will be given in Section 5, where for the ease of illustration, we have chosen some models with crystal structures for demonstration. However, the SDG method is not limited to these particular crystalline structures. It can also be applied to other organized structures and it can produce surface passivation results with structures consistent with the original model.



(a) (b)

Figure 4 Generating SDs from the given model. (a) The given atomistic model; (b) identified SDs from the given model.

4 Surface passivation with structure descriptors

4.1 SDG method

In order to extract SDs from a given model, all bonds in the model need to be scanned and classified into groups. This can be accomplished by the pseudo code in Algorithm 1.

Algorithm 1 Generation of structure descriptor

Input: Given model, M.

Output: Structure descriptors, Q.

$Q \leftarrow [\,]$;
for $i = 0$ **to** $M.getBondNum()$ **do**
  $start \leftarrow M.atoms[M.bonds[i].s]$; $end \leftarrow M.atoms[M.bonds[i].e]$;
  if $FullBonds(start)$ **and** $FullBonds(end)$ **then**
    $tSD \leftarrow$ **new** $SD()$; $tSD.\boldsymbol{O} \leftarrow RotVec(M.bonds[i].s, M.bonds[i].e)$;
    for $j = 0$ **to** $start.bonds.size()$ **do**
      if $i \neq start.bonds[j]$ **then**
        $tb \leftarrow M.bonds[start.bonds[j]]$;
        $tSD.V_S.append(RotVec(tb.s, tb.e))$;
      end if
      if $i \neq end.bonds[j]$ **then**
        $tb \leftarrow M.bonds[end.bonds[j]]$;
        $tSD.V_E.append(RotVec(tb.s, tb.e))$;
      end if
    end for
    if not $SDMatch(Q, tSD)$ **then**
      $Q.append(tSD)$;
    end if
  end if
end for
return Q.

In Algorithm 1, the atoms and bonds of the given model M are stored in $M.atoms$ and $M.bonds$ respectively. $FullBonds()$ checks whether the given atom is fully saturated or not. $RotVec()$ returns the orientation vector of the given bond. $SDMatch()$ checks whether the newly generated SD is in the Q already. Based on the pseudo code given, all SDs of the given model can be collected after the bonds are scanned.

As an example, consider the Si nanowire, which is depicted in Figure 4(a). For these well-terminated Si atoms, they should have four bonds around. The bonds without fully terminated atoms are discarded. For those bonds with well-terminated Si atoms, a different type is assigned to each bond after structure analysis. There are four types of SDs in this model, as depicted in Figure 4(b). These SDs can be used as guidance for passivating this device model. Besides directly generating SDs from the given model, users can assign exiting SDs for atomistic models to passivate surface.

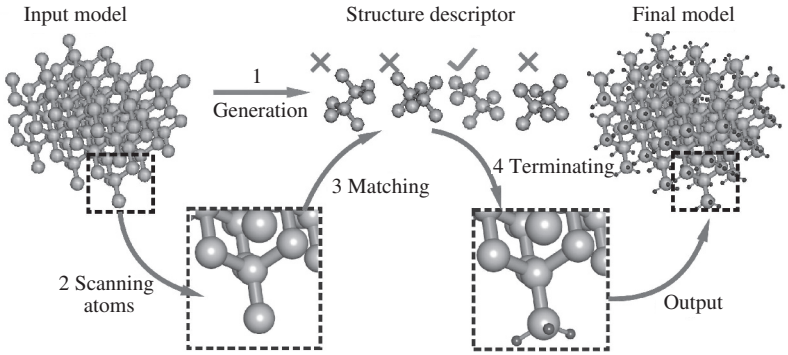


Figure 5 The pipeline of surface passivation.

4.2 Passivation pipeline

Because Algorithm 1 can generate all SDs of a given model, the SDs can be employed to accomplish surface passivation. There are four logical steps to finish the pipeline, as shown in Figure 5.

The pipeline for surface passivation is:

(1) SD generation. For each input model, all SDs are collected and put in a queue.

(2) Scanning atoms. Each atom in the model needs to be scanned to identify the ones without full bonds.

(3) Matching SDs. For these atoms not fully terminated, they are matched with the SDs to find the closest one.

(4) Terminating atoms. Add H atoms to the unsaturated atoms with their SDs and output the final result.

In the matching process, a function is defined to find a proper SD for each atom without full bonds. The evaluation function $f()$ is

$$f(Q_i, tSD) = h(Q_i.\boldsymbol{O}, tSD.\boldsymbol{O})[g(Q_i.V_S, tSD.V_S) + g(Q_i.V_E, tSD.V_E)], \tag{6}$$

$$g(Set_1, Set_2) = \sum_{k=0,\ldots,n} h(Set_1[k], Set_2[k]),$$

$$h(\boldsymbol{a}, \boldsymbol{b}) = \begin{cases} 0, & (1 - |\boldsymbol{a}| \cdot |\boldsymbol{b}|) > \epsilon, \\ 1, & (1 - |\boldsymbol{a}| \cdot |\boldsymbol{b}|) < \epsilon. \end{cases}$$

For each SD in the resulting Q array, the one with largest $f(Q_i, tSD)$ will be selected as the reference to finish the passivation. In the equation for calculating the value of $h(\boldsymbol{a}, \boldsymbol{b})$, ϵ is the tolerance used to reduce the floating point error and $|\boldsymbol{a}|$ is the normalized vector of $\boldsymbol{a}$. With Eq. (6), a proper SD will be selected and H atoms can be used to form bonds along the desired directions. The bond length between the H atom and Si atom is given by the user. Based on the pipeline above, surface passivation can be executed for any given model.

5 Performance and comparison

5.1 Application cases

The SDG method can be applied to various kinds of atomistic models. Besides the Si nanowire models mentioned above, it can also be applied to another group of nano-scale transistors, carbon nano-tube (CNT) [22]. CNTs can be used either as conductors or semiconductors, based on their chirality [23]. Those CNTs with semiconductor properties can be used to construct 10-nm-scale transistors or other devices [24]. The various properties of CNTs give rise to much interest for their possible applications [25].

Although CNTs have fewer dangling atoms, i.e., not fully bonded, than Si nanowires, the top and bottom carbons are not fully passivated, and therefore CNT models must still address the problem of

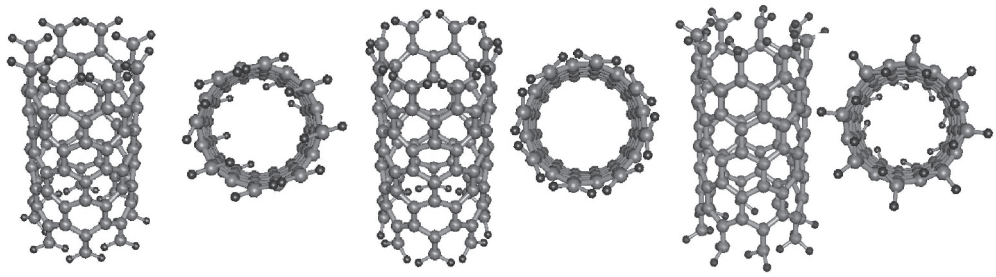


Figure 6 Surface passivation results from different methods, atoms with smaller radii are H atoms, larger ones are Carbon atoms. The result in (a) and (b) is generated by the BSA method. The result in (c) and (d) is generated by the SDG method. The result in (e) and (f) is rotate the H atoms in (c) for certain angle to make a larger distance between two nearby H atoms.

Table 1 Models Generated from both BSA and SDG methods

Model	Dimensions (nm×nm×nm)	Si/C	H	Diff. H	Total atoms
Si264	$3.26 \times 1.63 \times 1.09$	264	250	51	514
Si496	$4.20 \times 4.07 \times 0.54$	496	588	69	1084
Si1200	$10.96 \times 2.18 \times 1.19$	1200	928	132	2128
CNT(8,0)	$0.83 \times 0.83 \times 1.32$	96	32	32	128

passivation. For CNTs, each carbon atom should ideally have three bonds. With information from geometric analysis, the fully-bonded carbons can be used to complete the dangling atoms at two ends. The result from the BSA method is depicted in Figure 6(a), with a view from one end, as shown in Figure 6(b). It is clear that the H atoms at the tube end are added with no specified pattern.

The result from the SDG method is depicted in Figure 6(c), and the positions of these H atoms are closer to the shape of the original CNT. Because the distance between two H atoms, which should be larger than 0.1 nm in general cases, should not be as close as some of those seen in Figure 6 (a) and (c). All H atoms are rotated to a certain angle to increase the distance between two nearby atoms, as depicted in Figure 6(e). The models in Figure 6(e) can be used to carry out property simulations of the device. For the geometry optimization in the next subsection, the model in Figure 6(c) is used as the input model, since it is the result from the SDG method without any modification.

To show the performance of the SDG methods in different application cases, three silicon models and one CNT model are used for the testing. For Si nanowires, the bond length of a Si-Si bond is 0.23515 nm. For CNTs, the bond length of a C-C bond is 0.14210 nm. The composition of each model is given in Table 1.

In Table 1, the column Dimensions shows the size of the input model. the column Si/C lists the number of silicon or carbon atoms in the input model. H is the number of H atoms added to the input model, and Diff. H is the number of different H atoms between the results from the BSA method and SDG method. For Si atoms with two or three bonds, both BSA and SDG methods generate the same result. For the atoms with only one bond connected to another Si atom, SDG method will generate trimmer results, as depicted in Figure 7 (b) and (d). While these atoms are of the same structure of SDs as shown in Figure 3(b), some Si atoms passivated by the BSA method are in the same structure of the pattern shown in Figure 3(a). As depicted in Figure 7(a), the Si atoms on the bottom and the right side do not follow the pattern of their nearby Si atoms. Total atoms is the number of all atoms combined in the system.

5.2 Performance

Geometry optimization, which provides a good initial state, is an initial step for atomistic model simulations. When examining the same results from geometry optimization from the two methods, the surface

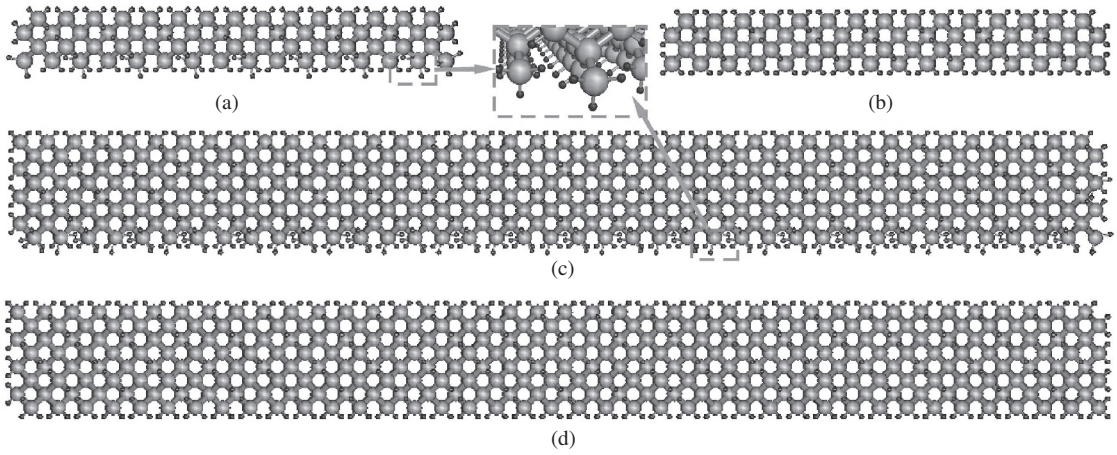


Figure 7 Passivation results. (a) Result of Si496 from the BSA method; (b) result of Si496 from the SDG method; (c) result of Si1200 from the BSA method; (d) result of Si1200 from the SDG method.

Table 2 Comparison of SDG and BSA methods for geometry optimization

Model	Method	Init. E_ϕ (kcal/mol)	Converged energy (kcal/mol)	Iterations	Simu. time (s)
Si264	SDG	0.0	339.879	599 (59.84%)	4.56
	BSA	15.925	340.518	1001	5.99
Si496	SDG	0.0	1030.413	2212 (69.58%)	28.28
	BSA	23.275	1030.416	3179	39.30
Si1200	SDG	0.0	1892.577	3852 (88.53%)	113.85
	BSA	106.858	1892.947	4351	129.17
CNT(8,0)	SDG	493.331	805.629	440 (82.86%)	2.65
	BSA	634.841	813.791	531	2.93

passivation method that lead to a generated model with less iterations during the optimization process should be recognized as the better one. The better surface passivation method will save a lot of time from the optimization process for large atomistic models or a device consisting of different atomistic models. In order to test the performance of the different surface passivation results for geometry optimization, the models generated from both the BSA and SDG methods are used as the initial model. The UFF 'forcite' optimization function in Material Studio [13] is employed to do the testing. The optimization target is to minimize the potential energy of E in (1). The testing platform is a common PC outfitted with Intel Xeon 3.33 GHz processors and 12.0 GB memory. The results of all test cases are shown in Table 2.

In Table 2, the Init. E_ϕ is the initial torsion angle energy of the model, which is calculated based on (2). The first four items listed in (1), E_R, E_θ and E_w are the same for both methods. Converged energy is the energy after geometry optimization, which is nearly the same of both methods. Iterations is the total number of iterations to obtain a convergent result. The convergence tolerance is set to 0.0001 kcal/mol for all tests. The percentage in the parentheses is the ratio of iteration times of the SDG method compared with that of the BSA method. Simu. time is short for simulation time, which is the duration for the geometry optimization process.

From the data listed in Table 2, it is clear that the models generated by the SDG method have less torsion energy, and require fewer iterations and less simulation time under the same convergence tolerance and with nearly same final converged energy. Overall, it can be concluded that the SDG method is superior to the BSA method. The ratio between the simulation time cost for different methods do not necessarily match with that of the number of required iterations. This is because there is an initialization process during the optimization.

For a smaller system, such as the Si264 model, the average initialization time is 1.39 s, which is quite

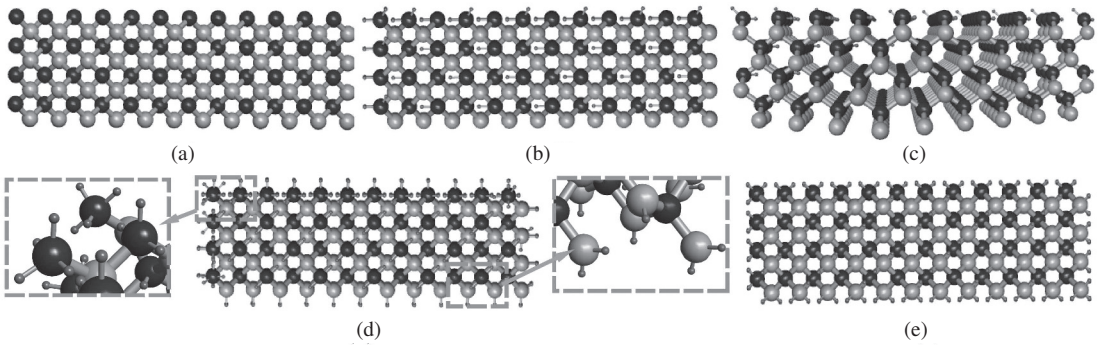


Figure 8 Surface passivation results of Ga-As nanowire, atoms in black are As atoms, gray ones are Ga atoms, and atoms with smaller radii are H. (a) The input model of a GaAs device; (b) and (c) show the result from Material Studio [13]; (d) shows the result from HyperChem [14]; (e) shows the result from our SDG method.

long compared to the total time cost. While for simulations with larger models, such as Si1200, the simulation time corresponds well to that of the number of iterations, since the similar time cost for initialization is negligible in this situation.

5.3 Application extension

Besides providing a more consistent surface and less torsion angle energy, the SDG method can also be applied to some special applications for device simulations. GaAs is a possible semiconductor material for metal-oxide-semiconductor field effect transistors (MOSFETs) [26]. It also requires surface passivation to maintain charge balance.

Moreover, most existing software cannot provide proper results, as shown in Figure 8 (b) and (d). The passivation result in Figure 8 (b) and (c) was obtained from Material Studio [13], which was not able to complete the passivation task. Some dangling atoms in the bottom and right side are still not passivated with enough H atoms. The passivation result in Figure 8(d) was obtained from HyperChem [14], which did complete passivation with the BSA method. However, the number of bonds for As (in black) and Ga (in gray) is 5 and 3, respectively, as can be seen in the left and right insets of Figure 8(d). This kind of surface passivation result is not desired. The desired result can be generated by the SDG method, which is shown in Figure 8(e). With the SDG method, both As and Ga atoms have four bonds after the passivation step.

6 Conclusion

Surface passivation is an essential step in the simulation of atomistic models. The passivation results are not unique if they only consider the conformation of atoms, which is the general approach for research projects and existing software. Based on structural analysis of the given models, the SDG method is proposed to generate trimmer results with less torsion angle energy. The structure descriptor is extracted from the model and constrains the bonding directions of H atoms. The experiment results validated the efficiency of using these models as the initial model to do geometry optimization, which require less iterations and time cost. This method can be applied to the surface passivation of materials with crystalline structures. Beyond the examples shown in this work, more complex systems, such as models consisting of more than two types of atoms with each having different bonding criteria is also interesting and important for us to study. Hence, the extension of current method to complex surface passivation will be pursued in the future.

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Conflict of interest The authors declare that they have no conflict of interest.

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