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Classical Atomistic Simulations in Materials Sciences: An Introduction

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The theory, use and limitations of classical potentials are presented, in the specific context of computational studies of materials. The general form of potentials is detailed, and several examples, used for educational purposes (Lennard-Jones) or giving good results for different kinds of materials (EAM, Stillinger-Weber, Tersoff), are described. Important issues related to classical potentials such as transferability, restrictions of use, and space and time limitations are also discussed. Three examples of theoretical studies, modeling of dislocations in zinc-blende materials, investigation of the dislocation formation from surface defects in a semiconductor, and study of the SiC/Si(001) interface, are presented.

Keywords: computational studies, classical potentials, dislocations, surface defects, semiconductor, interface.

1. INTRODUCTION

The last twenty years have seen a growing use of numerical simulations in materials science, thanks to the continuous improvement of computer performances. Indeed, complex calculations can now be performed even on low-price personal computers. Numerical simulations are interesting for several reasons. First, they could be considered as a necessary complement of experiments. For example, in spectroscopy or microscopy experiments, it is sometimes difficult to interpret directly the images. Useful insights may be obtained by comparing measurements with calculated images [1, 2]. Second, numerical simulations are also relatively cheap, a significant advantage for industrial research. A good example is provided by crash test simulations used for improving cars safety. It is now possible to get extremely reliable results from calculations. As a result, it is not necessary anymore to refine car prototypes in an expensive and slow iterative process of construction and crash test sequences. Third, numerical simulations allow us to explore easily a large range of system configurations, even for unusual or extreme conditions. For example, properties of matter under very high pressure or high temperatures, what occur inside stellar objects, can only be investigated with modeling. Finally, another advantage of simulations is prediction. Fast and cheap calculations could be carried out to test ideas about materials or processes, before building an expensive experiment.

However, one has to keep in mind that simulations, though of great help, will not provide answers in all cases. Hence, simulations are done in the frame of one theory, which is built from or validated by established experimental results. By definition, calculation results are then only valid in this frame, and one can not simulate one experiment violating this theory. Obviously, calculations should never be considered as a proof, and always be compared to experiments. Moreover, prediction from simulations may be used as a guide for experiments but not restrictively. Otherwise, new behaviors or properties of materials could be missed, for they were not obtained by calculations. In any case, the computational physicist has to know the liability range of each model, and whether computed results could be safely trusted or not.

Here, I focus on simulations in materials sciences. Typically, one wants to compute the behavior of solids in a scale roughly from 1 meter to 1 angstrom. It is hardly possible to consider such a large range (10^{10}) as a whole. Instead, one has to use different strategies depending on the problem dimensions. For example, at the macroscopic level, we know that the solid properties are well described by a continuum description and classical mechanics, if we exclude specific phenomena where quantum properties manifest themselves at this scale, such as superconductivity. Finite elements techniques are widely used for performing such calculations. At the other extremum, the atomic level, a continuum description of the matter is inadequate, and each atom must be considered as a definite entity, in the so-called atomistic approach. Also, quantum mechanics should be considered, and simulations done with first principles methods for example, allowing a very accurate description of the matter properties. However, only nanoscopic systems with less than about thousand atoms can be currently considered, even using the most powerful supercomputers, because of the tremendous difficulty to solve the Schrödinger equation for large systems. Obviously, there is a need for an intermediate description between the classical continuum and the quantum atomistic approaches, able to deal with systems whose characteristic dimensions are up to few tens of nanometers (i.e. about 10^6 atoms). This class of techniques exists and is commonly called “classical potential” or “atomistic” methods. They combine a classical mechanics approach with an atomistic description of the system. These methods can not model explicit quantum properties. However, the quantum contributions responsible for the atomic cohesion are implicitly included in the inter-atomic potentials. Therefore, typical applications in materials science focus on the atomic structure of specific systems: extended (dislocations) or localized (vacancies, interstitials) defects, surfaces, interfaces, etc... This

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approach allows the description of the atomic properties in a large number of physical problems, as well as a very good scalability of the needed computational power with the system size.

The purpose of this paper is to present the use of classical potentials for modeling materials. After a general description of the method and of the problems related to parameters fitting, I describe the two-body potentials as an introduction. Then many-body potentials are presented, focussing on recent potentials widely used for modeling metals and covalent materials. Important issues such as transferability and limitations of the method are then discussed. Finally, several applications of the method are shown.

2. GENERAL IDEA AND FORMALISM

In materials science, one wants to acquire the knowledge of the properties of condensed matter. In principle, both ionic and electronic structures should be known. Generally, ions are heavy enough to be considered as classical particles, except in very specific situations involving hydrogen. The energy of the system can then be written as

$$E = H(\varphi_1,\dots,\varphi_n,\boldsymbol{R}_1,\dots,\boldsymbol{R}_N)$$

φ_i being the wave function of the quantum electron i, and $\boldsymbol{R}_j$ the coordinates of the classical ion j. The electronic part is calculated using the fundamental quantum mechanics equation of Schrödinger. However, the large number of electrons in most systems of interest makes this determination almost impossible without serious approximations [3]. Even with these approximations, the calculation of the electronic structure remains a tremendous task. Fortunately, in a lot of physical problems related to atoms, the electronic structure is only implicitly required, for we only need to know the forces on ions due to electrons. The idea behind classical potentials methods is to not explicitly consider the electronic structure. The total energy of the system is then expressed as

$$E = F(\boldsymbol{R}_1,\dots,\boldsymbol{R}_N).$$

Now the total energy of the system will depend only on the ionic positions. Therefore, the function F should include explicitly the ion-ion contributions, and only implicitly the ion-electron contributions. F is not formally known and is only an approximate function of the ionic positions by definition. Usually, one tries to guess the best suitable form from empirical or physical insights. Because of the large diversity of behaviors observed in different class of materials such as insulator or metals, it is not possible to have a unique universal function F. Instead, several functions have been derived for each class of materials, and sometimes they also depend on the physical state of the material, whether it is amorphous or crystalline.

The function F is usually a mathematical formula including several numerical parameters, or in some cases, a set of tabulated functions. Parameters or tabulated functions are calculated or fitted, using experimental data when available or results obtained from more precise methods. The number of parameters or tabulated functions solely depends on the function of the classical potential. If N parameters have to be determined, at least N independent data are needed. It is possible to use more data than parameters, and in that case several sets of parameters may be determined by using fitting procedures like least squares optimization.

The knowledge of F is enough to characterize the system. Given a set of atomic positions, the force on each atom is obtained from the gradient of F, and the system could be relaxed to the state of minimal energy. This state is of course not the true ground state of the physical system, but rather an approximation, the accuracy depending on the choice of the function F. Following Born-Oppenheimer, the total energy could also be written in the following form:

$$E = \sum_i F_1(\boldsymbol{R}_i) + \sum_{i,j} F_2(\boldsymbol{R}_i,\boldsymbol{R}_j) + \sum_{i,j,k} F_3(\boldsymbol{R}_i,\boldsymbol{R}_j,\boldsymbol{R}_k) + \dots$$

F_1 contributions depend only on the position of a single atom. These are generally set to zero, since they are irrelevant in an isolated system, where the coordinate's origin is not uniquely defined. However, they could be non zero in the case of the study of a system under the influence of an external field. In that case, the field will change the system energy according to the atoms positions. The second term in the expression involves two-body F_2 contributions, which depend on the distance between two atoms. These energies, called pair energies, are generally the most important contribution to the total energy, for all materials, especially when the two concerned atoms are close together. F_3 terms will be related to the position of three atoms, and then they will depend on the angle between them. Torsion angle contributions are described by F_4 terms. The next terms in the expansion express higher order contributions to the total energy, but are not used in practice.

3. EXAMPLES OF POTENTIALS

In this section, I describe different kinds of potentials, beginning with pair potentials. Though not qualitatively accurate for most of the materials, they are still widely used in specific cases, or for educational purpose, due to their simplicity. As an example, I will focus on the Lennard-Jones potential, originally designed for rare gas, which is a standard and model potential in computational physics [4]. The pair potential total energy of the system is

$$E = \sum_{i,j} F_2(\boldsymbol{R}_i,\boldsymbol{R}_j) = \sum_{i,j} F_2(|\boldsymbol{R}_{ij}|)$$

and, for the Lennard-Jones potential,

$$F_2(R) = 4\varepsilon\left[\left(\frac{\sigma}{R}\right)^{12} - \left(\frac{\sigma}{R}\right)^{6}\right]$$

The first term is a short range positive contribution, modeling the electrostatic repulsion between atoms. The second term is a negative contribution to the energy, representing the long range anisotropic van der Waals dispersion. The exponent 12 has been chosen for computational reason, the first term being the square of the second one. There are only two parameters, ε and σ, which correspond to the energy and time scale of the potential.

The Lennard-Jones potential is well suited for rare gas, but yields only a crude description of other materials, due to its two-body function. Largest deviations from experiments are obtained in the case of elements for which many-body contributions play an important role, like metals or semiconductors. For instance, it is known that the so-called Cauchy relation $C_{12} = C_{44}$ is always verified in cubic systems for elastic constants obtained with pair potentials, while this is not the case experimentally. For the most studied materials, better potentials, with functions including either higher order contributions, or local environment effects, are available.

For metals, potentials derived from the Embedded Atom Model (EAM) are widely used, for reasons of simplicity, efficiency and quality [5]. EAM potentials have the following form:

$$E = \sum_i F_i(\rho_i) + \frac{1}{2}\sum_{i \neq j} \varphi_{ij}(R_{ij}).$$

F_i is the energy to embed the atom i into the background electron density ρ_i, and Φ_{ij} is the electrostatic repulsion pair energy [6]. The background electron density is approximated by the superposition of atomic densities:

$$\rho_i = \sum_{j \neq i} \rho_j^a(R_{ij}) .$$

The functions F and φ can be obtained from first principles, but in practice, it is customary to use empirical analytical functions, fitted to several bulk properties of the material [7]. Compared to pair potentials, EAM derived potentials include higher-body interactions. The interaction between two atoms depends on the slopes of their embedding functions F, which depends on the background density ρ. Therefore, the effective interactions within the EAM are environment-dependent. They are called bond order interactions, since EAM is able to describe correctly the effect of the coordination on the bond strength: less coordinated atoms, such as in surface, have stronger bonds and shorter bond lengths. The concepts behind the EAM are also used in other methods, such as the 'glue' model [8] or the Effective Medium Theory [9].

EAM class of potentials is well adapted for metals, because of the bond order term that mimics the hardness of metallic bonds as a function of the coordination. This approach has proved to be inadequate for semiconductors, in which covalent bonds have a complicated dependence on coordination and bond angles. This is actually the case for semiconductors of group IV, such as diamond, silicon, germanium or silicon carbide, stable in a cubic diamond or zinc-blende structure. Due to their technological importance, several kinds of potentials have been designed for these materials. For example, an extended version of the EAM model has been developed [10], with angle-dependent electron densities. Another one, the Stillinger-Weber (SW) potential, for which sets of parameters for Si and Ge are available, has been widely used [11]. Its function is written below:

$$E = \sum_{i,j} \varepsilon F_2\left(\frac{|\boldsymbol{R}_{ij}|}{\sigma}\right) + \sum_{i,j,k} \varepsilon F_3\left(\frac{\boldsymbol{R}_i}{\sigma}, \frac{\boldsymbol{R}_j}{\sigma}, \frac{\boldsymbol{R}_k}{\sigma}\right),$$

$$\begin{aligned} F_3(\boldsymbol{R}_i, \boldsymbol{R}_j, \boldsymbol{R}_k) = {} & h(R_{ij}, R_{ik}, \theta_{jik}) + h(R_{ji}, R_{jk}, \theta_{ijk}) \\ & + h(R_{ki}, R_{kj}, \theta_{ikj}) \end{aligned} .$$

F_2 and h are two analytical functions, vanishing beyond a given cutoff. F_3 is a three-body contribution introducing an angular dependence in the energy. Here, the energy gain is maximal for the bond angle of the cubic diamond structure. Compared to pair potentials, an additional term of the Born-Oppenheimer development is included in the potential function, what improves the accuracy of interatomic forces description. In addition, this term bears an angular dependence, particularly well suited for covalent materials where bonds are directional.

In this last example, the dependence of the interactions on the local environment is strengthened by taking into account three-body terms. However, this approach requires a larger computational effort, since during the calculation interactions have to be computed for all atomic triplets. It is possible to use a two-body function while introducing environment dependence by modifying the interactions as a function of the atomic environment of the atoms. An example is given by the potential of Tersoff [12], which is available for diamond, Si, Ge and compounds such as silicon carbide SiC and SiGe alloys [13].

$$E = \frac{1}{2}\sum_{i \neq j} f_C(|\boldsymbol{R}_{ij}|)\left[f_R(|\boldsymbol{R}_{ij}|) + b_{ij} f_A(|\boldsymbol{R}_{ij}|)\right] .$$

Here, f_R and f_A are repulsive and attractive functions, respectively, while f_C is a function going smoothly to zero beyond a given cut-off. The bond order contributions are included through b_{ij}, which is modified according to local environment as a function of interatomic distances and angles. The Tersoff potential is different from the EAM approach in the sense that the two-body Tersoff interactions are directly modified by local environment, while bond order is obtained in EAM via electron distributions. Note that EDIP, a recent potential for Si and diamond, built from the same concepts that the Tersoff potential, has been recently proposed and is supposed to be qualitatively superior [14, 15].

4. TRANSFERABILITY

A classical potential provides a rough description of the physical system. It is interesting to define the domain of validity, i.e. which physical quantities can be calculated with a reasonable precision, and the physical phenomena that can be modeled. This determination is often done empirically by extensive investigations [16]. In addition, several informations may be obtained from the analysis of the set of data used in the fitting procedure of the potential. For example, the database of a potential designed for studying solid phase transitions would include known structural data related to one or more structure. Or, for studying liquid state, one would take into account the melting temperature. The examination of the database will then provide several insights on the validity domain of the potential, though test calculations can not be avoided. The ability of a potential to model several physical mechanisms and to reproduce a lot of different properties, for a given material, is called its transferability. Usually, potential designer tries to get the highest transferability, to the detriment of a better precision in specific cases.

Transferability is closely related to the fitted parameters and function of the potential, and also depends on modeled species. It could be tempting to widen the database, by including all the measured available quantities. The idea is to get the largest validity domain, with a potential fitted for several states of matter, and able to model correctly a lot of physical mechanisms. However, in fundamental research, this approach is not recommended, for three reasons. First, though it is possible to use more measured quantities than parameters during the fitting procedure, using a wide database requires a large number of parameters, and then a complicated function *F*. It is unlikely that one could build such a function from physical concepts only. Keeping a small function with different terms, each related to a unique physical contribution (like repulsive and attractive energies) is much more satisfactory from the point of view of the physicist. Second, with a complex function, the probability to get non-physical behaviors increases. For example, more local minima will exist in the configuration space of the atomic structure, and unstable phases may become stable. Finally, using a complicated function increases the required computational time, and the advantage of using an approximated analytical function is reduced.

Usually designed for a specific element, it is sometimes possible to use the same potential for different species. This chemical transferability is not related to the parameters, which are fitted to material properties, but only to the function. Of course, given the variety of physical states and the difference in bond chemistry between all species, it is clear that there is no universal potential, giving optimal results. However, in the case of a family of elements sharing several properties, the same function may be used. For example, semiconductors of the group IV such as diamond, silicon and germanium, are correctly modeled by the Tersoff potential, since they are very similar, and the function of the potential is built on physical concepts. Another example is given by the EAM potentials, giving good results for a large set of metals.

5. LIMITATIONS

It is important to know the limitations in size and simulation time associated with classical potentials computations, the precision one can obtain, as well as shortcomings and failures. Regarding the size limitation or the maximum atoms that can be considered, it obviously depends on the computer resources available, and also on the complexity of the potential. With state-of-the-art massively parallel super-calculator and simple potential, it is nowadays possible to treat systems including at most one hundred millions of atoms [17, 18]. Despite this large number, potential simulations are still restricted to the submicroscopic scale, since a cube including all these atoms would have typically an edge length of about 100 nm. In some specific cases where the system is two-dimensional, it is possible to have larger dimensions. Using standard computers and potentials with a high computational cost greatly lowers these numbers. Typical simulations are performed with less than one hundred thousands of atoms, which is still largely enough to model a wide range of physical systems and mechanisms.

In the case of molecular dynamics simulations, the simulation time, or the maximum number of iterations, is also an important parameter, and depends of the size of the system. With a small number of atoms, it is possible to perform calculations with more than 10^7 iterations, i.e. about 10 ns (the integration time step is typically about 1 fs). But for large systems, the simulation time is at most of the order of the picosecond [19, 20].

The choice of classical potentials for performing simulations depends on the size of the investigated system, simulation time as well as computational resources available. For small systems, first principles methods should be favored, though classical potentials calculations may be used to obtain very good initial configurations [21]. Several physical problems cannot be investigated by classical potentials, such as quantities and mechanisms closely related to the electronic structure, since the potentials we have described here allows only the modeling of the atomic structure. For example, important electronic effects such charge transfer mechanisms are out of reach of classical interatomic potentials. Also, classical potentials simulations are not adequate for physical mechanisms occurring on a long time scale, or relying on rare events. This concerns particularly diffusion, growth, etc… Best results are obtained by calculating accurately the probability of each event with first principles, then performing kinetic Monte Carlo calculations.

6. EXAMPLE OF APPLICATIONS

In this section, some results of classical potentials calculations, recently obtained by the author and co-workers, are presented. A first example concerns the modeling of extended defects in bulk silicon, such as screw dislocations. Although it is known that at high temperature, silicon plasticity occurs mainly through slip of dissociated dislocations [22], recent low temperature experiments revealed the presence of undissociated dislocations with screw or 60° orientations [23]. We have then performed numerical simulations of undissociated screw dislocations in silicon, for characterizing the structure and extension of its core, which is a pre-requisite to the study of dislocation mobility. A picture of several possible atomic configurations, relaxed using classical potentials, potential is shown in the Figure 1. The structure A has the lower energy with Tersoff and EDIP potentials [24], which is confirmed by ab initio calculations [25]. We also considered the configuration C, which has the peculiar feature of a sp^2 hybridization in the dislocation core. Even if this configuration is not the most stable for silicon, it may play an interesting role for the plasticity of material where sp^2 is favored, such as diamond. In fact, recent calculations with the Tersoff potential indicate that the configuration C is the most stable one in diamond.

In a second example, I present large scale calculations with almost hundred thousand atoms, prohibitive for ab

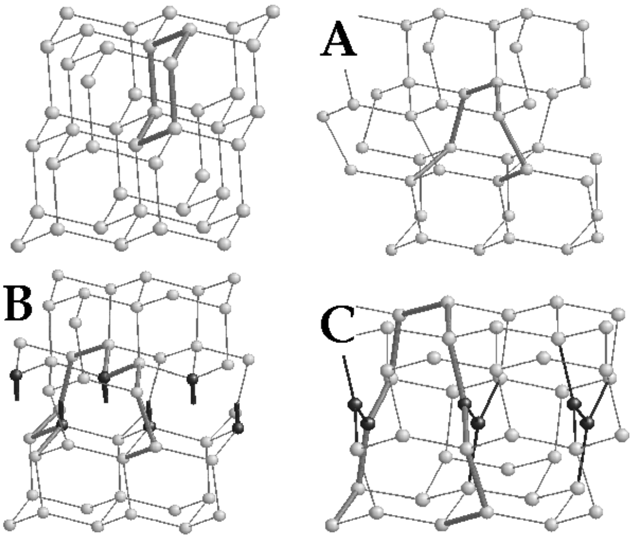

Fig. 1. Ball-and-stick representation of the perfect zinc-blende structure (upper left) and of three different relaxed configurations for perfect screw dislocations. The grey thick sticks show the Burgers circuit for each core. Black spheres are atoms with dangling bonds (B) or with hybridization sp^2 (C)

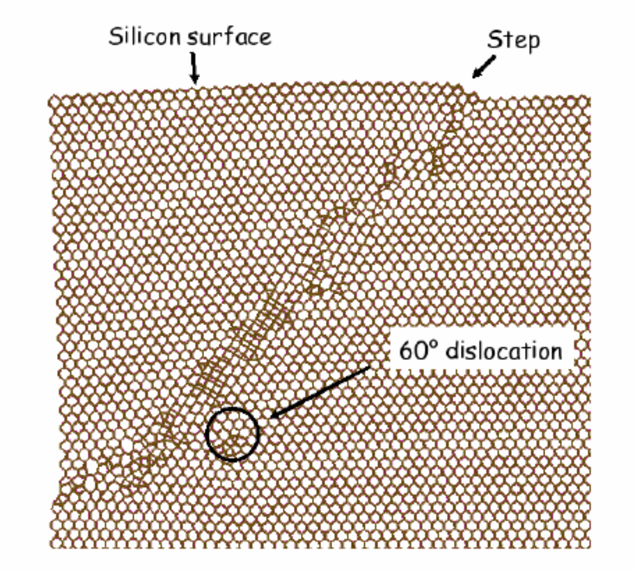

Fig. 2. Cross-section view of a silicon surface with a monoatomic step, submitted to a uniaxial compression of 10% (disoriented by 22.5° with respect to the step line), after relaxation at 0K

initio calculations. Here, we aimed at the understanding of dislocations nucleation in epitaxied semiconductor films. The typical dimensions of these films are too small to allow the formation of the observed dislocations by usual mechanisms, such as the Franck-Read sources [22]. One hypothesis is that nucleation occurs from the surface, with an important role devoted to surface defects like steps or kinks. We focused on the role of a step in a silicon (001) surface submitted to a uniaxial stress. The SW potential was selected, as the most suited for this study [26]. We found that if the stress orientation is perpendicular to the step, a micro-twin along the [111] direction may be formed, starting from the step. It is also clear that the orientation of the applied stress is very important. Indeed, if the stress is now disoriented of 22.5° versus the step, a perfect 60° dislocation is nucleated from the step (Figure 2). The relation between the stress orientation and the dislocation type can be explained from the analysis of the calculated Schmidt factors [27].

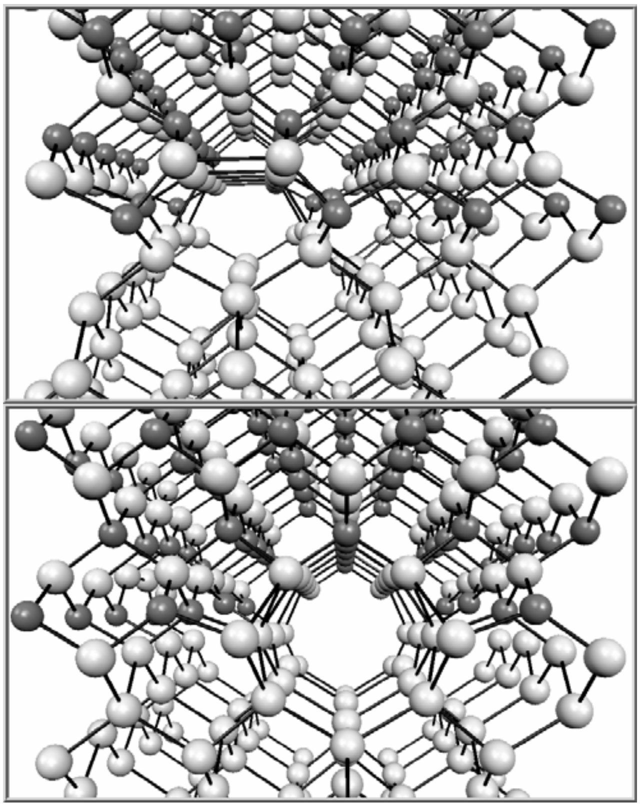

Fig. 3. Ball-and-stick representation along directions [110] (up) and [1-10] (down) of the most stable atomic configuration calculated for the SiC/Si(001) interface. Light grey (dark grey) spheres represent silicon (carbon) atoms

Finally, my last example shows that classical potentials are a valuable tool for exploring quickly the space of configurations, and providing results with a good accuracy. We investigated the structure of the SiC/Si(001) interface using the Tersoff potential. This system may be considered as a model of a highly mismatched interface, owing to the difference of about 20 % between silicon and cubic silicon carbide lattice constants. In addition, this system may be used in electronic devices, SiC being increasingly considered for applications in high temperature or harsh environments. High resolution microscopy experiments revealed that the stress due to the lattice mismatch is released by the introduction of an array of misfit dislocations at the interface [28]. The structure remains unknown, although it has to be characterized before computing the electronic structure of the interface. Because no information were available regarding the location of the misfit dislocation cores compared to the interface, their structures as well as the stoichiometry of the interface, we investigated a large number of possible configurations [21], what is possible with classical potentials simulations. The most stable solution is represented in the Figure 3. Our analysis showed that this configuration is favored because it combines three important characteristics [29]. First, the SiC layer at the interface is carbon-like, which is energetically favored by chemistry. Then, the core is perfectly reconstructed, almost all atoms being fully saturated. Finally, there are no carbon atoms in the core. In fact, atomic bonds are stretched in the core, with a high cost in energy, especially for carbon bonds. These findings, obtained with a classical potential, have been confirmed by ab initio calculations [30].

7. FUTURE / PERSPECTIVES

Classical potentials are widely used in materials science, and it is probable that this interest will not decrease in the future. In fact, even if the power of computers is continuously growing, more accurate first principles calculations are still restricted to systems including several hundreds of atoms, and short timescale. Moreover, classical atomistic computations also benefit from better performance, which allows larger and more complex systems, and longer timescale. For example, even with potentials, it is still difficult to model a material with a realistic microstructure and including several structural defects such as dislocations.

It is clear that in general classical potentials suffer from a lack of transferability. The development of potentials for new materials is then required. There are still many elementary materials for which there are no available potentials. In the case of complex materials, including several elements, the development of potentials remains challenging. Another working direction concerns the combination of classical potentials together with other methods. For example, the modeling of fracture in bulk silicon has been obtained from a complex simulation involving simultaneously three methods [31]. The crack tip is described by an accurate first principles technique. The area surrounding the crack is modeled by classical potentials, while finite elements are used for the area far from the crack, weakly perturbed. This so-called multi-scale modeling is definitely an interesting and exciting research area, and several applications are expected in the near future.

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