Density Functional Theory and Molecular Dynamics Study of 3C Silicon Carbide

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***Abstract*—The aim of the following report was to conduct simple study of silicon carbide (SiC) by means of Density Functional Theory (DFT) and Molecular Dynamics (MD). DFT was used to calculate geometry and electronic structure of pristine and two gallium doped SiC structures. In the MD approach, the influence on lattice lengths of nine available force-fields for SiC was tested.**

***Index Terms*—silicon carbide, density functional theory, molecular dynamics, doping, force-field benchmark.**

I. Introduction

The silicon carbide is still today mostly used in demanding mechanical applications as turbine components, bearings, cutting tools, car parts etc. However, the silicon carbide is a very promising semiconductor not only for mechanical but also electronic applications. Similarly to diamond, the SiC has a variety of extreme electronic properties as large breakdown electric field strength, large saturated electron drift velocity, small dielectric constant, high electron mobility, and high thermal conductivity. These properties are making silicon carbide attractive for usage in high power electronics [2].

In this report 3C-SiC polytype was chosen as the subject matter of the study. This polytype is the most extreme in regards of most of the above mentioned properties (except e.g. thermal conductivity) out of the SiC polytypes. One of the other features of 3C-SiC polytype is that it has diamond lattice and the smallest bandgap (2.36 eV) among SiC polytypes [1].

II. Density Functional Theory

A. Calculation Setup

The goal of the Density Functional Theory part of the study was to determine what changes the introduction of the gallium dopant can create in the geometry and electronic structure if we substitute either carbon or silicon atom in a 16 atom supercell.

As the first step pure 3C-SiC structure was chosen from the Crystallography Open Database [3]. The second step was to run a series of convergence benchmarks to find optimal input parameters for the calculation. The optimal setup parameters determined during the convergence tests are listed in Table I (abinit variables are in brackets).

After obtaining relaxed pure structure two 16 atoms supercells were created by multiplying the primitive cell by $2\times2\times2$. Then, gallium defect was introduced into both structures by substituting one carbon (the first structure) or one silicon (the second structure) atom creating dopant concentration of 6.25%. Computational setup remained the same; the only changed parameter was the k-mesh which was reduced to $9 \times 9 \times 9$ because of the multiplication of the cell.

Parameter	Value
k-mesh (ngkpt)	$17 \times 17 \times 17$
Energy cutoff (ecut)	65 Ha (1769 eV)
PAW doublegrid energy cutoff (pawecutdg)	130 Ha (3537 eV)
Exchange-correlation functional (ixc)	GGA [5]
Energy difference between SCF steps stopping criterion (toldfe)	10^{-11} eV
Tolerance for maximum force below which structural relaxation stops (tolmx)	5×10^{-7} eV/Å

TABLE I
SUMMARY OF USED PARAMETERS FOR STRUCTURE RELAXATION.

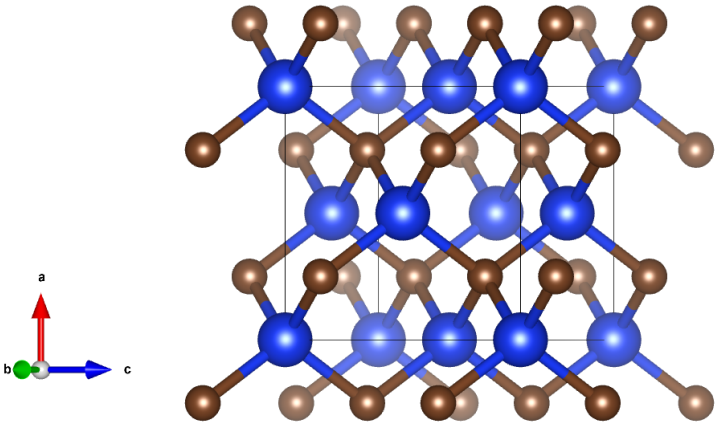

Fig. 1. The FCC lattice of 3C-SiC prior to relaxation.

B. Results

The relaxed doped structures' interatomic distances between dopant and its neighbour and between Si and C which are not neighbouring the first coordination shell of the dopant are reported in Table II. The Si and C distance in pure SiC is reported as the first row.

Substituted atom	Dopant - Neighbour [Å]	Si-C [Å]
-	-	1.885
Si	1.985	1.90018
C	2.168	1.94158

TABLE II
INTERATOMIC DISTANCES BETWEEN DOPANT AND ITS NEIGHBOURS AND BETWEEN SI AND C FARTHER FROM THE DOPANT. THE FIRST ROW REPRESENTS PURE SIC STRUCTURE.

The geometries seem to be consistent with expectations. Substitution of the C atom caused larger distortion in the cell as differences between atomic radii of Ga and C are significant.

On the other hand, atomic radii of Si and Ga are much more similar; resulting in similar interatomic distances as in the pure structure.

In the following paragraphs electronic properties of the studied systems are reported. To this aim, band gap, density of states and band structure are sequentially compared. Firstly, band gaps are compared in Table III.

Substituted atom	Fundamental gap [eV]	Minimum direct gap [eV]
-	1.357	4.559
Si	1.362	1.362
C	-	-

TABLE III
FUNDAMENTAL AND MINIMUM DIRECT BAND GAPS OF THE STUDIED SYSTEMS.

Calculated fundamental band gap of the pure 3C-SiC is consistent with other researchers' DFT calculations [4]; although, may seem underestimated in comparison with experiments. The significant difference of behaviour appears between the two doped structures. The fundamental band gap of the structure with substituted silicon is nearly unchanged. On the other hand, minimum direct band gap changed significantly as now the fundamental band gap is a direct band gap. As can be seen in Figure 2, density of states is similar to the undoped case. The situation is completely different in the case of structure with substituted carbon. In this case the Fermi level lies deeply in the band (Figure 2 and Figure 5), band gap disappeared completely, and the system is showing metallic behaviour. The density of states appears shifted in comparison with pure structure.

The cause of this behaviour can be that silicon is already acting like an electron acceptor in SiC structure and replacing it with another electron acceptor, gallium, is not changing situation notably. However, replacing carbon is creating center with gallium in the middle and silicon atoms in the first coordination shell which probably contributes to conductivity remarkably.

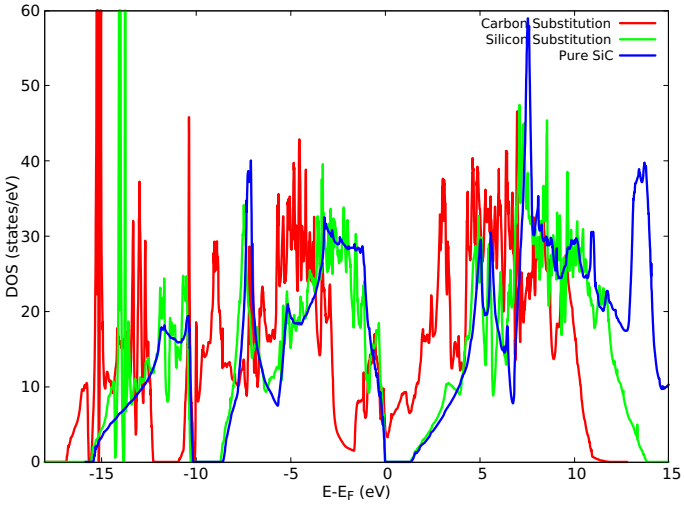

Fig. 2. Densities of states of all three systems. All plots are normalized according to number of the atoms in the primitive cell.

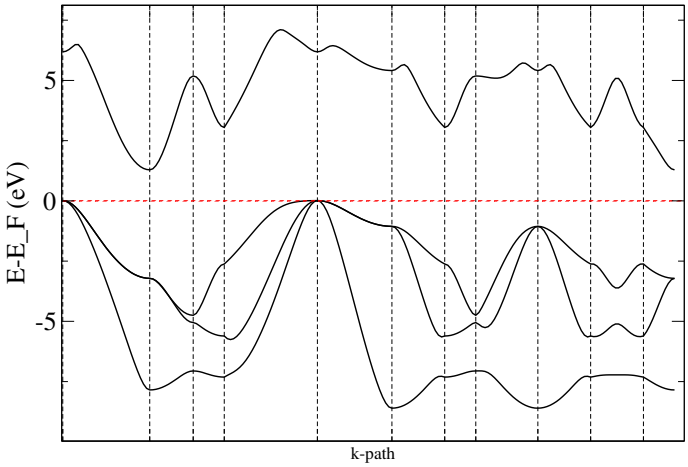

Fig. 3. Band structure of the pure 3C-SiC calculated along standard FCC k-path (Γ-X-W-K-Γ-L-U-W-L-K|U-X).

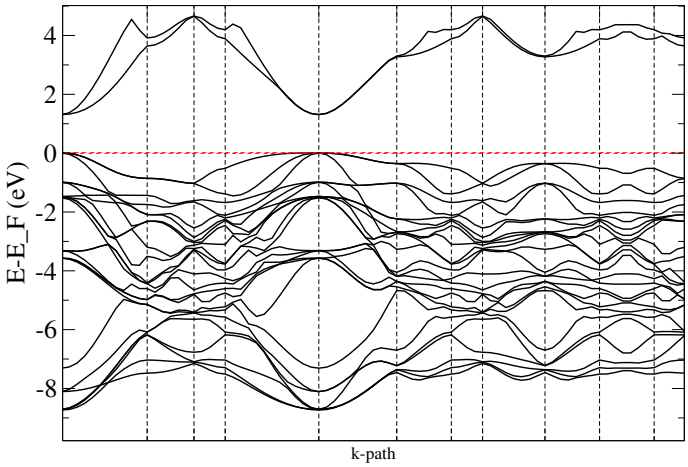

Fig. 4. Band structure of the 6.25 % doped 3C-SiC with substituted silicon calculated along standard FCC k-path.

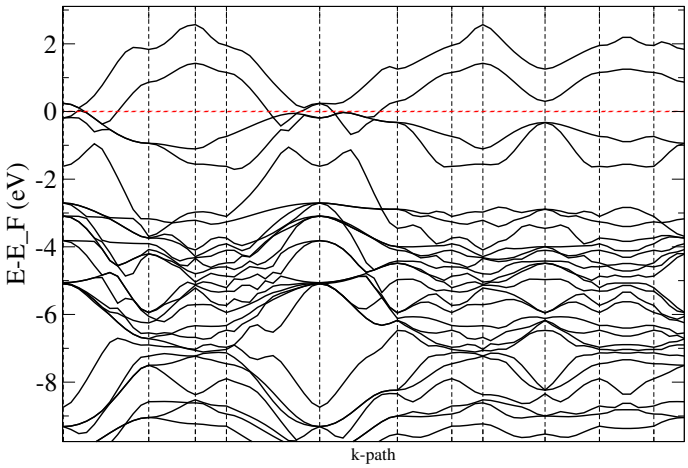

Fig. 5. Band structure of the 6.25 % doped 3C-SiC with substituted carbon calculated along standard FCC k-path.

III. Molecular Dynamics

A. Calculation Setup

The goal of the Molecular Dynamics part of the study was to analyse the influence of the chosen force-field on lattice lengths of silicon carbide. To this aim, all of the available SiC force-fields at Interatomic Potentials Repository were collected and tested.

As the first step to setup the simulation the lattice length of 3C-SiC was found [1]. Then a series of tests was conducted to determine the optimal minimization parameters. The stopping criterion was chosen as energy tolerance. The number of used replicas was chosen as $17 \times 17 \times 17$ to be similar to k-mesh in DFT calculation; although, using even just one cell ($1 \times 1 \times 1$) seemed to be sufficient. Change of the box was allowed during the minimization with 0 external pressure and couple xyz keywords. The summary of the used simulation parameters is in Table IV with LAMMPS variable in brackets.

Parameter	Value
Units	metal
Minimization energy tolerance (minimize)	10^{-20}
Lattice parameters (lattice)	diamond 4.3596 Å
Number of replicas used (region)	box block $17 \times 17 \times 17$
Minimization algorithm (min_style)	conjugate gradient (cg)
Fixations (fix)	relax all box/relax
	x 0.0 y 0.0 z 0.0
	nreset 1 couple xyz

TABLE IV
Summary of used parameters for structure relaxation.

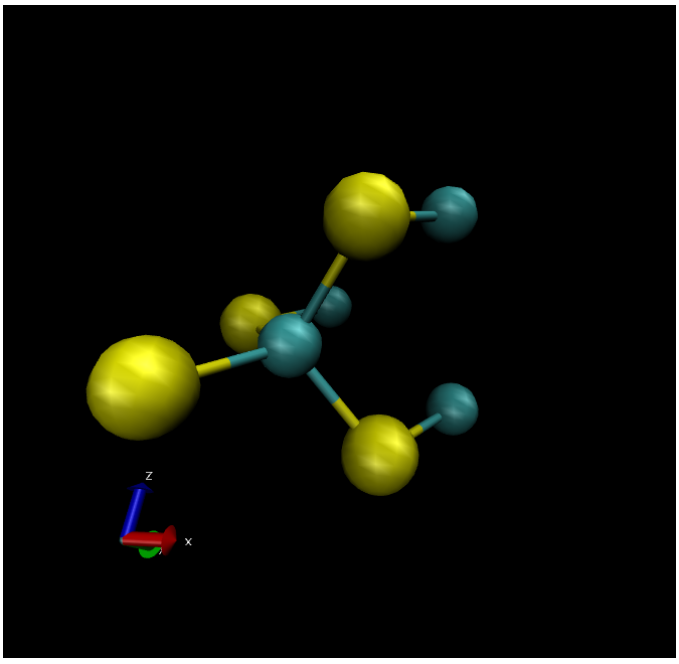

Fig. 6. Picture of single 3C-SiC cell used in the calculation.

B. Results

Calculated lattice lengths with usage of all the available force-fields and their comparison with lattice length calculated by DFT are reported in Table V.

Used force-field	Potential type	Lattice length [Å]
1989-Tersoff-J	Tersoff	4.321
1990-Tersoff-J	Tersoff	4.307
1994-Tersoff-J	Tersoff	4.280
1998-Devanathan-R-Diaz -de-la-Rubia-T-Weber-W	Tersoff.zbl	4.280
2005-Erhart-P-Albe-K (I)	Tersoff	4.359
2005-Erhart-P-Albe-K (II)	Tersoff	4.359
2007-Vashishta-P-Kalia-R-K-Nakano-A-Rino	Vashishta	4.358
2012-Jiang-C-Morgan-D-Szlufarska-I	Edip	4.362
2014-Kang-K-H-Eun-T-Jun-M-C-Lee-B-J	Meam	4.359
DFT	-	4.353

TABLE V
Calculated lattice lengths.

If we take experimental value of 4.3596 Å as a reference then the tersoff potentials from year 2005 (2005-Erhart-P-Albe-K I and II) and meam potential (2014-Kang-K-H-Eun-T-Jun-M-C-Lee-B-J) are the most accurate ones. In general, the newer potentials are more accurate than tersoff potentials from years 1989-1998. The change of type of the potential from years after 2005 is not making any significant change in the lattice legths.

IV. Conclusion

In this study, the 3C-SiC polytype was studied by means of Density Functional Theory (DFT) and Molecular Dynamics (MD). DFT was used to calculate geometry and electronic structure of the pure 3C-SiC and two gallium doped 3C-SiC structures. The doped structures were created by substituting 1 in 16 SiC atoms with gallium creating 6.25 % dopant concentration. The notice of differences in properties between substitution of carbon and silicon was of primary importance. MD was used to calculate lattice lengths with usage of all available force-fields at Interatomic Potentials Repository and the results were compared with experimental data.

The calculated geometry and electronic properties of pure 3C-SiC match the experimental or published DFT calculated data. A significant difference between electronic properties of doped structures was found. The system with substituted silicon did not change notably after introduction of gallium defect. On the other hand, the system with substituted carbon became conductive. According to the benchmark of force-fields on lattice lengths, the newer force-fields (after 2005) perform better than old ones and there is no significant performance difference between different potential types.

References

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