

PROPERTY ENHANCEMENT OF VANADIUM DOPED SILICON CARBIDE: A COMPUTATIONAL STUDY

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Abstract

Dilute magnetic semiconductors (DMS) are those semiconductors that show magnetic behaviour when some impurities are doped in them. The DMS has found applications in spintronic devices. Among all the materials for DMS, Silicon Carbide (SiC) is a promising one as it shows stronger coupling and high Curie temperature. One of the important polytypes of SiC is cubic silicon carbide. This work investigates the transition metal, vanadium (V) doped 3C-SiC by using the *first-principle* energy code, Quantum Espresso, which uses pseudopotential within density functional theory (DFT). Here, it is observed that when V is doped with a Si site substitution of 3C SiC, then two deep levels will be introduced, out of which one is a deep donor and another deep acceptor state. When vanadium is doped with C site substitution of 3C-SiC, the half-metallic character is introduced. Again, formation energy for both before and after relaxation is also calculated. The calculation of formation energy indicates V impurity prefers the Si site to C site in cubic SiC.

Keywords: Density Functional Theory; Density of States; DMS; LDA; Silicon Carbide; Vanadium Impurity

Introduction

Carrier-induced ferromagnetism in dilute magnetic semiconductors (DMS) is of interest as they have found applications for the material in spintronics (Das *et al.*, 2006). DMS is a class of material in which a fraction of constituent ions is replaced with magnetic impurities. Transition metals, when added to SiC, introduce magnetic properties in it (Averous and Balkanski, 2012). Amongst various materials for DMS, SiC having the properties for achieving stronger magnetic coupling and higher Curie temperature, is a promising material for spintronics (Los and Los, 2011). In the case of dilute magnetic semiconductors, the ground state, which is

generally stable state shows various types of magnetic properties such as paramagnetic, ferromagnetic, or antiferromagnetic properties. The magnetic properties of cubic SiC (3C SiC) doped with vanadium are discussed here by using the first principle density functional theory (DFT).

Silicon carbide is a wide-bandgap semiconductor that contains both silicon and carbon. The building block diagram of SiC indicates it is a tetrahedral structure and electron sharing between Si and C atom takes place. The building block diagram also shows each atom of SiC is 88% covalently bonded and 12% is ionically bonded with

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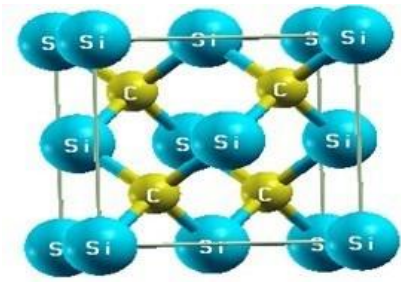


Figure 1. Crystal structure of 3C-SiC

their very nearest atoms; here, four Si atoms are bonded with one C atom covalently in a tetrahedron manner. It is also referred to as Beta (β) SiC. Silicon carbide is generally an artificial high-performance material. 3C SiC is the only cubic polytype of SiC; it shows high hardness, which is nearly close to the Mohs hardness of the diamond (diamond-10 Mohs hardness). In the case of cubic silicon carbide, hardness is in the range of 9.5-9.75 (Bugge, 2012). Cubic silicon carbide shows some extreme properties such as excellent chemical stability, high electro-drift speed, low thermal expansion coefficient, high thermal conductivity, high-temperature resistance, and wide band gap (Abderrazak *et al.*, 2011). These properties make it popular to use for power electronic devices, cutting tools and many more. Figure 1 shows the unit cell of cubic SiC.

Transition metal (TM), when added to SiC, introduces magnetic properties in it (Backes *et al.*, 1996), which are found to be impurity and site-dependent (Miao and Lambrecht, 2003). Full potential LMTO technique with lattice relaxation used to compare electric and magnetic properties of 3C and 4H SiC doped with early TMs shows a spin polarization for V, Cr, and Mn doped SiC (Miao and Lambrecht, 2006). Semi-insulating SiC has its application in devices for high-power electronics. Now a days, due to the establishment of the power electronics, which has the ability to control and conversion of electric power, performs under some extreme conditions.

Power generation devices and power electronic systems are generally performed under extreme conditions. High temperature and field are the primary necessities for these power generation devices and power electronics.

Although SiC contains such extraordinary properties but to enhance the performance it is generally doped with transition metal. In condensed matter physics the meaning of doping is generally to introduce an impurity in the material to get some new properties. Generally, concentration less than 10% considered the limit of doping more than this

percentage of concentration termed as alloying. The main difference between alloying and doping is, in the latter case, higher concentration changes its structural properties and develops new structural phases. But in the case of doping, i.e., lesser percent of impurity, the host matrix does not lose its structural properties. There are several types of doping present, one of them is magnetic doping. In the case of magnetic doping, it is carried out by substitution of open-shell atoms of 3d, 4s, 5d, 4f, and 5f in the host matrix (Majid *et al.*, 2019). One of the transition metals, vanadium, is found to be an electrically active impurity in SiC, and high-quality semi-insulating SiC crystal can be obtained with vanadium (Mynbaeva *et al.*, 2003).

V doped with SiC introduced localized magnetic moments, which allow the spin manipulation of the materials and can be used as a potential application in spintronic devices. (Majid, *et al.*, 2020). V doped with 4H-SiC was significantly used for different applications as the addition of vanadium impurities in 4H-SiC modified the electrical conductivity used for photodetectors and quantum emitters (Kramer *et al.*, 2020). Due to the excellent material properties of 4H-SiC and 6H-SiC at high temperatures and high electric fields, these are frequently utilized in high-power electronic devices. Wide band gap, high thermal conductivity, high saturation drift velocity, and mechanical and chemical stability of 4H-SiC and 6H-SiC enable them to function at temperatures significantly higher than other silicon-based devices (Casady *et al.*, 1998; Hornberger *et al.*, 2004). Matsunami (2020). V doped Poly types of SiC (4H-SiC and 6H-SiC) are utilized in different optoelectronic and high-power electronic devices, so V-doped cubic polytype of SiC (3C-SiC) may be a promising material for different optoelectronic devices. The impurity level of vanadium can act as acceptor and deep donor state in 4H-SiC and 6H-SiC (Kunzer *et al.*, 1995; Kimoto *et al.*, 1996). V impurities introduced an additional hole carrier and ferromagnetism at room temperature on different doping concentrations in 4H-SiC (Lin *et al.*, 2018).

Materials and Methods

Silicon Carbide is a wide band gap semiconductor consisting of three major polytypes, 3C-SiC, 4H-SiC, and 6H-SiC, having band gaps of 2.36 eV, 3.23 eV, and 3.05 eV, respectively. 3C-SiC is the only cubic poly-type of SiC, whereas both 4H-SiC and 6H-SiC are hexagonal structures. Cubic SiC is considered in this work. Different sizes of crystal structures having different numbers of atoms with Vanadium doping are considered for calculations.

SiC is doped with V either at Si site or C site and calculations were done. Supercells of different sizes ($2 \times 2 \times 2$ and $3 \times 3 \times 3$) were developed to add the impurity. This simulation is done for V-doped SiC supercells with primitive cells having atoms 8, 16, and 54 atoms. Figure 2 shows the SiC doped with V at Si and C site. The top line has two figures: unit cell of SiC with V at the Si site (left) and V at the C site (right). The lower line of Figure 2 shows the SiC doped with V at the Si site in the $3 \times 3 \times 3$ supercell with 54 atoms. In these figures, light blue colours are the Si atoms, yellow colours are the carbon atoms and dark blue colours are the V atoms. Bigger size cell ensures the minimization of interaction between the impurity atoms.

Computational Details

These calculations are based on the DFT with the local density approximation (LDA). Vanderbilt ultra-soft pseudopotentials (Vanderbilt, 1990) are used in choosing only the valence electrons for calculations. The code chosen here is the Quantum Espresso (Giannozzi *et al.*, 2009) code. It's suitable for first principles of electronic structure calculations and modeling of various materials based on DFT (Panda and Patnaik, 2022; Patnaik, *et al.*, 2022). It uses both norm-conserving and Vanderbilt pseudopotential. The pseudopotential scheme used allows the expansion of the single particle wave functions into a plane wave basis set. It is restricted by a kinetic energy cut off of 32.0 Ry. A set of special $2 \times 2 \times 2$, $4 \times 4 \times 4$ and $8 \times 8 \times 8$ k-points generated by the Monkhorst and Pack (1976) scheme is used for BZ sampling.

The Monte Carlo results of Ceperley and Alder (1980) method are used to describe the exchange and correlation potential energy of the electrons in the Perdew and Zunger (1981) parametrization. While generating the pseudopotentials nonlinear core correction is applied to the exchange correlation energy. This is done to minimize the errors arising due to the consideration of frozen cores. The single particle Kohn-Sham (Kohn and Sham, 1965) equations are solved, and the eigenvalues are taken to interpret bulk band structure and the vacancy levels.

Results and discussion

Cubic SiC is considered a host, and vanadium is a substitutional impurity in Si and C placed separately. Spin polarized calculations are done in all cases to check the magnetic behaviour of the sample. The distance between two consecutive impurity atoms is $13.08 \text{ \AA}$. The effect of relaxation is also checked.

Figure 3 shows the DOS and the PDOS for pure SiC. The top of the valence band is taken as zero on the energy axis, and all other values are plotted accordingly. The partial density of states plot shows that most of the contribution for the top portion of the valence band is from p state electrons. The conduction band consists of contributions both from s-states and p-state electrons. The total density of states of pure 3C-SiC points out that spin bands of pure SiC are symmetric in nature, which means both up spin and down spin bands show a symmetric

Table 1. Formation and Fermi energy of V doped cubic SiC

Cubic SiC Substitution site	Formation energy (eV / at)		Fermi energy in Ry	
	Before relaxation	After relaxation	Before relaxation	After relaxation
Si	1.04	1.45	1.65	1.36
C	19.7	13.35	1.02	1.85

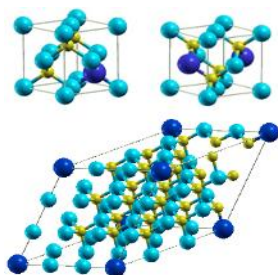


Figure 2. Top line left figure shows V at Si site in 8 atom cell, top-line right figure shows V at C site in 8 atom cell, bottom line figure is primitive cell of 54 atoms with V at Si site

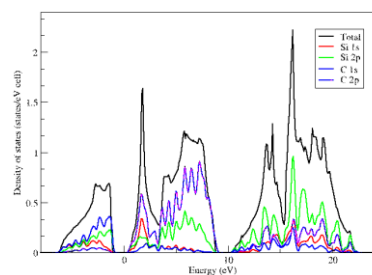


Figure 3. Total and partial density of states of 3C SiC

nature. These symmetries suggest magnetism is absent in intrinsic 3C-SiC. But when doped with transition metal like vanadium then magnetic property is introduced in it. Formation energy is calculated for both before relaxation and after relaxation and presented in Table 1.

Formation energy provides the valuable insights regarding the stability of a particular crystal structure or materials. Lower the formation energy indicates more stability of the materials. The formation energy of 'V' doped SiC is expressed as following:

$$E_f = E_f^{Defect} - E_f^{SiC} + \sum n_i \mu_i$$

E_f^{Defect} and E_f^{SiC} are the total energy of 'V' doped SiC and intrinsic SiC supercell respectively. μ_i be the chemical potential of i^{th} atom and n_i be the number of i^{th} atom (Reunchan *et al.*, 2017; Charoenphon *et al.*, 2023).

Formation energy calculations are done for both before and after relaxation. The simulation starts with experimental data without relaxing the structure. In this phase, the simulation does not carry out any geometry optimization and atomic positions are fixed. After relaxation phase involves the geometry optimization which provide the most favorable and stable configuration to the materials. This allows to alter the atomic position and cell parameters. After relaxation, it minimizes the total energy by adjusting the cell parameters and atomic positions.

3C SiC

It generates the most stable structure after the simulation and we can extract various structural properties such as bond length, bond angle, lattice parameters from it. Further simulation is done with these lattice parameters to get more exact results.

These values indicate Si site is preferable over C site substitution by V atom. These results are same even after relaxing the structure. This indicates that Si site substitution of V is more stable than C site substitution. The value of the Fermi level position obtained in this calculation is mentioned in Table 1. These values are with respect to valence band top.

To understand the magnetic behavior of the sample we have looked for its magnetic moment. Most of the magnetic moment of the sample is found to be concentrated on the vanadium (V) atom. The total magnetic moment for Si substitution is 1 μ B and the local moment is 0.97 μ B. However, this is not the case for C site substitution with the values 3.06 and 2.02 μ B, respectively. To understand the spin state, we can have look at the density of states

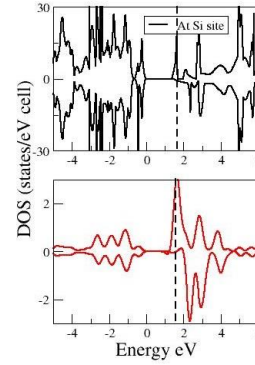


Figure 4. Total DOS and PDOS of V at Si site in cubic SiC are shown. Valence band maximum is taken at zero of energy axes. The dashed line shows the position of the Fermi level

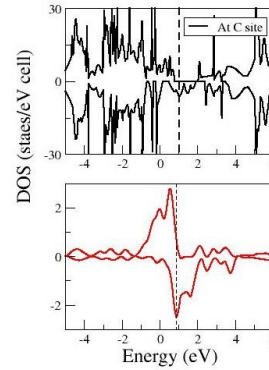


Figure 5. Total DOS and PDOS of V at C sites in cubic SiC are shown. Valence band maximum is taken at zero of energy axes. The dashed line shows the position of the Fermi level

(DOS). Figures 4 and 5 show the density of states (DOS) on the top panel and the partial density of states (PDOS) on the bottom panel of impurity d states. Significant 3d-character is observed in the band due to the hybridization of d states on V with s and p states of its neighborhood atoms. For Si site substitution impurity level is seen just below the conduction band maximum. Presence of this partially filled impurity level decreases the band gap. This filled impurity state at energy value is at 1.5eV above the valence band which is experimentally found to be 1.7eV (Achtziger *et al.*, 2000). The Fermi level is located inside the conduction band.

Since we are using LDA that reduces the band gap so considering the experimental band gap we can observe two deep levels inside it which is an agreement with other published results (Kunzer

et al., 1995; Bathen *et al.*, 2019). The broadening of the impurity levels is due to the coupling with dangling bonds and interaction between the neighboring impurities. Very small spin splitting is observed for both the cases. The situation is different for C site substitution. Here, the valence band gets contribution from 3d states of the V atom. The contributions from spin down go to the conduction band and also to the band gap, as seen in Figure 5. The band gap for the up spin is decreased, and there is no band gap for the down spin. This DOS plot shows V at C place in cubic SiC shows half-metallic character. Since the SiC with a Si vacancy shows high spin state in various studies (Itoh *et al.*, 1997; Torpo *et al.*, 1999; Wimbauer *et al.*, 1997) the combination of V-doped with Si or C vacancy can then be expected to give a DMS (Kukushkin and Osipov, 2021; Zhang *et al.*, 2020).

Conclusion

Cubic silicon carbide SiC doped with vanadium (V) is studied with density functional theory using pseudopotentials. It is a very tough and complicated process to describe an interacting multi-particle system. To find the solution of the Schrodinger's equation of this system needs the involvement of various approximations. First principle method takes care of all these. Cubic SiC doped with transition metal vanadium by using DFT, we observed two deep levels for V at Si site substitutions as a deep donor and deep acceptor levels. This may indicate semi-insulating behavior. V at C site substitution shows half-metallic character of cubic SiC. The calculation value of formation energy indicates V impurity prefers Si site than C site in cubic silicon carbide (3C-SiC). The presence of V at C site induces magnetic properties as can be seen from the total magnetic moment of the material. For C site substitution the sample shows magnetic behavior. So V at C site can be more investigated for a potential candidate as a DMS.

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