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# AB-INITIO CALCULATION OF THE STRUCTURAL AND ELASTIC PROPERTIES OF THE ALLOY $SiGe_XC_{1-X}$

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## Abstract

In this work, we studied the structural and elastic properties of the SiC, SiGe binary compounds and their ternary alloy, $SiGe_xC_{(1-x)}$ , in the zinc blende phase. Throughout the study, we used an ab-initio calculation based on the density functional theory (DFT) [1,2] combined with the pseudopotential method [3]. This work focuses on a purely numerical study that uses the VCA (virtual crystal approximation) method with the ABINIT code [4]. In the treatment of the exchange and correlation term, we used the local density approximation (LDA) [5].

We performed the convergence tests, determining the cutoff energy as well as the number of special points of the material under investigation namely the (SiC, SiGe and $SiGe_XC_{(1-X)}$). We have calculated the properties of the ground state namely: the equilibrium lattice parameter, the compressibility modulus and its first derivative. We have also calculated the elastic properties. Our results are in good agreement with the experimental data available and with those published in the literature [6-8], by other forms of pseudo-potential and exchange-correlation energies.

For the elastic constants as a function of the concentration, the same trend of variation was found for the three elastic constants and it was found that the hardness increases with the increase of the carbon concentration in the alloy.

**Keywords:** SiC, SiGe et $SiGe_XC_{1-X}$, Abinit, elastic properties, Dft, Structural properties.

## 1. Introduction

$Si_{1-x}Ge_x$ semiconductor alloys have a great interest in nanoelectronic applications, photovoltaic technology, optical devices, and many other applications. Many types of $Si_{1-x}Ge_x$ / Si heterostructure-stripped electronic and optoelectronic devices have been realized [9]. Alloys and Si-Ge compounds also have particular optoelectronic properties for the applications of inter-subband transitions in quantum wells [10]. Several companies already offer SiGe circuits on the market with considerable advantages over the performance of conventional devices [11]. SiGe brings many advantages over all-silicon technology. However, the use of SiGe has disadvantages, for example, the incorporation into germanium is not sufficient to obtain steep profiles of dopants. The high levels of germanium needed to improve the performance of TBH (heterojunction bipolar transistors), can also lead to the relaxation of SiGe layers according to the deposited thickness. It is for these reasons that the silicon-germanium-carbon ternary alloy has been (and still is) studied.

The addition of a high concentration of carbon in SiGe films is recognized to provide several advantageous effects on the performance of the device. The main interest of the incorporation of carbon atoms into bipolar transistors with Si / SiGe / Si heterojunction is a significant reduction in boron diffusion [12]. Obtaining very steep and highly doped boron profiles is possible, allowing bipolar devices to achieve better dynamic performance.

At the same time, the addition of carbon in the binary alloy makes it possible to reduce the stress caused by the SiGe / Si matrix and to delay the generation of adaptation dislocation. The atomic volume of carbon is lower than that of the silicon atom. This property is used in the realization of the SiGeC alloy which behaves like a binary SiGe alloy whose crystalline parameter is decreased, and the constraint partially reduced, by the incorporation of carbon. The incorporation of carbon in SiGe opens up a field of very attractive possibilities.

## 2. Calculation method ab initio

Calculations were performed using density functional theory (DFT) combined with the pseudopotential method implemented in the ABINIT code. The code ABINIT (URL http://www.abinit.org) is a software based on the method (DFT), it is developed firstly by Xavier Gonze, Jean-Michel Beuken [13] of the unit Physico-Chemistry, and Physics of Materials at the Catholic University of Louvain, Belgium.

ABINIT is based on a plane wave development of electronic wave functions, under periodic boundary conditions (Bloch). This representation is particularly suitable for crystal studies. For pseudopotentials that eliminate the explicit processing of core electrons, and focus on bond formation and response properties of valence electrons. ABINIT has an extensive library of conserved standard pseudopotentials for the entire periodic table. In our work we have used those proposed by Hartwigzen-Goedecker-Hutter (HGH) [14]. The form proposed by Teter and Pade [15] (1993) is used for the exchange and correlation energy in the context of the local density approximation, this form reproduces that of Perdew Wang, which in turn reproduces that of Ceperley Alder. Integrations in the reciprocal lattice were made using the Monkhorst and Pack k-point generation method [16].

Before starting the calculations, tests must be performed to ensure convergence. First and foremost, we did convergence tests on two essential parameters:

- The cutoff energy "Ecut"
- The choice of the number of k points, taken into account in the integration through the 1st Brillouin zone.

We found that a cutoff energy equal to 75 Hartree and 50 Hartree is largely sufficient to obtain a good convergence of the total energy and to carry out the rest of the calculations for the SiC and SiGe compounds respectively. the choice of a mesh of 6x6x6 k points (28 points) for the number of special points is more than enough to obtain a very good convergence of the total energy for the two SiC and SiGe compounds.

## 3. Structural properties

### 3.1. SiC and SiGe compounds

The second step is to make a total energy calculation for different mesh parameter values; From these calculation it is possible to obtain the static structural properties such as the equilibrium lattice constant obtained from the volume which gives the minimum energy, the modulus of rigidity, as well as its derivative, by adjustment of the values of the total energy calculated using the Murnaghan state equation given by this relation [17]:

$$E(V)-E(V_0)=\frac{B_0 V}{B}\left[\frac{(V_0/V)^{B'}}{B-1}+1\right]-\frac{B_0 V_0}{B-1} \qquad (1)$$

$$B_0=V\frac{\partial^2 E}{\partial V^2}=\frac{4}{9\mathrm{a}}\frac{\partial^2 E}{\partial \mathrm{a}^2} \qquad (2)$$

Where at P = 0, $B_0$ is the stiffness modulus given by relation (2), $V_0$ is the equilibrium volume E ($V_0$) is the equilibrium volume energy and B' is the derivative of the stiffness modulus depending on the pressure P:

$$B'=\frac{\partial B}{\partial P} \qquad (3)$$

This equation gives a very good fit of the energy according to the volume.

The results obtained are shown in Table 1 in comparison with the experimental results and other Ab-initio calculations.

We note that our calculated lattice parameter, for SiGe compound, is in excellent agreement with the theoretical values available [18,19,20]. The calculated SiC lattice parameter is in agreement with the results obtained experimentally [19] and theoretically [18,6].

**Table 1: The mesh parameter, the modulus of rigidity and its derivative in comparison with the experimental and theoretical values.**

| | **Lattice parameter (A°)** | **$B_0$(GPa)** | ***B'*** |
|---|---|---|---|
| **SiC** | 4.31 | | |
| | 4.31 (fitted) | 226.07 | 3.817 |
| | 4.329 [18] | 225 [6] | 3.430 [6] |
| | 4.36 [19] | 224 [19] | 3.532 [18] |
| | 4.31 [20] | 227 [18] | |
| **SiGe** | 5.472 | | |
| | 5.47 (fitted) | 84.69 | 4.391 |
| | 5.506 [18] | 84.16 [18] | 4.48 [20] |
| | 5.527 [6] | 84.85 [6] | 3.88 [6] |
| | 5.53 [20] | 87.4 [20] | 4.266[18] |

### 3.2. SiGe$_x$C$_{1-x}$ alloy

For the calculation of the structural properties (no gratings, modulus of rigidity and its derivative) at the equilibrium of the SiGe$_x$C$_{1-x}$ alloy we fixed the cutoff energy at 90 Hartree to obtain a good convergence, the energy total was calculated in a self-consistent manner with 28 k in the reduced Brillouin area.

To study the SiGe$_x$C$_{1-x}$ alloy, we preferred to follow the virtual crystal approximation (VCA). The VCA considers that the alloy is approximately represented by a monatomic (virtual) periodic array with an average atomic potential [21].

This approximation provides a linear variation of the main parameters in the alloy. In particular, the crystalline potential is defined by linear interpolation between those components constituting the crystal.

$$V_{VCA} = (1-x)V_{SiC} + xV_{SiGe} \qquad (4)$$

Where x is the atomic concentration of the SiGe type atom. $V_{SiC}$, $V_{SiGe}$ is the atomic potential of the SiC atom, SiGe respectively. This method is simple and has shown its efficient in several scientific works to study different system of alloys of semiconductors, superconductors and ferromagnetic materials.

Vegard's law is used to calculate the initial lattice parameters of the alloys considered. It is an empirical relationship. It states that the lattice parameter of a solid solution of two constituents is approximately a weighted mean of the two constituents' lattice parameters at the same temperature:

$$a_0 = (1-x)a_{SiC} + xa_{SiGe} \qquad (5)$$

The equilibrium lattice parameter, modulus of rigidity and its derivative were calculated for several concentrations x (x [0, 0.2, 0.4, 0.6, 0.8, 1]), by minimizing the total energy calculated for different lattice constant values by the same method used for SiC and SiGe compounds. The results obtained are given in Table 2.

**Table 2: Mesh parameter, stiffness modulus and its derivative for SiGexC1-x alloy**

| X | $V_0$ ($A^{\wedge 3}$) | $a_0$ (A) | $B_0$ (GPa) | $B_0$’ |
|---|---|---|---|---|
| **0** | 20.07318 | 4.3141 | 226.07 | 3.78 |
| **0.2** | 27.45491 | 4.7888 | 142.02 | 4.05 |
| **0.4** | 32.98147 | 5.0907 | 104.48 | 4.27 |
| **0.6** | 36.80479 | 5.2803 | 92.44 | 4.34 |
| **0.8** | 39.28747 | 5.3964 | 87.29 | 4.37 |
| **1** | 40.96664 | 5.4722 | 84.70 | 4.39 |

To our knowledge, there is no experimental data or theoretical calculation to compare our results of the variation of modulus of rigidity $B_0$, as well as its derivative B’ as a function of the concentration (x) for alloy $SiGe_xC_{1-x}$ so our results can be taken as predictions.

The values found for the lattice parameters of the alloy indicate that the introduction of carbon decreases the SiGe lattice parameter. Figure 1 shows the values of the lattice parameter as a function of concentration x.

Using a polynomial fit at 30 points gets the following equation:

$$a(A°) = 0.8085x^3 - 2.4297x^2 + 2.7795x + 4.3137 \qquad (6)$$

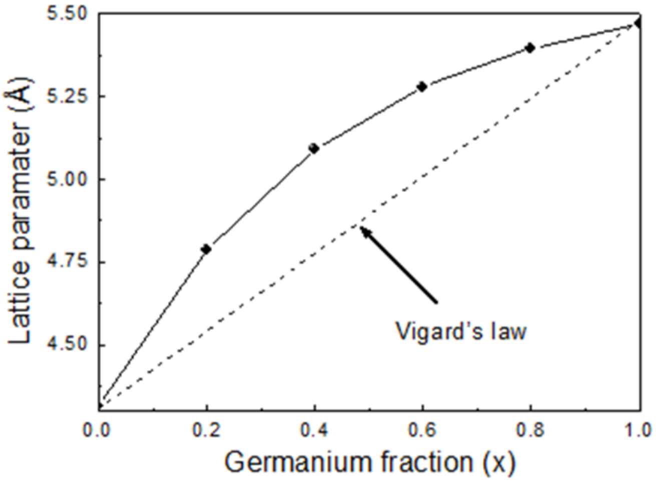

**Figure 1 : The variation of lattice parameter versus germanium fraction x for SiGe (x) C (1-x) alloy**

## 4. The mechanical properties of SiC compounds, SiGe and SiGexC1-x alloy

### 4.1. The elastic constants Cij

It is very important to study the elastic properties of the materials, because they allow to express a relation between the mechanical and dynamic behavior of the crystals, and to give important information on the nature of the forces that act in the solids.

When a stress is applied to the crystal, it deforms, modifying the parameters that describe it. In the region close to equilibrium, the quadratic development of energy makes it possible to express a linear relation between stress and strain: this is Hooke's law. This relationship is defined by elastic constants. The elastic constants also make it possible to define the mechanical stability of the crystal in the face of the deformations. In fact, for the equilibrium point to be a point of stable equilibrium, the quadratic form of the energy must be positive definite, which imposes conditions on the elastic constants.

Calculations of elastic constants are performed using a method introduced in 2005, it uses the density functional perturbation (DFPT) theory [22] combined with the pseudopotential method, with a base of waves planes (PPW). Its principle is based on the use of the first derivatives of the wave functions with respect to the perturbation (here the deformation or the atomic displacement) to evaluate the second derivatives of the energy [23,24].

Because of its ease of use and low computing times, this method is a standard, and has quickly become a method of choice for evaluating the elastic constants of materials.

The cubic crystalline structures have three independent elastic constants: $C_{11}$, $C_{12}$ and $C_{44}$. The calculated values of elastic constants Cij at (Gpa) are shown in Table 3 and plotted in Figure 2.

**Table 3 : Calculated values of elastic constants $C_{11}$, $C_{12}$, $C_{44}$ in (GPa)**

| **Composition** | **$C_{11}$(GPa)** | **$C_{12}$ (GPa)** | **$C_{44}$ (GPa)** |
|---|---|---|---|
| **SiC** | 395,55 | 134,45 | 252,93 |
| | 390 [26] | 134 [7] | 259 [26] |
| | 399.6 [6] | 138 [6] | 253 [7] |
| | 395 12[8] | 132±9 [8] | 236±7 [8] |
| **$SiGe_{0.2}C_{0.8}$** | 251,32 | 81,98 | 142,59 |
| **$SiGe_{0.4}C_{0.6}$** | 189,26 | 62,86 | 101,67 |
| **$SiGe_{0.6}C_{0.4}$** | 164,06 | 56,86 | 85,58 |
| **$SiGe_{0.8}C_{0.2}$** | 152,81 | 54,99 | 78,27 |
| **SiGe** | 142,39 | 54,96 | 70,75 |
| | 147.8 [25] | 56.1[25] | 41[6] |

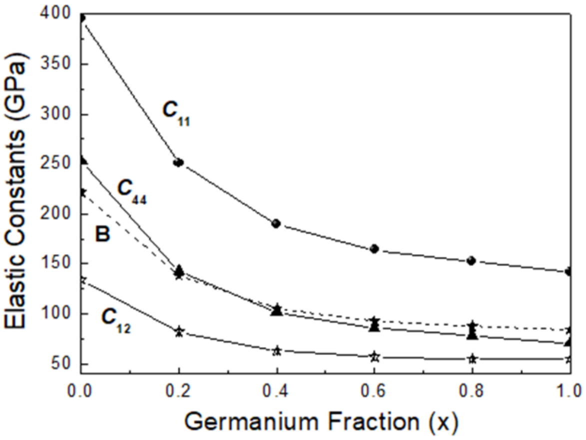

**Figure 2 : The variation of elastic constants versus germanium fraction x for $SiGe_XC_{1-X}$ alloy**

We can notice that our result for the elastic constants is in good agreement with the theoretical calculations made by [6.7.25.26] for SiC and SiGe, but for the elastic constant $C_{44}$ of SiGe, our calculated value is higher in comparison with the results. theories made by S. Goumri-Said et al. [6]
Our elastic constants and the calculated compressibility modulus of SiGexC1-x satisfy the requirements of mechanical stability [27] of cubic crystals.

$C_{11}+2C_{12}>0$ , $C_{11}>C_{12}$ , $C_{44}>0$ , $C_{11}>B>C_{12}$

When comparing the values of the elastic constants obtained for SiC and SiGe, we can see that all the elastic constants for SiC are almost triple those of SiGe, which indicates that SiC is a material much harder than the SiGe.

The incorporation of carbon in SiGe increases the hardness of this compound.

To our knowledge, there is no experimental data or theoretical calculation to compare our results of the variation of the elastic constants as a function of the concentration (x) for the alloy $SiGe_XC_{1-X}$ so our results can be taken as predictions.

### 4.2. Rigidity modulus B and shear modulus G

For the cubic system, the stiffness modulus B and the shear modulus G can be expressed as a linear combination of the two elastic constants $C_{11}$ and $C_{12}$: [28]

$$B = (C_{11} + 2C_{12})/3 \qquad (7)$$

$$G = (C_{11} - C_{12})/2 \qquad (8)$$

The Pugh **B / G** ratio [29] was originally introduced to distinguish between ductile behavior (high **B / G** values) and brittle behavior (low **B / G** values). To distinguish between the fragile or ductile nature of materials a critical value of Pugh's ratio is found to be 1.75. [30]

The values found for this report are listed in Table 4 and plotted in Figure 3. All values calculated for this alloy in the range of 1.14 to 1.44 are less than 1.75 indicating the fragile nature of the alloy.

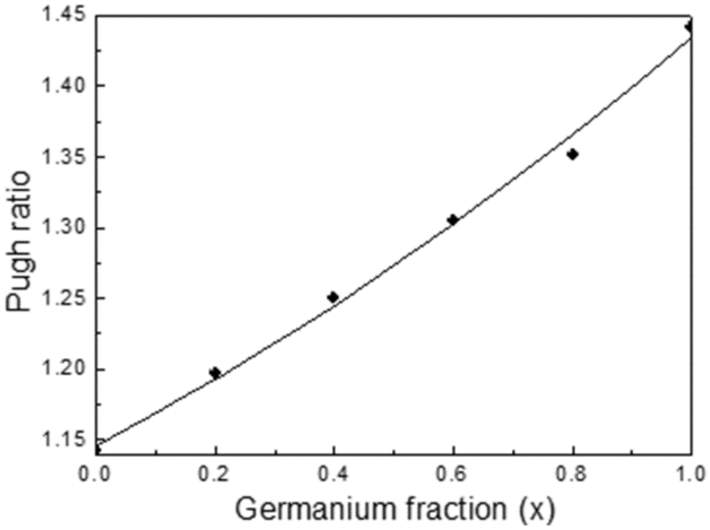

**Figure 3 :** ***Evolution of Pugh ratio versus germanium fraction*** **for $SiGe_xC_{1-x}$ alloy**

**Tableau 4 : Calculated values of volume density, Pugh ratio, Poisson's ratio (σ) and Young's modulus (E) for the $SiGe_xC_{1-x}$ alloy**

| X | Densité (g/cm$^3$) | B/G | *E (GPa)* | *σ* |
|---|---|---|---|---|
| **0** | 3.31704 | 1.14 | 450.41 | 0.16 |
| **0.2** | 3.15856 | 1.20 | 271.45 | 0.17 |
| **0.4** | 3.23978 | 1.25 | 198.99 | 0.18 |
| **0.6** | 3.45024 | 1.31 | 169.53 | 0.19 |
| **0.8** | 3.74483 | 1.35 | 155.99 | 0.20 |
| **1** | 4.08287 | 1.44 | 142.13 | 0.22 |

### 4.3. Young's modulus and Poisson's ratio

There is considerable interest in the effect of mechanical stresses on the growth of semiconductor crystals and electronic devices and consequently on their behavior and reliability. The accurate calculation of such constraints requires knowledge of Young's modulus and Poisson's ratio, especially for specific crystallographic orientations defining the surface of the semiconductor [31].

Designated by the Greek letter ν and dimensionless, here is the principal Poisson coefficient, another constant characteristic of the elastic behavior of the material. This coefficient makes it possible to characterize the contraction of the material perpendicular to the direction of the force applied (ν = unitary transverse contraction / unit axial elongation). Theoretically this coefficient is equal to 0.25 for a perfectly isotropic material and is in practice very close to this value. It is always less than or equal to 1/2. If it is equal to 1/2, the material is perfectly incompressible.

These two constants, Young's modulus and the Poisson's principal coefficient are given by the following relations:

$E = 9BG / (3B + G)$ (9)

$\sigma = (3B-2G) / (6B + 2G)$ (10)

Frantsevich's rules [30] also suggest that a value of ν = 0.26, is the boundary that separates fragile and ductile materials. If the main coefficient of Poisson is greater than this value the material is classified as ductile. In the opposite case the material is classified as fragile, this is the case of the $SiGe_xC_{1-X}$ alloy where the main Poisson's ratio is less than 0.26.

Calculated Young's modulus and Poison coefficient values are tabulated in Table 4 and plotted in Figure 4.

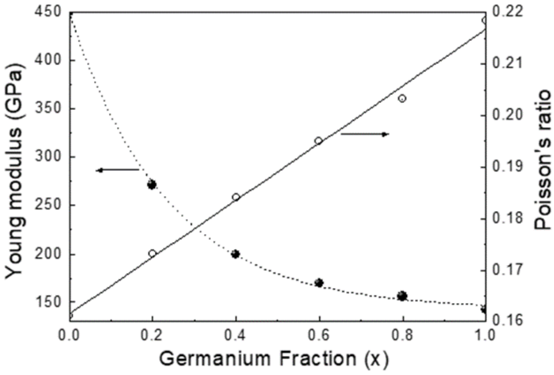

**Figure 4 :** ***Variation of Young's modulus and Poisson's ratio versus x concentration for $SiGe_xC_{1-x}$ alloy***

At present, the focus is on the search for new materials having a high Young's modulus while remaining light, the latter is ensured by the low density values found for this alloy. And for high carbon concentrations the Young's modulus of the alloy is high.

## 4.4. Elastic wave propagation velocities and Debye temperature

A perfectly isotropic material is a material for which A (isotropic factor) = 1.0, most of the crystalline solids are not perfectly isotropic in their elastic properties. The propagation velocities of elastic waves in these materials are strongly dependent on the directions of propagation. If the crystal density g and the elastic constants Cij of a cubic crystal are known, the propagation velocities of the elastic waves can be easily calculated in certain specific crystallographic directions.

If we know the stiffness modulus B, the shear modulus G, and the crystal density g of a solid, we can easily calculate the Debye temperature, which is an important fundamental parameter, closely related to many physical properties such as that: specific heat, elastic constants, melting temperature, etc.

At low temperature the vibratory excitation results only from the acoustic modes, and therefore, the Debye temperature (the temperature above which a certain crystal behaves conventionally; ie above which the vibrations thermal values are larger than the quantum effects) calculated from the elastic constants is the same as that determined from the measurements of the specific heat.

One of the standard methods for calculating the Debye temperature ($\theta_D$) is that of the elastic constants, since $\theta_D$ can be estimated from the mean velocity of the elastic waves $v_m$ by the following equation [32]

$$\theta_D = \frac{h}{k_\beta}(3/4\pi V_a)^{1/3} V_m \qquad (11)$$

Where: h is the Planck constant, kB is the Boltzmann constant, νm is the mean velocity of the elastic waves, and Va is the atomic volume. For the cubic zincblende phase: Va = V / 8, from which equation (11) becomes:

$$\theta_D = \frac{0.59548}{a} V_m \qquad (12)$$

Where: a represents the mesh parameter (Å)

The average velocity ν m of the elastic waves is given by [32, 33, 34]

$$v_m = \left[\frac{1}{3}\left(\frac{2}{v_t^3} + \frac{1}{v_l^3}\right)\right]^{-1/3} \qquad (13)$$

Or :

νl and νt are respectively the propagation velocities of the longitudinal and transverse elastic waves. They are obtained using rigidity modulus B, shear modulus G and crystalline density g from the Navier equation [32, 33, 35]:

$$v_l = \left(\frac{3B+4G}{3g}\right)^{1/2} \qquad (14)$$

$$v_t = \left(\frac{G}{g}\right)^{1/2} \qquad (15)$$

If one writes: [B = (C11 + 2C12) / 3] and [G = (C11-C12) / 2], one finds that the propagation velocities of the longitudinal waves νl and transverse νt are respectively these in the direction [100] (with a plane of polarization [100] L), and these which have wave vectors parallel to the direction [110] and creating displacements of the particles perpendicular to this direction, i.e. a plane of polarization [001] T), so they can be rewritten by the following formulas:

$$v_l = \left(\frac{C_{11}}{g}\right)^{1/2} \qquad (16)$$

$$v_l = \left(\frac{C_{11}-C_{12}}{2g}\right)^{1/2} \qquad (17)$$

The results obtained from these parameters for this alloy are summarized in Table 5.

**Tableau 5 : Values of the propagation velocities of elastic waves $\nu_l$, $\nu_T$, $\nu_m$ and $\theta_D$ for $SiGe_xC_{1-x}$ alloy**

| X | *vl* (km/s) | *vt* (km/s) | *vm* (km/s) | Debye temperature (K) |
|---|---|---|---|---|
| **0** | 12.031 | 7.647 | 8.408 | 1161 |
| **0.2** | 9.626 | 6.052 | 6.663 | 828 |
| **0.4** | 8.185 | 5.093 | 5.613 | 657 |
| **0.6** | 7.366 | 4.534 | 5.003 | 564 |
| **0.8** | 6.817 | 4.160 | 4.595 | 507 |
| **1** | 6.297 | 3.780 | 4.181 | 455 |

The Debye temperature $\theta_D$ is one of the most important parameters that determines the thermal characteristics of materials. In general, a high value of this temperature implies a greater associated thermal conductivity and a high melting temperature. Knowledge of such a numerical value is essential for the development and manufacture of electronic devices. For the alloy considered in this study the temperature of Debye increases with the increase of the carbon concentration.

## 5. Conclusion

In this work, we have studied the structural and elastic properties of the **SiC**, **SiGe** binary compounds and their ternary **$SiGe_XC_{1-X}$** alloy in the blende zinc phase. Throughout the study, we used an ab-initio calculation based on the DFT density functional theory combined with the pseudopotential method. In the treatment of the exchange and correlation term, we used the local density approximation LDA.

We performed the convergence tests, determining the cutoff energy as well as the number of special points of the material under investigation. We have calculated the properties of the ground state: the equilibrium network parameter, the compressibility modulus and its first derivative. We have also calculated the elastic properties. Our results are in good agreement with the experimental data available and with those published in the literature, by other forms of pseudo-potential and exchange and correlation energies.

For the elastic constants, the same tendency of variation as a function of concentration was found for the three elastic constants and it was found that the hardness increases with the increase of the carbon concentration in the alloy.

Calculated values of Pugh ratio and Poisson's ratio for this alloy indicate the brittle nature of the alloy and finally the large values of Debye temperatures for large carbon concentrations indicative of high melting temperatures and high conductivities thermal for this alloy.

A work of computation of these elastic constants as a function of the pressure, the phase transition as well as the effect of the pressure on the different physical properties is envisaged to have a complete set of data on this alloy.

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