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First-Principles Calculations of Elastic and Optical Properties of $SrSi_2$

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Abstract: **The different properties of $SrSi_2$ have been calculated using the plane wave ultra soft pseudo potential technique which is based on the first-principles Density Functional Theory (DEF) with Generalized Gradient Approximation (GGA). The study involves the calculations of elastic and optical properties of $SrSi_2$. The optimized lattice parameters, three independent elastic constants (C_{11}, C_{12}, and C_{44}), bulk modulus (B), shear modulus (G), Young's modulus (Y), Pugh's ratio (G/B), Poisson's ratio (v) and elastic anisotropy (A) are estimated and discussed. This is the first quantitative theoretical prediction of the elastic properties of $SrSi_2$ compound. Finally the optical properties of $SrSi_2$ are obtained and discussed in detail.**

Keywords**: $SrSi_2$; First-principles; Elastic properties; Optical properties.**

I. INTRODUCTION

Silicon is a primary material in modern solid-state electronics and semiconducting silicides which are composed of non- or less toxic and naturally abundant elements from earth's crust have attracted considerable attention because of their practical applications in photoelectric and thermoelectric [1-3] devices, such as a light-emitting diode and as candidates of new thermoelectric materials because they are environmentally friendly. Thermoelectric materials are capable of converting waste heat into electricity [4]. It is very important for developing alternative energy technologies in the reduction in our dependence on fossil fuels [5] to utilize the technology of energy conversion. The effectiveness of a material for thermoelectric applications is determined by the dimensionless figure of merit, $ZT=S^2\sigma T/k$, where S is the Seebeck co-efficient, σ the electrical conductivity, k the thermal conductivity and T the absolute temperature [6]. Photoelectric devices give an electrical signal in response to visible, infrared, or ultraviolet radiation. They are often used in systems which sense objects or encoded data by a change in transmitted or reflected light. Photoelectric devices which generate a voltage can be used as solar cells to produce useful electric power. Among alkaline-earth metals disilicides, very recently $SrSi_2$ was reported to be a narrow-gap semiconductor with a band gap of 0.035 eV estimated by the Hall coefficient measurements ranging from 10 to 300 K and the electrical resistivity measurements ranging from 2 to 760 K [7]. Elastic properties of solids are closely related to many fundamental solid state properties, such as equation of state EOS, specific heat, thermal expansion, Debye temperature, Gruneisen parameter and melting point. From the elastic constants, one can obtain valuable information about the binding characteristics between adjacent atomic planes, the anisotropic character of the bonding, and the structural stability. Furthermore, elastic properties are of great interest for the material science of SCs; for example, elastic constants can be linked to such important physical parameters of SCs as the Debye temperature QD and the electron–phonon coupling constant λ. Besides, mechanical properties are important for technology and advanced applications of superconducting materials [8–10]. On the other hand, the study of the optical functions helps to give a better understanding of the electronic structure. At present, there are a few reports about dielectric function, absorption coefficient, loss function on optical properties [28], the other optical properties such as conductivity, reflectivity, refractive index and even the elastic properties of $SrSi_2$ have not studied. Therefore, in this paper, we calculate the elastic constant, conductivity, reflectivity, refractive index, absorption coefficient of the cubic $SrSi_2$ using the planewave pseudopotential methods based on density functional(DFT) and the results are analyzed in detail. The rest of the paper is organized as follows: in Sec. 2, description of the method of calculation is given; Sec. 3

contains our results and discussion, involving elastic and optical properties for $SrSi_2$ composition. Finally, the conclusion is given in Sec. 4.

II. COMPUTATIONAL METHODS

The considered semiconducting $SrSi_2$ phase possesses the cubic structure with space group $P4_332$ (no. 212). It contains four Sr atoms and eight Si atoms, each Si atom is surrounded by three Si atoms and seven Sr atoms, and each Sr atom is surrounded by fourteen Si atoms and six Sr atoms see Fig.1. The positions of atoms in $SrSi_2$ are Sr: 4a(0.125, 0.125, 0.125) and Si: 8c(0.423, 0.423, 0.423). All calculations were performed by employing PP–PW approach based on DFT [11, 12] and implemented in Cambridge Serial Total Energy Package (CASTEP) code [13]. The major advantages of this approach are: the ease of computing forces and stresses; good convergence control with respect to all computational parameters employed; favorable scaling with number of atoms in the system and the ability to make cheaper calculations by neglecting core electrons. The exchange correlation potential is treated within the LDA, developed by Ceperly and Alder and parameterized by Perdew and Zunger [14, 15]. The presence of tightly bound core electrons was represented by non-local ultra-soft pseudo-potentials of the Vanderbilt-type [16]. Two parameters that affect the accuracy of calculations are the kinetic energy cut-off which determines the number of plane waves in the expansion and the number of special k-points used for the Brillouin zone (BZ) integration. We performed convergence with respect to BZ sampling and the size of the basis set. Converged results were achieved with 8x8x8 special k-points mesh [17]. The size of the basis set is given by cutoff energy equal to 350 eV.

III. RESULTS AND DISCUSSION

3.1. Lattice constant and elastic properties

The geometry optimization was carried out as a function of the normal stress by minimizing the total energy for the compound $SrSi_2$. The procedures lead to successful optimization of the $SrSi_2$ structure. For $SrSi_2$, our calculated value of the lattice constant (6.556 Å) is in good agreement with experimental value, [18]. The optimized lattice parameter and atomic coordinates of $SrSi_2$ are shown in Table 1.

Table 1: Lattice parameters and atomic coordinates for $SrSi_2$

System	Phase	Lattice parameters (Å)	Atomic coordinates
Cubic	$SrSi_2$	$a=b=c$=6.556, 6.545[a] $\alpha=\beta=\gamma$=90	Sr: 4a(0.125, 0.125, 0.125) Si: 8c(0.423, 0.423, 0.423)

[a]Expt.[18].

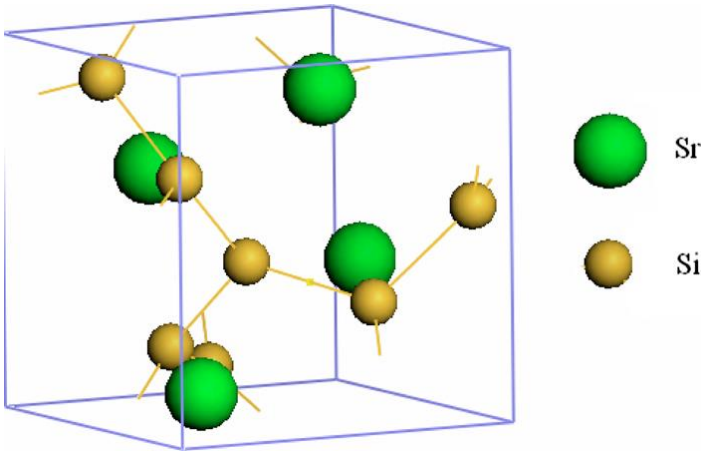

Fig.1. Structures of cubic $SrSi_2$.

The values of three independent elastic constants (C_{11}, C_{12} and C_{44}) for cubic lattice were calculated by applying a proper strain to the equilibrium structure from different directions [19–22]. These values are included in Table 2. All these values are positive and satisfy the generalized criteria [23] for mechanically stable crystals: $(C_{11}-C_{12})> 0$, and $(C_{11}+2C_{12})> 0$, $C_{44}> 0$. These conditions also lead to a restriction on the value of the bulk modulus B, which is required to be between C_{11} and C_{12}, i.e., $C_{12} < B < C_{11}$.

Table 2: Single crystal elastic constants (C_{ij} in GPa).

Compound	C_{11}	C_{44}	C_{12}
$SrSi_2$	84.79	44.92	42.59

Polycrystalline elastic constants are more attractive in technological characterizations of materials, to obtain such quantities ; we have used the Reuss assumption to estimate the bulk modulus *B*, shear modulus *G*, Young modulus *Y*, Poisson ratio υ, and anisotropy factor *A*, according to the following relations:

$$B= (C_{11}+2C_{12}) / 3 \quad (1.1)$$

$$G = 5(C_{11}-C_{12}) C_{44}/ (4C_{44}+3(C_{11}-C_{12})) \quad (1.2)$$

$$Y = 9BG / (3B+G) \quad (1.3)$$

$$\upsilon = (3B-2G)/ 2 (3B+G) \quad (1.4)$$

$$A = 2C_{44}/ (C_{11}-C_{12}) \quad (1.5)$$

The calculated bulk modulus *B*, shear modulus *G*, Young's modulus *Y*, Poisson ratio υ and anisotropy factor *A* of $SrSi_2$ compound are given in Table 3. The Young's modulus, also known as the tensile modulus *Y*, is defined as the ratio between stress and strain and used to provide a measure of stiffness, i.e., the larger the value of *Y*, the stiffer the material. From our calculation, we have the value of *Y* for $SrSi_2$ is 53.63 GPa. So we conclude that this is a stiff material. A simple relationship, which empirically links the plastic properties of materials with their elastic moduli, was proposed by Pugh [24]. The shear modulus *G* represents the resistance to plastic deformation while *B* represents their resistant to fracture [25]. If $G/B<0.5$ the material will behave in a ductile manner, and vice versa, if $G/B>0.5$ the material demonstrates brittleness. In our case, we have found that G/B ratio is 0.57, classifying this material as brittle. An additional argument for the variation in the brittle/ductile behavior of $SrSi_2$ phase follows from the calculated Poisson's ratio *v*, Table 3. Indeed, for brittle materials these values are small enough, whereas for ductile metallic materials *v* is typically 0.33[26]. In our case, the obtained value of *v* is 0.258 which indicates that the examined compound belongs to brittle material.

Table 3: Polycrystalline elastic constants

Compound	*B* (GPa)	*G* (GPa)	*Y* (GPa)	*v*	*A*	*G*/*B*
$SrSi_2$	58.21	33.53	53.67	0.258	2.41	0.57
$SrSi_2$	50.30[a]					

[a]Ref. [27]

Elastic anisotropy of crystals is a very important factor for material science of SCs, since it correlates with the possibility of appearance of microcracks in these materials [30, 31].The anisotropy factor *A* provides a measure of the degree of anisotropy in the bonding in the different planes. For an isotropy crystal, the value of *A* should be equal to the unity, while any deviation from the unity is a measure of the degree of elastic anisotropy possessed by the crystal [27]. There are different ways to estimate elastic anisotropy theoretically. For example, the so-called shear anisotropy ratio $A=2C44/(C_{11}-C_{12})$ is widely used for this purpose. The factor $A_1=4C_{44}/ (C_{11}+C_{33}-2C_{13})$ is also used as a measure of the degree of anisotropy for the {100} shear planes between [011] and [010] directions. Our estimations (Table 3) demonstrate that the examined phase is an anisotropic.

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3.2. Optical Properties

The study of the optical functions helps to give a better understanding of the electronic structure. Here the optical properties such as complex conductivity $\sigma(\omega)$, reflectivity, refractive index and absorption coefficient are calculated. We have used a 0.5 eV Gaussian smearing for all calculations. The calculated optical properties at the equilibrium lattice constants are presented in Figs. 2(I) and 2(II).

(i) Conductivity: The photoconductivity $\sigma(\omega)$, which is directly related to the energy band structure of solids. In Fig. 2(II)(a) photoconductivity starts with photon energy 0.47 eV. This shows that the material has a band gap of about 0.47 eV. The real part of the conductivity is zero below 0.24 eV and above 22.37 eV. Moreover, the photoconductivity and hence electrical conductivity of a material increases as a results of absorbing photons [29].

(ii) Reflectivity: The reflectivity can be expressed by n_1=1, n_2= n+ ik. The reflectivity is derived from $R(\omega) = [(n-1)^2+k^2]/[(n+1)^2 + k^2]$. Fig. 2(II)(b) shows the reflectivity of $SrSi_2$. From the reflectivity spectrum it can be seen that large reflectivity is obtained in the low-energy region, which is the characteristics of high conductance.

(iii) Refractive index: The refractive index n and extinction coefficient k are derived from $n^2-k^2= \varepsilon_1$.$2nk = \varepsilon_2$. The refractive index is shown in Fig. 2(II)(c). The static refractive index n_0 is 5.05. The real part of the refractive index reaches a maximum value of 5.34 at 1.17 eV and then reduces sharply.

(iv) Absorption coefficient: The dielectric function [Ref.28] and absorption coefficient are derived from $\propto(\omega) = \omega\,\varepsilon_2(\omega)/ne$, Fig. 2(I)(b) shows the curve of the absorption coefficient. Two main absorption peaks are observed at 5.11eV and 20.52 eV, which are ascribed to interband transition between Sr 3*d* states at the conduction band (CB) and Si 3*P* in the valence band (VB) states. When the photon energy is below 0.11 eV and above 22.50 eV, $SrSi_2$ is transparent. For first absorption peak, the absorption coefficient increases from 1.05 eV to 5.11 eV, it reaches the maximum value 2.2 x 10^5 cm^{-1} at 5.11 eV and then decreases with the increasing of photon energy till zero and 14.17 eV. For second absorption peak, the absorption coefficient increases from 17.29 eV to 20.52 eV, it reaches the maximum value 1.41 x 10^5 cm^{-1} at 22.52 eV and then decreases with increasing of photon energy till zero, and 22.61 eV corresponds to the value of indirect band gap.

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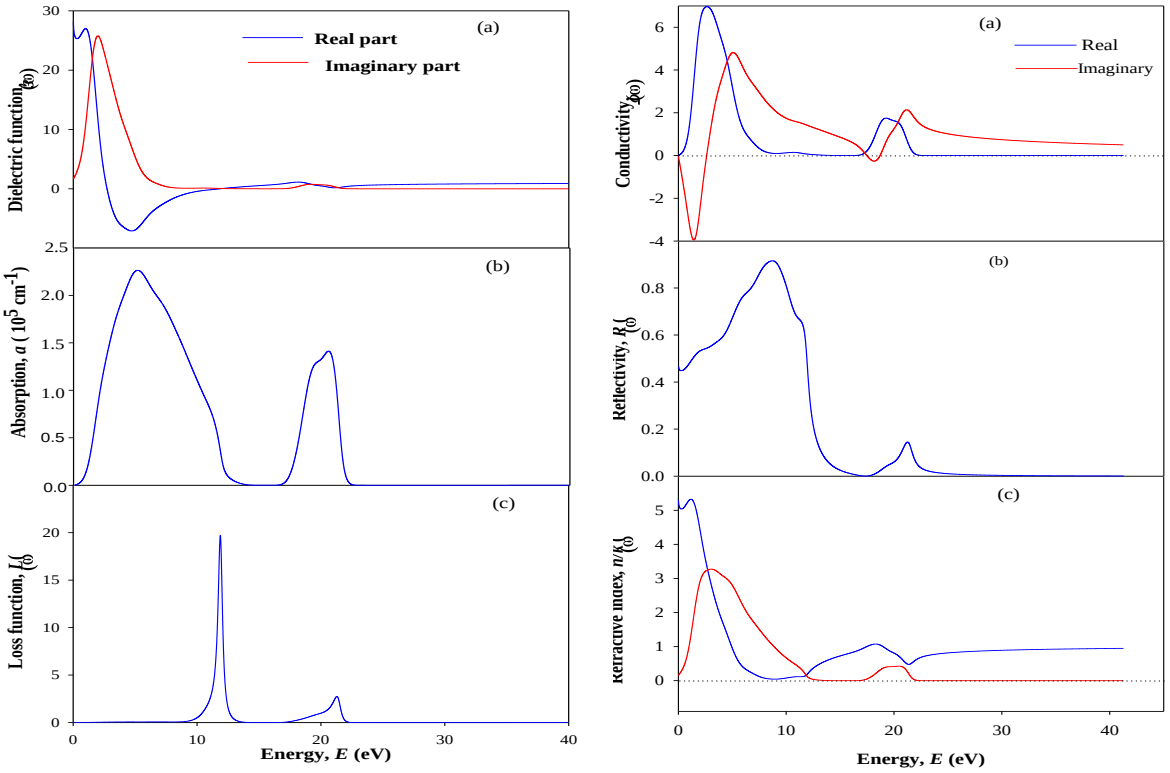

Fig. 2: The optical properties of $SrSi_2$: (a) conductivity $\sigma(\omega)$, (b) reflectivity $R(\omega)$, (c) refractive index n/k (ω).

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IV. CONCLUSION

In summary, the elastic and optical properties of $SrSi_2$ have been investigated using planewave pseudopotential density functional theory within the generalized gradient approximation (GGA). The evaluated elastic parameters allow us to conclude that $SrSi_2$ phase is mechanically stable. The small value of bulk modulus indicates that the material is soft. The obtained Poisson's ratio value indicates that this material possesses brittle behavior. Further the large reflectivity in the low energy region (with moderately good reflectivity up to 10-20 eV) indicates suitability of the compound for use in the solar cell to remove solar heating. Finally we observe that the photoconductivity and hence the electrical conductivity of the material increases as a result of absorbing photons.

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