

# Semi-classical electronic transport properties of ternary compound $\text{AlGaAs}_2$ : role of different scattering mechanisms

Soubhik Chakrabarty<sup>1</sup>, Anup Kumar Mandia<sup>2</sup>, Bhaskaran Muralidharan<sup>2</sup> ,  
Seung Cheol Lee<sup>1,3</sup> and Satadeep Bhattacharjee<sup>1,3</sup> 

<sup>1</sup> Indo-Korea Science and Technology Center, Bangalore 560065, India

<sup>2</sup> Indian Institute of Technology, Mumbai 400076, India

E-mail: [seungcheol.lee@ikst.res.in](mailto:seungcheol.lee@ikst.res.in) and [satadeep.bhattacharjee@ikst.res.in](mailto:satadeep.bhattacharjee@ikst.res.in)

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## Abstract

Using Rode's iterative method, we have investigated the semi-classical transport properties of the  $n$ -type ternary compound  $\text{AlGaAs}_2$ . Four scattering mechanisms have been included in our transport calculation, namely, ionized impurity, piezoelectric, acoustic deformation and polar optical phonon (POP). The scattering rates have been calculated in terms of *ab initio* parameters. We consider  $\text{AlGaAs}_2$  to have two distinct crystal geometries, one in tetragonal phase (space group:  $p4m2$ ), while the other one having body centered tetragonal crystal structure (space group:  $I42d$ ). Higher electron mobility has been observed in the body centered tetragonal phase, thereby making it more suitable for high mobility device application, over the tetragonal phase. In order to understand the differences in electron mobility for these two phases, curvatures of the  $E$ - $k$  dispersion of the conduction bands for these phases have been compared. At room temperature, the dominant contribution in electron mobility was found to be provided by inelastic POP scattering. We have also noted that mobility is underestimated in relaxation time approximation compared with the Rode's iterative approach.

Keywords: semiclassical transport, III–V semiconductor, electronic structure

 Supplementary material for this article is available [online](#)

(Some figures may appear in colour only in the online journal)

## 1. Introduction

III–V compound semiconductors such as GaAs, GaSb, AlAs, InP etc possessing direct band gap have drawn enormous attention of the scientific community over the past few decades because of their strong potential for application in high mobility electronic and high-performance optoelectronic devices [1–9]. As mentioned by Adachi *et al* [1] there have been avalanche of reports on the growth and development on III–V ternary and quaternary compound semiconductors [1–5] as they provide natural way of tuning the energy band gap and

the band structure. In case of ternary  $\text{AB}_x\text{C}_{1-x}$  compounds the band structure is strongly dependent on the alloy composition  $x$ . In order to exploit the application potential of a material in electronic transport devices such as field effect transistors, high electron mobility transistors it is essential to have a precise knowledge of its energy band dispersion, forbidden band gap, density of states and some other parameters such as phonon frequency, elastic constants, piezoelectric constants.

In an ideal, perfect periodic crystal there is no scattering of electrons. However, in real crystals, electrons are scattered due to lattice vibrations, presence of impurities, dislocations etc which determines the electron distribution function. We need to solve Boltzmann transport equation (BTE) to obtain

<sup>3</sup> Author to whom any correspondence should be addressed.

the electron distribution function which governs the electron transport properties viz. mobility, conductivity etc. Thus modeling of semi-classical electron transport through semiconductors hinges on the numerical solution of BTE [10–25].

Most of the available models for solving BTE employ relaxation time approximation (RTA) [12, 13, 16–22]. There are some semi-empirical models that considers input parameters viz. effective mass, band gap, polar optical phonon (POP) frequency, dielectric constant from experimental data for calculating the scattering rates [10–15]. In these type of models parabolic or Kane energy-momentum dispersion relation is considered. The relaxation time is assumed to follow a power law distribution of energy. However this basic assumption fails for inelastic scattering for which scattering rate does not satisfy such power law dependency on energy [10, 15, 20]. Moreover these models rely on the availability of experimental data, thereby limiting the predicting ability of these models for new materials. There are some other RTA models that rely on *ab initio* band structure [26, 27]. The basic assumptions of these models are consideration of the electron–phonon scattering to be elastic, the distribution function to be unchanged from its equilibrium form and relaxation time to be a constant (c-RTA). Madsen and Singh [27] have witnessed that this c-RTA models work good for materials having scattering rates moderately constant. However the over simplified assumptions of these models ruins the predictive power of these approaches.

The RTA models are suitable when the scattering mechanisms are elastic and isotropic, and as a consequence relaxation time becomes independent of the distribution function. POP scattering has significant influence on the distribution function at room temperature for polar III–V compounds [9, 28, 29]. In III–V compounds oscillating electric dipole is generated because of the movement of charged ions in the unit cell and the corresponding vibrational mode is known as the POP mode. The interaction of the conduction electron with POP is inelastic and nonrandomizing, making RTA inappropriate [10, 15, 20, 22] for describing transport phenomena of the III–V materials at room temperature. Rode’s iterative method [10, 15, 20–25] is an effective solution for the incorporation of POP scattering in order to simulate semi-classical transport phenomena of III–V materials.

In the present work we have calculated the mobility of *n*-type ternary compound AlGaAs<sub>2</sub>, with Al:Ga:As ratio being 1:1:2 using Rode’s iterative method. The input parameters viz. band dispersion, DOS, dielectric constant, deformation potential, POP frequency, wave function admixture, required for calculating different scattering rates have been calculated using density functional based approach in which the only input is the crystal geometry. In our previous work [30] we computed the mobility of *n*-type ZnSe using Rode-*ab initio* approach and observed good agreement with the experimental results. In this present work we have considered ternary AlGaAs<sub>2</sub> compounds having two distinct crystal structures. This paper aims to provide a comparison of electron mobility of the two ternary compounds having different atomic arrangement with same stoichiometry and predict the better one for high-speed electronic devices on the basis of electron mobility.

## 2. Methodology

### 2.1. Solution of BTE

Semi-classical transport calculations have been performed using our code AMMCR [31]. Brief methodology of solving the BTE is presented below.

Under the application of a low electric field  $E$ , BTE for the electron distribution function  $f$  is given by

$$\frac{df}{dt} + \mathbf{v}(\mathbf{k}) \cdot \nabla_{\mathbf{r}} f + \frac{e\mathbf{E}}{\hbar} \cdot \nabla_{\mathbf{k}} f = \left( \frac{\partial f}{\partial t} \right)_s \quad (1)$$

where  $\mathbf{v}(\mathbf{k})$  represents group velocity of electron and  $\left( \frac{\partial f}{\partial t} \right)_s$  denotes change in the distribution function due to all scattering processes.

Under steady state condition,  $\frac{df}{dt} = 0$ , and under the absence of thermal driving force (spatial homogeneity) the second term in equation (1) vanishes. Under these two conditions equation (1) can be rewritten as

$$\frac{e\mathbf{E}}{\hbar} \cdot \nabla_{\mathbf{k}} f = \int \{s(\mathbf{k}', k) f(\mathbf{k}') (1 - f(\mathbf{k})) - s(\mathbf{k}, \mathbf{k}') f(\mathbf{k}) (1 - f(\mathbf{k}'))\} d\mathbf{k}' \quad (2)$$

where  $s(\mathbf{k}', k)$  represents scattering rate for an electron making a transition from a state  $k$  to a state  $k'$ .

Due to the application of low electric field the distribution function is assumed (linear response) to get perturbed as follows

$$f(\mathbf{k}) = f_0[\varepsilon(\mathbf{k})] + xg(\mathbf{k}) \quad (3)$$

where  $f$  is the actual perturbed distribution function,  $f_0$  represents the equilibrium part of the distribution given by the Fermi–Dirac distribution function,  $g(\mathbf{k})$  is the perturbation part caused by the application of low electric field and  $x$  denotes the cosine of the angle between  $\mathbf{k}$  and the electric field. In order to calculate low-field electron transport properties we need to calculate the perturbation  $g(\mathbf{k})$ . For simplicity we expressed the energy of the electron in the conduction band as a function of distance  $k$  from the CBM. After performing some mathematical steps and assuming  $x = 1$ , BTE can be expressed to yield  $g(k)$  as follows

$$g_{i+1}(k) = \frac{S_i(g_i(k)) - \frac{eE}{\hbar} \frac{\partial f}{\partial k}}{S_0(k) + \frac{1}{\tau_{el}(k)}} \quad (4)$$

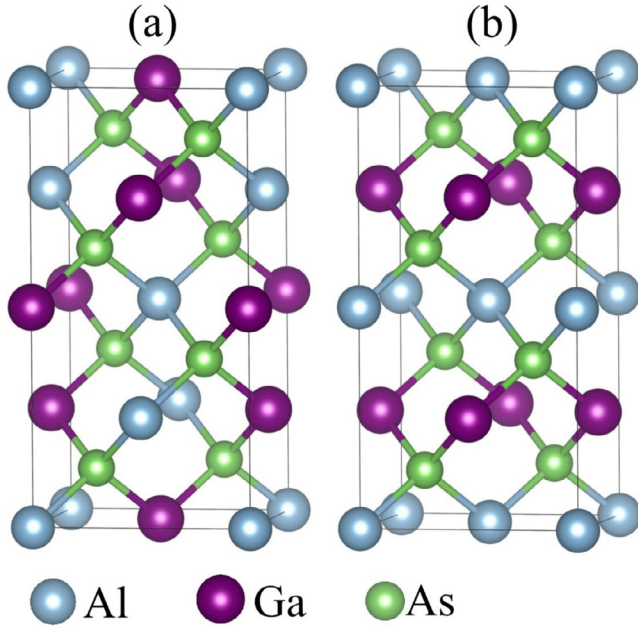
The scattering rates in equation (2) have two components; elastic part ( $s_{el}$ ) and the inelastic part ( $s_{in}$ ). i.e.  $s(\mathbf{k}, \mathbf{k}') = s(\mathbf{k}, \mathbf{k}')_{el} + s(\mathbf{k}, \mathbf{k}')_{in}$ .

$S_i, S_0, \tau_{el}$  appearing in equation (4) are given by

$$S_i(g_i(k)) = \int Xg_i(k') [s_{in}(k', k) (1 - f(k)) + s_{in}(k, k') f(k)] d\mathbf{k}' \quad (5)$$

$$S_0(k) = \int [s_{in}(k, k') (1 - f(k')) + s_{in}(k', k) f(k')] d\mathbf{k}' \quad (6)$$

$$\frac{1}{\tau_{el}} = \int (1 - X) s_{el}(k, k') d\mathbf{k}' \quad (7)$$



**Figure 1.** Conventional unit cell of AlGaAs<sub>2</sub>: (a) BCT phase, (b) TET phase. Blue, purple and green spheres respectively corresponds to Al, Ga and As atoms.

where  $X$  in equation (7) corresponds to the cosine of the angle between final and initial wave vectors.

$S_i$  and  $f$  are functions of  $g$ , hence equation (4) has to be solved iteratively using Rode's iterative method in order to get the converged value of  $g(k)$ . The two term  $S_i$ ,  $S_0$  deal with the inelastic POP scattering and the term  $\tau_{el}$  captures the effect of all the elastic scattering processes. According to Matthiessen's rule the total elastic scattering rate  $\frac{1}{\tau_{el}(k)}$  can be written as the sum of the momentum relaxation rates off all the scattering processes.

$$\frac{1}{\tau_{el}(k)} = \frac{1}{\tau_{ii}(k)} + \frac{1}{\tau_{pz}(k)} + \frac{1}{\tau_{ac}(k)} \quad (8)$$

where the subscripts  $ii$ ,  $pz$ ,  $ac$  respectively corresponds to the ionized impurity, piezoelectric, acoustic deformation potential scattering processes. It is worth mentioning here that independence of the scattering events is considered e.g. while calculating  $\tau_{ii}(k)$  we have only considered ionized impurity scattering and neglected all other scattering processes.

The rates of the different elastic scattering processes have been calculated in terms of electron group velocity and density of states as discussed in the literature [30–32]. Inelastic POP scattering rate has been calculated iteratively using Rode's iterative formalism details of which is presented in the previously published reports [30–32]. In our previous work [30] we have followed identical formalism for calculating low-field transport properties of  $n$ -ZnSe.

The carrier mobility has been computed using the following expression

$$\mu = \frac{1}{3E} \frac{\int v(\varepsilon) D_s(\varepsilon) g(\varepsilon) d\varepsilon}{\int D_s(\varepsilon) f(\varepsilon) d\varepsilon} \quad (9)$$

**Table 1.** Calculated material properties of AlGaAs<sub>2</sub> in both BCT and TET phases.

Parameters	AlGaAs <sub>2</sub> configurations	
	BCT	TET
Primitive lattice vectors	$a$ (Å)	7.03
	$b$ (Å)	7.03
	$c$ (Å)	5.74
Angle between primitive lattice vectors	$\alpha$ (°)	131.84
	$\beta$ (°)	131.84
	$\gamma$ (°)	70.48
$\varepsilon_0$	13.73	13.87
$\varepsilon_\infty$	11.56	11.71
$E_D$ (eV)	15.25	14.2
$E_g$ (eV)	0.99	0.86
$\omega_{po}$ (THz)	10.4	10.70
$c_l$ ( $10^{10}$ N m <sup>-2</sup> )	11.78	11.79
$c_t$ ( $10^{10}$ N m <sup>-2</sup> )	4.04	4.05
$P$	0.111	0.084
$\rho$ (gm cm <sup>-3</sup> )	4.33	4.33

$\varepsilon_0$  = low frequency dielectric constant,  $\varepsilon_\infty$  = high frequency dielectric constant,  $E_D$  = acoustic deformation potential,  $E_g$  = electronic band gap,  $\omega_{po}$  = polar optical phonon frequency for the longitudinal mode,  $c_l$  = longitudinal elastic constant,  $c_t$  = transverse elastic constant,  $P$  = dimensionless piezoelectric coefficient,  $\rho$  = density.

where  $D_s(\varepsilon)$  is the density of states. The group velocity of electron is calculated from *ab initio* band dispersion of the conduction band by using the following expression

$$v(k) = \frac{1}{\hbar} \frac{d\varepsilon}{dk}. \quad (10)$$

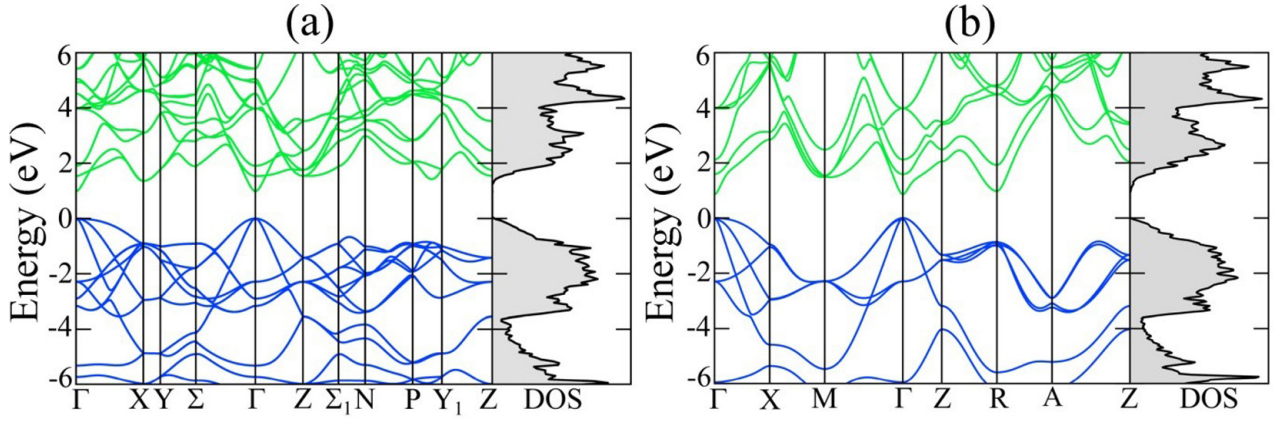
## 2.2. Ab initio inputs

Band structure and density of states of the ternary AlGaAs<sub>2</sub> compounds have been computed using density functional theory as implemented in Vienna *ab initio* simulation package (VASP) [33–35]. In order to calculate carrier velocities we have calculated the band structures using a highly dense  $k$  mesh around the conduction band minimum (CBM) and then we expressed the average electron energies for the conduction band as a function of distance  $k = |k|$  from the CBM. After performing the numerical fitting of the conduction band with a six degree polynomial we computed carrier group velocity using equation (10). This approach produces a smooth curve for mobility and has been reported earlier by Alireja *et al* [32]. For the carrier concentration ( $n$ ) we have considered the following equation

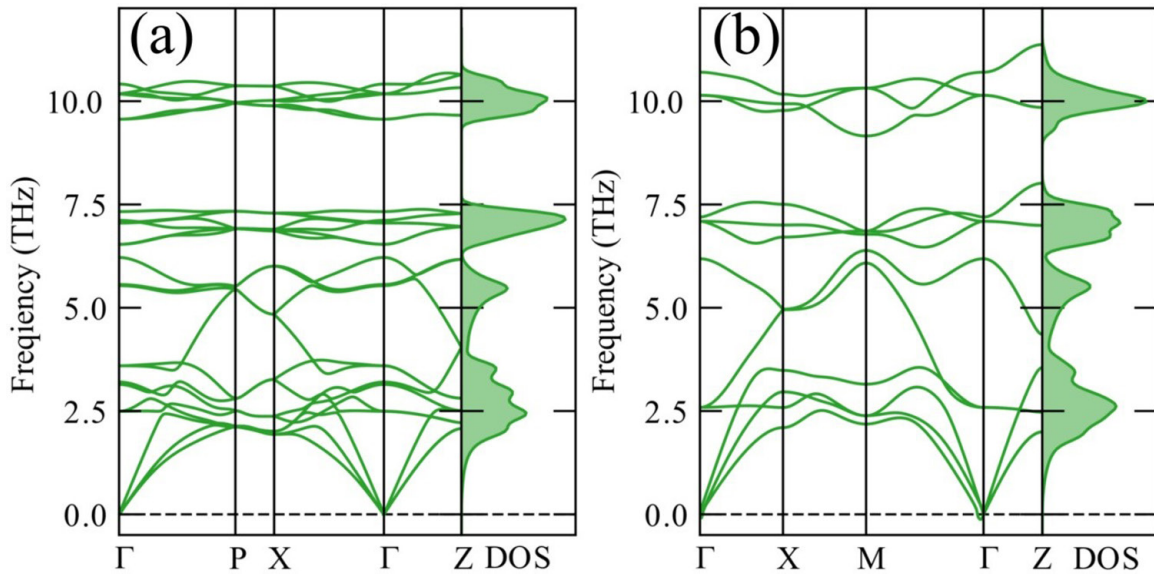
$$n = \frac{1}{V_0} \int_{\varepsilon_c}^{+\infty} D_s(\varepsilon) f(\varepsilon) d\varepsilon \quad (11)$$

where  $V_0$  is the volume of the relaxed unit cell. Fermi level for a given carrier concentration is computed by matching the concentration according to equation (11).

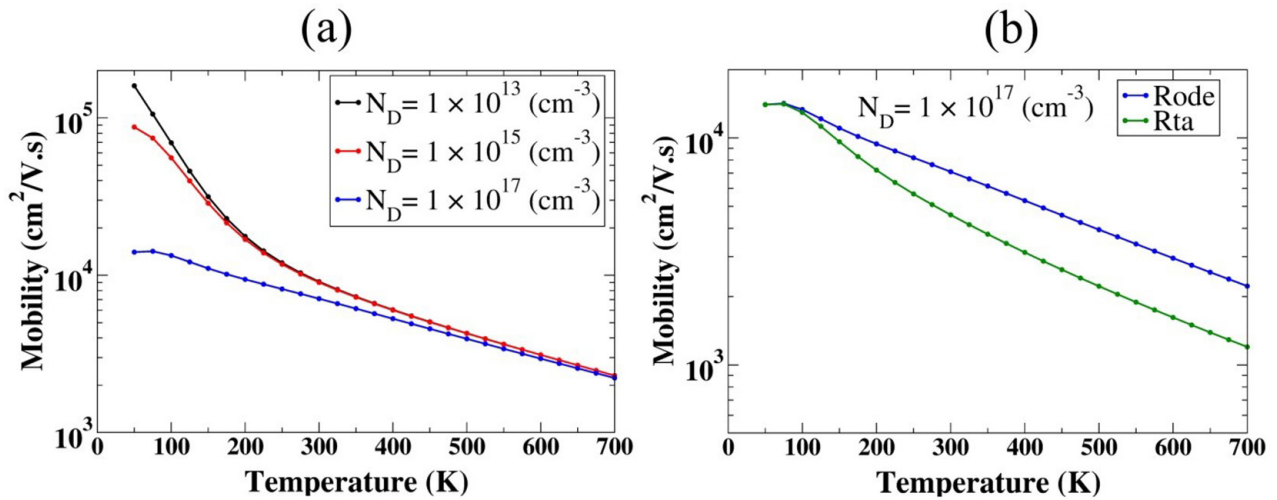




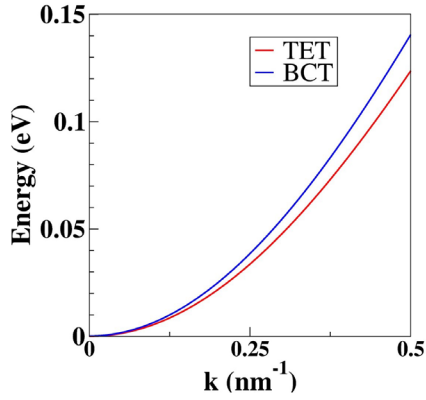
**Figure 2.** Band structure and density of states of AlGaAs<sub>2</sub>: (a) BCT-AlGaAs<sub>2</sub> (b) TET-AlGaAs<sub>2</sub>. Zero energy is set to valence band top. Density of states is in arbitrary unit.



**Figure 3.** Phonon dispersion of (a) BCT-AlGaAs<sub>2</sub> and (b) TET-AlGaAs<sub>2</sub>.



**Figure 4.** Variation of mobility with temperature for BCT-AlGaAs<sub>2</sub>. (a) shows the mobility versus temperature at different doping concentration with mobility computed using Rode's iterative method. The black, red and blue line indicates the corresponding plots for doping concentration  $1 \times 10^{13} \text{ cm}^{-3}$ ,  $1 \times 10^{15} \text{ cm}^{-3}$  and  $1 \times 10^{17} \text{ cm}^{-3}$ , respectively. (b) shows the comparison of mobilities calculated using Rode's method and RTA at the doping concentration  $1 \times 10^{17} \text{ cm}^{-3}$ . The blue line corresponds to the mobility estimated using Rode's method and the green line corresponds to RTA estimated mobility.



**Figure 5.** Energy of the electron in conduction band versus  $k$ -distance plot. Blue and the red line are respectively the corresponding plots for the BCT and TET phases.

For calculating deformation potential ( $E_D$ ) we calculated the changes in the CBM by changing the volume of the unit cell and calculated  $E_D$  using the following expression

$$E_D = -V \left( \frac{\partial E}{\partial V} \right) \bigg|_{V=V_0}. \quad (12)$$

We used density functional perturbation theory [36, 37] for calculating piezoelectric constants, low and high frequency dielectric constants, frequency of POPs as impediment in the VASP code. For obtaining elastic tensor, finite distortions of the lattice were considered and the elastic constants were derived from the stress–strain relationship [38]. The elastic tensor has been computed for both, fixed atoms, as well as performing relaxation of them. After obtaining the elastic matrix from VASP output, we used MechElastic [39] script to obtain the longitudinal and transverse elastic constants.

### 2.3. *Ab initio* computational details

We have considered ternary AlGaAs<sub>2</sub> compounds of two different crystal geometries. One of the configurations crystallizes in tetragonal (TET) lattice with space group type  $p\bar{4}m2$  (115). The other one crystallizes in body centered tetragonal (BCT) lattice with space group type  $I\bar{4}2d$  (122). We obtained the ternary structures through cation substitution in a GaAs supercell, using Site-Occupation Disorder package [40]. For geometry optimization and electronic structure calculation we have used DFT based approach as implemented in VASP code. We considered generalized gradient approximation (GGA) of Perdew, Burke, and Ernzerhof (PBE) [41] to approximate the exchange–correlation part. In order to describe the electron–ion interaction we have employed projector augmented wave (PAW) method [42]. We used conjugate-gradient method [43] for ionic relaxation. The Hellman–Feynman forces on the constituent atoms were minimized with the tolerance of 0.005 eV Å<sup>−1</sup>. For electronic structure calculation we have considered primitive unit cells. The lengths of the primitive basis vectors for the TET-AlGaAs<sub>2</sub> are  $a = b = 4.06$  Å and  $c = 5.74$  Å and the corresponding parameters for BCT-AlGaAs<sub>2</sub> are  $a = b = c = 7.03$  Å. Hence, we considered  $23 \times 23 \times 15$  and  $13 \times 13 \times 13$  Monkhorst–Pack [44]  $k$ -mesh for sampling

the Brillouin zones (BZ) of the TET and BCT configurations, respectively. In order to calculate group velocity of the electrons in the conduction band we performed band structure calculation with a high dense  $k$ -mesh around the CBM. In order to obtain phonon dispersion, we considered finite displacements of atoms in a  $3 \times 3 \times 3$  supercell and the force sets were obtained using Phonopy [45] code from VASP output.

## 3. Results and discussion

### 3.1. Electronic structure

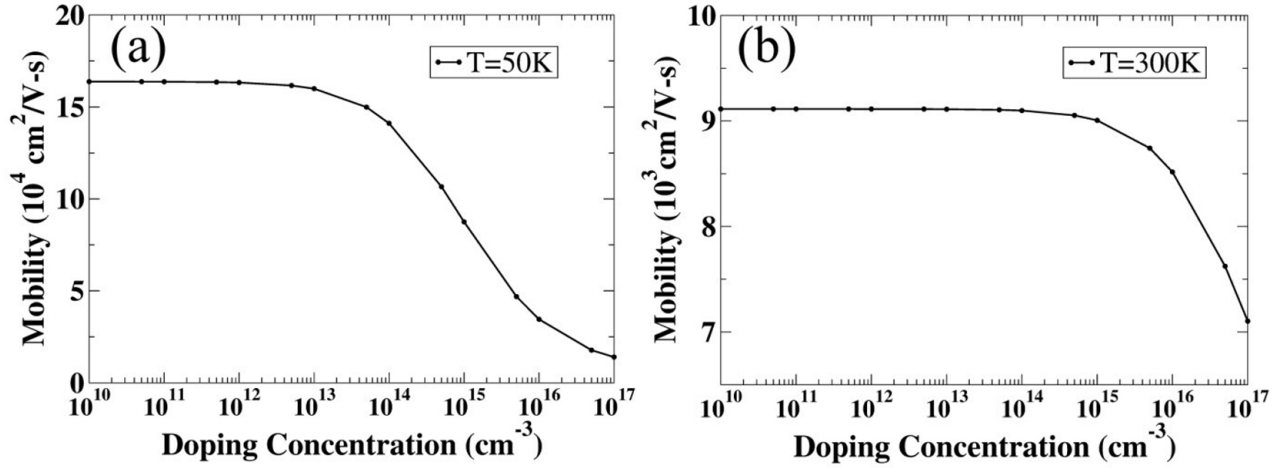
16 atom unit cell with Al:Ga:As ratio being 1:1:2 for the two phases is shown in figure 1. We consider primitive unit cells (figure S1 ([stacks.iop.org/JPhysCM/32/135704/mmedia](http://stacks.iop.org/JPhysCM/32/135704/mmedia)) of supplementary material) for electronic structure calculations. The primitive unit cells were obtained by imposing symmetry on the 16 atom unit cells as implemented in Phonopy code. The primitive unit cells of the TET and BCT phases consist of 4 and 8 atoms respectively. Optimized lattice parameters of the primitive cell and the angles between the primitive translation vectors are given in table 1. PBE estimated band structure for both the TET and BCT configurations predicts semiconducting nature. Both the configurations are found out to be direct band gap ( $E_g$ ) semiconductors with valence band maximum and CBM situated at the BZ centre (figure 2). PBE estimated band gap values for the TET and BCT configurations are found out to be 0.99 eV and 0.86 eV. We have analyzed atom and orbital projected DOS (figure S2) in order to investigate the contribution of different atoms and orbitals on the valence and conduction bands. For both the TET and BCT configurations we observed that As- $p$  states has the dominant contribution to the valence band. However, the major contribution in the conduction band is coming from Ga- $s$  and As- $p$  states.

### 3.2. Stability

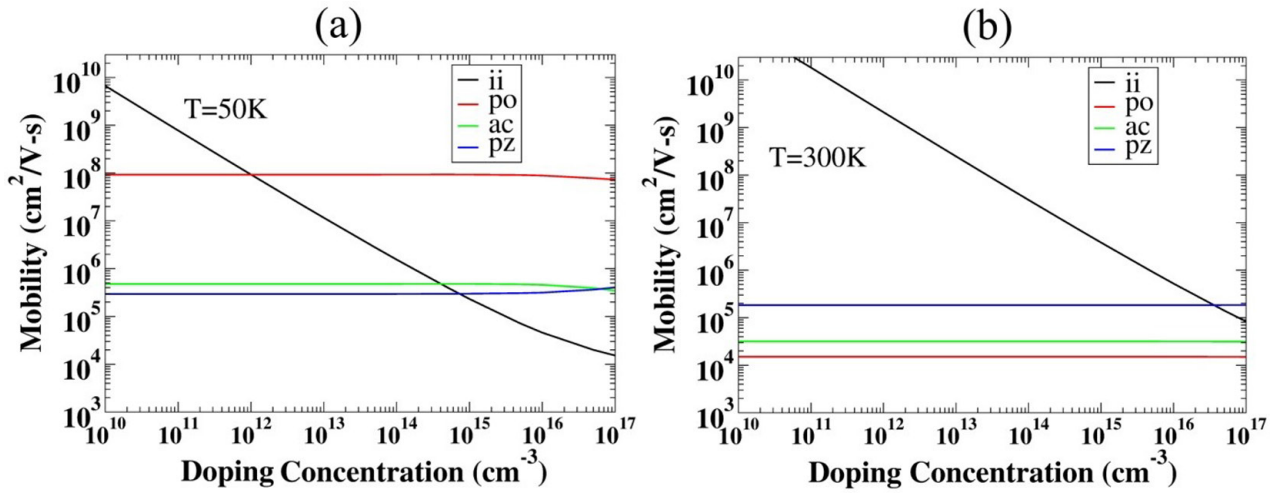
In order to analyze dynamical stability of the two configurations we have plotted the phonon dispersion in figure 3. No imaginary frequency has been observed for the BCT phase. However, for the TET phase imaginary frequency of magnitude less than 4 cm<sup>−1</sup> has been observed around the BZ centre. This small imaginary acoustic phonon appearing near the zone center do not correspond structural instability. The negligible imaginary frequency of the acoustic mode is a numerical error, arising due to violation of translational invariance in approximated calculation [46, 47]. The phonon dispersion plots, hence confirms the structural stability of the both the phases.

We have studied mechanical stability of the two phases using Born stability criteria [48]. The necessary stability criteria for tetragonal systems are given by

- (i)  $C_{11} - C_{12} > 0$
- (ii)  $2C_{13}^2 < C_{33}(C_{11} + C_{12})$
- (iii)  $C_{44} > 0$



**Figure 6.** Variation of mobility with doping concentration at (a)  $T = 50$  K and (b)  $T = 300$  K for BCT-AlGaAs<sub>2</sub>.



**Figure 7.** Contribution of different scattering mechanism to the mobility for BCT-AlGaAs<sub>2</sub> at (a)  $T = 50$  K and (b)  $T = 300$  K. The contributions from the ionized impurity, POP, acoustic deformation potential and piezoelectric scatterings are indicated by the black, red, green, and blue lines, respectively.

- (iv)  $C_{66} > 0$
- (v)  $2C_{16}^2 < C_{66}(C_{11} - C_{12})$

Coefficients of the elastic matrix  $C_{ij}$  obtained with DFT-PBE calculations for both phases have been found to satisfy all the above mentioned criteria, thereby suggesting their mechanical stability.

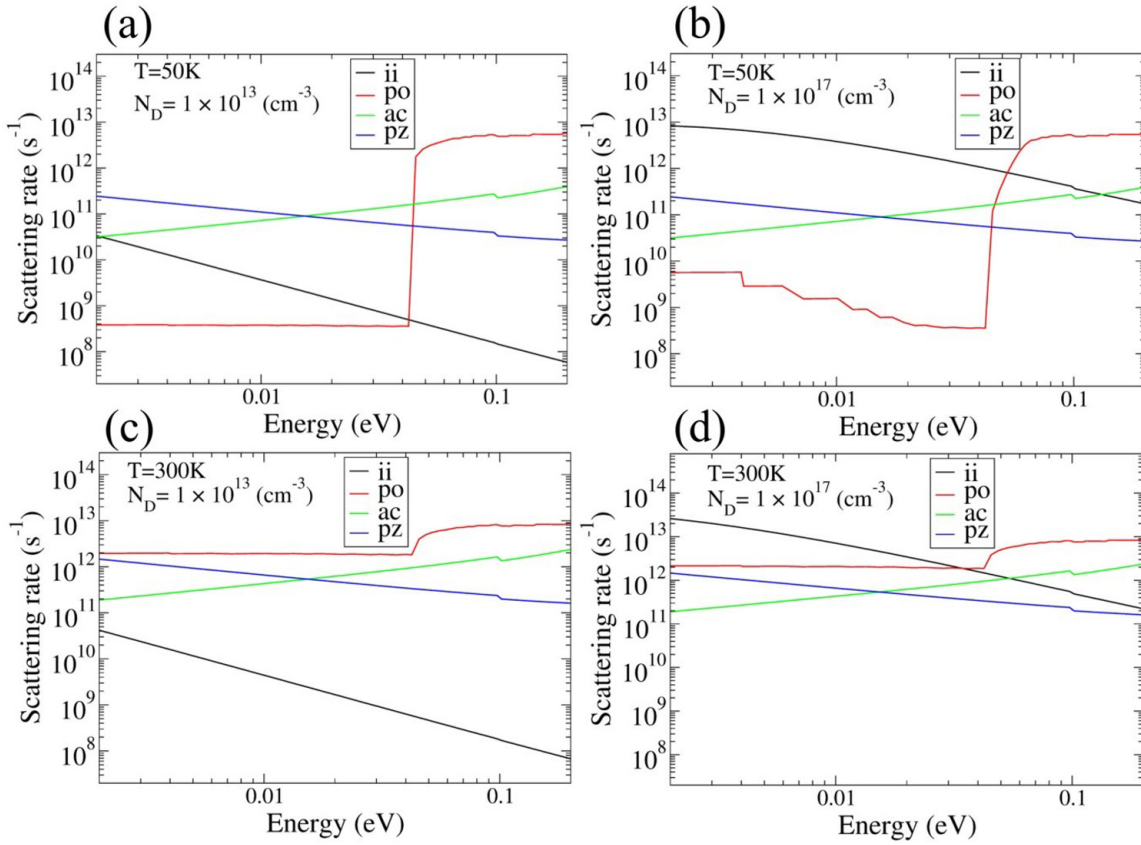
### 3.3. Transport properties

**3.3.1. Mobility versus temperature.** The variation of mobility versus temperature for different carrier concentration is shown in figure 4 for the BCT configuration. Mobility continuously decreases with temperature as expected. Mobility values do not differ much for low carrier concentration viz.  $1 \times 10^{13} \text{ cm}^{-3}$  and  $1 \times 10^{15} \text{ cm}^{-3}$ . This is because of the fact that at low carrier concentration ionized impurity is less significant. Figure 4(b) shows the comparison of mobility estimated using RTA method and Rode's scheme. In RTA approach the mobility is underestimated. This is attributed to the fact that, POP scattering is inelastic and nonrandomizing and hence the

perturbation in the distribution function using relaxation time (either constant or power law dependency on energy) cannot be defined. At low temperature POP scattering become insignificant, as a result of which mobility estimated using RTA and Rode's iterative method become almost equal. The variation of mobility with temperature for the TET is given in figure S3 which shows similar trend as that of the BCT phase. Comparing the mobility for the TET and BCT configurations at a carrier concentration of  $1 \times 10^{17} \text{ cm}^{-3}$  (figure S4) we observed that the BCT configuration shows higher mobility as compared with the TET configuration for the entire range of temperature. In figure 5 we have plotted the average energy of electron for the conduction band versus the  $k$ -distance from the CBM for both the configurations. The curvature of the  $E$ - $k$  curve for the BCT is higher as compared with the TET, and this attributes to the higher mobility of the BCT structure.

**3.3.2. Mobility versus carrier concentration.** In figure 6 we have plotted the variation of mobility with doping concentration ( $n$ ) at 50 K and 300 K temperature for the BCT configuration. We have observed that for both of the configurations mobility





**Figure 8.** Scattering versus electron energy plot for BCT-AlGaAs<sub>2</sub> at (a)  $T = 50$  K and doping concentration =  $1 \times 10^{13} \text{ cm}^{-3}$  (b)  $T = 50$  K and doping concentration =  $1 \times 10^{17} \text{ cm}^{-3}$  (c)  $T = 300$  K and doping concentration =  $1 \times 10^{13} \text{ cm}^{-3}$  (d)  $T = 300$  K and doping concentration =  $1 \times 10^{17} \text{ cm}^{-3}$ .

does not change significantly for  $1 \times 10^{10} \leq n \leq 1 \times 10^{13}$  at  $T = 50$  K and  $1 \times 10^{10} \leq n \leq 1 \times 10^{15}$  at  $T = 300$  K. At  $T = 50$  K/300 K when  $n$  is increased beyond  $10^{13}/10^{15} \text{ cm}^{-3}$  mobility starts decreasing. In order to gain an insight we have analyzed the variation of different components of mobility with doping concentration. According to Matthiessen's rule

$$\frac{1}{\mu} = \frac{1}{\mu_{ii}} + \frac{1}{\mu_{po}} + \frac{1}{\mu_{ac}} + \frac{1}{\mu_{pz}} \quad (13)$$

where  $\mu$  is the total mobility and the suffixes *ii*, *po*, *ac*, *pz* are used to indicate ionized impurity, POP, acoustic deformation potential, piezoelectric scattering mechanism.  $\mu_{ii}$  is the mobility of the material considering only the ionized impurity scattering mechanism;  $\mu_{po}$  is the mobility, if the scattering occurs only through POP scattering mechanism and so on.  $\mu_{po}$ ,  $\mu_{ac}$  and  $\mu_{pz}$  almost remains constant for the entire range of doping concentration where as  $\mu_{ii}$  strongly depends on  $n$ , as is evident from figure 7 for the BCT configuration. As the different components appears in reciprocals in equation (13), the component showing the smallest value is the most significant one. At  $T = 50$  K, the dominant contributions comes from  $\mu_{ac}$ ,  $\mu_{pz}$  for  $n \leq 1 \times 10^{13} \text{ cm}^{-3}$ . For  $n \geq 1 \times 10^{13} \text{ cm}^{-3}$ ,  $\mu_{ii}$  becomes comparable with  $\mu_{ac}$  and  $\mu_{pz}$ .  $\mu_{ii}$  is a decreasing function of  $n$  hence  $\mu$  starts decreasing when  $n$  is increased beyond  $1 \times 10^{13} \text{ cm}^{-3}$ . At  $T = 50$  K,  $\mu_{ii}$  has the dominant contribution to the total mobility for  $n \geq 1 \times 10^{15} \text{ cm}^{-3}$ .  $\mu_{po}$  is very high at

$T = 50$  K indicating the fact that POP scattering is insignificant in low temperature. At  $T = 300$  K, POP scattering is significant and has the dominant contribution in mobility. Figure 7 also indicates that at high temperature and high doping concentration  $\mu_{pz}$  become less significant. We have observed similar trend for the TET phase (figures S5 and S6).

**3.3.3. Scattering rates.** In order to have a better understanding of the observed transport properties we have analyzed scattering rates of different mechanisms at different temperature and carrier concentrations. Figure 8 shows the scattering rate versus electron energy plots for the BCT configuration. We observe that all the scattering rates increases when the temperature rises. At low temp and low doping concentration piezoelectric scattering dominates in the low energy region (figure 8(a)). At  $T = 50$  K, the average electron energy is roughly  $\frac{3}{2}kT = 0.0064 \text{ eV}$ . Hence piezoelectric scattering has been observed to have dominant contribution in the mobility at low temperature and low doping concentration. On the other hand POP energy is  $\hbar\omega_{PO} = 0.04 \text{ eV}$ . At  $T = 50$  K most of the electrons are in low energy region, making POP insignificant. At low temperature there is a predominant jump in the POP scattering rate. It is because of the fact that if the energy of an electron is less than  $0.04 \text{ eV}$  then it can be scattered only by absorption of an optical phonon. But, if electron energy is greater than  $0.04 \text{ eV}$  then scattering process involve

both emission and absorption of POPs. POP scattering rate increases at  $T = 300$  K and has the dominant contribution in the total mobility. Piezoelectric scattering rate also increases when temperature increases from 50 K to 300 K but POP scattering rate suppresses it, thereby making it insignificant at higher temperature. When the temperature is 50 K but the doping concentration increases, ionized impurity scattering rates is also found to increase and suppresses the contribution from piezoelectric scattering as is evident from figure 8(b) for  $n = 1 \times 10^{17} \text{ cm}^{-3}$ . The scattering rates of the TET configuration show similar behaviour (figure S7).

## 4. Conclusion

We have computed electron mobility of  $n$ -type AlGaAs<sub>2</sub> using Rode's iterative method with transport parameters calculated from DFT based approach. We have considered two different geometries of AlGaAs<sub>2</sub>, viz. BCT-AlGaAs<sub>2</sub> and TET-AlGaAs<sub>2</sub>. Both the TET and BCT phases are direct band gap semiconductors having PBE estimated band gap of 0.99 eV and 0.86 eV, respectively. Absence of mode with imaginary frequency in the phonon dispersions for both the phases confirms their stability. We have observed that the curvature of energy versus  $k$ -distance curve is higher for the BCT phase compared with the TET phase which results in higher electron mobility in the BCT phase than the TET phase. Therefore we can predict that the BCT phase will be more suitable for high mobility device applications as compared with the TET phase. We notice that piezoelectric scattering dominates in the low temperature and low doping concentration situation. At high doping concentration contribution from ionized impurity scattering significantly increases which suppresses the piezoelectric scattering contribution. Moreover we have also noted that at low temperature POP scattering is insignificant, however at room temperature POP scattering dominates.

## ORCID iDs

Bhaskaran Muralidharan  <https://orcid.org/0000-0003-3541-5102>

Satadeep Bhattacharjee  <https://orcid.org/0000-0002-6717-2881>

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