A First-principles study on the impact of doping and vacancies in $\beta - Ga_2O_3$

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Abstract

Ga_2O_3 is a wide band gap semiconductor, allowing us to operate at larger voltages than its better-known competitors Sic and GaN. The project deals with first print- caplet DFT based modelling and investigation on the performance by the impactof various structural phases, number of layers and impact of doping and impu- reties on Ga_2O_3. The advantage of using hybrid functions in the first principal calculations over the DFT based calculations is observed. Gallium oxide has low conductivity compared to other semiconductor devices due to its large band gap.In this project we try to analyses the ballistic conduction in the semiconductor channel. Ballistic transport means transport of carriers over long distances in the channel without any scattering. Lindauer's approach allows to analyze about transport of carriers in semiconductor materials. By using this approach, we can find the number of modes or channels contributing for current flow in the channel.If many channels conduct, we get the maximum ballistic conduction which meansthe maximum current density of the device. The project analyses the variation of ballistic conductance by moving from bulk to 2D layers on $\beta - Ga_2O_3$ and by different dopants on gallium oxide.

1. Related work

According to L. Chen [1] Gallium oxide (Ga2O3) is an emerging wide bandgap semiconductor that has attracted a large amount of interest due to its ultra-large bandgap of 4.8 eV, a high breakdown field of 8 MV/cm, and high thermal stability. These properties enable Ga2O3 a promising material for a large range of applications, such as high-power electronic devices and solar-blind ultraviolet (UV) photodetectors. In the past few years, a significant process has been made for the growth of high-quality bulk crystals and thin films and device optimizations for power electronics and solar blind UV detection. However, many challenges remain, including the difficulty in p-type doping, a large density of unintentional electron carriers and defects/impurities, and issues with the device process (contact, dielectrics, and surface passivation), and so on. The purpose of this article is to provide a timely review on the fundamental understanding of the semiconductor physics and chemistry of Ga2O3 in terms of electronic band structures, optical properties, and chemistry of defects and impurity doping. Recent progress and perspectives on epitaxial thin film growth, chemical and physical properties of defects and impurities, p-type doping, and ternary alloys with In2O3 and Al2O3 will be discussed

According to Mohi Uddin Jewel Ultrawide [2] bandgap gallium oxide (Ga2O3) is a promising material for power semiconductor devices and deep ultraviolet (UV) solar-blind photodetectors. Understanding the properties of point defects in Ga2O3 is necessary to realize better-performing devices. A comprehensive study based on density functional theory (DFT), using the generalized gradient approximation (GGA): Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional, of point defects in corundum (α), monoclinic (β), and orthorhombic (ε) phases of Ga2O3 is presented. The point defects include vacancies, interstitials, antisites, and extrinsic impurities in various phases of Ga2O3. Defect formation energies, charge transition energy levels, and defect concentrations variation with temperature are listed and presented under both gallium-rich (Ga-rich) and oxygen-rich (O-rich) growth conditions. The formation energy diagrams predict that the Ga2O3 phases favor the formation of Ga and O vacancies and the incorporation of extrinsic impurities. The calculations also show that the charge transition levels are deep inside the bandgap regardless of the Ga2O3 phase and

growth environment. The impacts of temperature on the intrinsic point defects are analyzed by probing the vibrational modes of β-Ga2O3 thin films grown in a metal-organic chemical vapor deposition (MOCVD) system at 700 oC temperature and annealed at 1100 oC in an O-rich environment.
According to R. Anvari [3] It is known that the terminating polymorph native oxide is responsible for the chemical reactivity and pH sensitivity of the AlGaN/GaN heterostructure-based chemical sensor. Surprisingly, the details of the role of the surface Ga2O3 in the behaviour of GaN-capped AlGaN/GaN based chemical sensors remains largely unknown. In addition, there is a discrepancy in the reported experimental data for the effect of thermally grown surface Ga2O3 on the channel electron density and the channel conductivity of AlGaN/GaN heterostructure based electronic devices. The aim of this thesis is to explore the role of the most energetically favorable surfaces of the crystalline phase Ga2O3 in the sensing mechanism of the AlGaN/GaN heterostructure-based chemical sensors in aqueous solutions. To achieve this goal, different levels of abstraction and various theoretical tools are used to study the effect of the hydration, equilibration with aqueous solutions, thickness, interfacial defect density as an indication of the material quality and chemical stability of two of the energetically favorable surfaces of Ga2O3.
According to J. Zhang [4] the discovery of two-dimensional (2D) Ga2O3 has provided an efficient way to design high performance Ga2O3 devices. Here, mechanical and thermodynamic properties of 2D Ga2O3 are important parameters in device design but very few studies are investigated by density functional theory. Results show that 2D Ga2O3 retains the monoclinic character with thirteen independent elastic constants which meet with the mechanical stability criteria, and irrespective of its thickness. Interestingly, although the elastic constant C11 is lower than C22 and C33, 2D Ga2O3 may be harder to be compressed along a direction. Meanwhile, the elastic constant C44 is larger than C55 and C66, in contrast to that of bulk β-Ga2O3. Upon decreasing the thickness of 2D Ga2O3, the elastic properties continue reduce and lower than those of 2D layered materials, but their compressive anisotropic properties are enhanced and larger than those of bulk β-Ga2O3. The thermal conductivity and capacity of monolayer Ga2O3 are enhanced to 0.49 W·cm−1 ·K−1, and 27.58 J·mol−1 ·K−1, respectively. Such variations of bulk-transition-2D Ga2O3 are opposite to those of bulk-transition-2D GaN due to the recombined orbitals of GaN. These results are crucial to the device design based on 2D Ga2O3.
According to Z. Zhang [5] A novel 2D Ga2O3 monolayer was constructed and systematically investigated by first-principles calculations. The 2D Ga2O3 has an asymmetric configuration with the quintuple-layer atomic structure, the same with the well-studied α-In2Se3, and is expected to be experimentally synthesized. The dynamic and thermodynamic calculations show excellent stability properties for this monolayer material. The relaxed Ga2O3 monolayer has an indirect band gap of 3.16 eV, smaller than that of β-Ga2O3 bulk, and shows tunable electronics and optoelectronics properties with biaxial strain engineering. An attractive feature is that the asymmetric configuration spontaneously introduces an intrinsic dipole and thus the electrostatic potential difference between the top and bottom surfaces of Ga2O3 monolayer, which helps to separate photon-generated electrons and holes within the quintuple-layer structure. By applying compressive strain, the Ga2O3 monolayer can be converted to a direct band gap semiconductor with a wider gap reaching 3.5 eV. Also, enhancement of hybridization between orbitals leads to the increase of electron mobility, from the initial 5000 cm2V-1s-1 increasing to 7000 cm2V-1s-1. Excellent optical absorption ability is confirmed, which can be effectively tuned by strain engineering. With the superior stability, as well as the strain-tunable electronic properties, carrier mobility and optical absorption, the studied novel Ga2O3 monolayer sheds light on low-dimensional electronic and optoelectronics device applications.
According to M. J. Tjader [6] β-gallium oxide (β-Ga2O3) and hexagonal boron nitride (h-BN) heterostructure-based quasi-two-dimensional metal-insulator-semiconductor field-effect transistors (MISFETs) were demonstrated by integrating mechanical exfoliation of (quasi)-two-dimensional (2D) materials with dry transfer process, where nano-thin flakes of β-Ga2O3and h-BN were utilized as the channel and gate dielectric, respectively, of the MISFET. The h-BN dielectric, which has extraordinary flat and clean surface, provides a minimal density of charged impurities on the interface between β-Ga2O3 and h-BN, resulting in superior device performances (maximum transconductance, on/off ratio,

subthreshold swing, and threshold voltage), compared with the conventional back-gated configurations. Also, double-gating of the fabricated device was demonstrated by biasing both top and bottom gates, achieving the modulation of the threshold voltage. This heterostructure wide bandgap nanodevice shows a new route toward stable and high-power nano-electronic devices.

According to G. Kresse [7] The formal relationship between ultrasoft (US) Vanderbilt-type pseudopotentials and Bloch's projector augmented wave (PAW) method is derived. It is shown that the total energy functional for US pseudopotentials can be obtained by linearization of two terms in a slightly modified PAW total energy functional. The Hamilton operator, the forces, and the stress tensor are derived for this modified PAW functional. A simple way to implement the PAW method in existing plane-wave codes supporting US pseudopotentials is pointed out. In addition, critical tests are presented to compare the accuracy and efficiency of the PAW and the US pseudopotential method with relaxed core all electron methods. These tests include small molecules (H2, H2O, Li2, N2, F2, BF3, SiF4) and several bulk systems (diamond, Si, V, Li, Ca, CaF2, Fe, Co, Ni). Particular attention is paid to the bulk properties and magnetic energies of Fe, Co, and Ni.

According to L. Dong [8] The structural, electronic, and optical properties of β-Ga2O3 with oxygen vacancies are studied by employing first-principles calculations based on density function theory. Based on the defect's formation energies, we conclude the oxygen vacancies are most stable in their fully charge states. The electronic structures and optical properties of β-Ga2O3 are calculated by Generalized Gradient Approximation + U formalisms with the Hubbard U parameters set 7.0 eV and 8.5 eV for Ga and O ions, respectively. The calculated bandgap is 4.92 eV, which is consistent with the experimental value. The static real dielectric constants of the defective structures are increased compared with the intrinsic one, which is attributed to the level caused by the Ga-4s states in the bandgap. Extra peaks are introduced in the absorption spectra, which are related to Ga-4s and O-2p states. Experimentally, β-Ga2O3 films are deposited under different O2 volume percentage with ratio-frequency magnetron sputtering method. The measured results indicate that oxygen vacancies can induce extra emission peaks in the photoluminescence spectrum, the location of these peaks are close to the calculated results. Extra O2 can increase the formation energies of oxygen vacancies and thus reduce oxygen vacancies in β-Ga2O3.

According to Y. Zhang [9] Recent fundamental advances in the density-functional theory of electronic structure are summarized. Emphasis is given to four aspects of the subject: (*a*) tests of functionals, (*b*) new methods for determining accurate exchange-correlation functionals, (*c*) linear scaling methods, and (*d*) developments in the description of chemical reactivity

According to P. De´ak [10] Defects influence the electronic and optical properties of crystals, so their identification is crucial to develop device technology for materials of micro-/optoelectronics and photovoltaics. The identification requires the accurate calculation of the electronic transitions and the paramagnetic properties of defects. The achievable accuracy is strongly limited in the case of the (semi)local approximations to density functional theory, because of the underestimation of the gap and of the degree of localization. In the past two decades, hybrid functionals, mixing semi local and nonlocal exchange semi empirically, have emerged as an alternative. Very often, however, the parameters of such hybrids have to be tuned from material to material. In this paper, we describe the theoretical foundations for the proper tuning and show that if the relative positions of the band edge states are well reproduced, and the generalized Koopmans's theorem is fulfilled by the given parameterization, the calculated defect levels and localizations can be very accurate. As demonstrated here, this can be achieved with the two-parameter Heydt-Scuderia-Brinkerhoff hybrid, HSE(α,μ) for diamond, Si, Ge, TiO2, GaAs, CuGaS(Se)2, GaSe, GaN, and Ga2O3. The paper describes details of the parameterization process and discusses the limitations of optimizing HSE functionals. Based on the gained experience, future directions for improving exchange functionals are also provided.

2. Introduction

Gallium oxide (Ga2O3) is evolving as a feasible candidate for certain classes of power electronics and opto-electronics, due to its ultra-large band gap (4.4-4.9eV). Photo detectors based on Ga2O3 have the cutoff wavelength range of 250–280nm, which meets the requirements for detection over a deep ultra-

violet (DUV) region and can be seen as an emerging star in the field of solar-blind UV photo detectors. The theoretical critical field strength (Ec) of Ga2O3 is 8 MV/cm and value of Baliga figure of merit (BFOM) is over 3000, which is very high than other WBG semiconductors like GaN, SiC. This makes it as a promising candidate in future power electronic applications. There are 5 polymorphs of Ga2O3, namely α, β, γ, δ and ε. Among which, the monoclinic (β) phase of Ga2O3 denotes the most stable, most widely studied and utilized the project deals with the first principles study on the structure and electronic properties of this β − Ga2O3. Although it has high breakdown voltage and high band gap, but it has an intrinsic mobility which is less than GaN and SiC . It also gives a low hole mobility which makes it difficult to get p-type conductivity. Many theories have shown that 2D materials performance are dependent on their thickness. Therefore, we look forward in this project on how performance of gallium oxide can be improved by moving to 2D β − Ga2O3 layers and effect of different dopants on bulk gallium oxide.

3. Objective and Scope

The project aim is to achieve the following:

1.A study on the optimal conditions for generating maximum ballistic drive current in β − Ga2O3 FETs.

2.Study on the impact of doping and vacancies in β − Ga2O3

3.1 High electric field breakdown and BFOM:

The electric field in the depletion region of semiconductors can become extremely high when a high voltage is applied. Even in a pure semiconductor, current willflow when the applied electric field reaches the critical value *Ec*, then system will have experience electrical breakdown ultimately failure of device. So, the amount of electricity required to convert an insulator to a conductor is called theBreakdown voltage (*Ec*). The breakdown voltage determines how much power the device can handle. The higher the breakdown voltage, more power the device canhandle.

The band gap of the semiconductor is related to the electrical breakdown value.The graph obtained by using this condition as shown in Fig. 1.1 and we can observe the theoretical value breakdown field of around 8MV/cm assuming the band gapof Ga_2O_3 From the figure we can observe, the breakdown field for diamond is around 10MV/cm indicating Diamond has more band gap thanGa_2O_3.

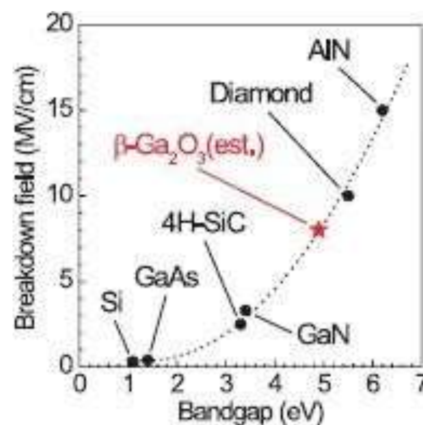


Figure 2.1: Breakdown Field variation with Band gap

The universal relationship that can be used for finding the breakdown voltage is in the form of $E_c = a (E_G)^n$ with the coefficient a and index n (a and n have a fixed values for direct and indirect materials) The band gap and breakdown field strength are related exponentially, so small increase in band gap increases the Breakdown field strength largely For the output of power semiconductor devices, several FOM (Figure of Merit) methods have been defined which are helpful to identify the device performance. High FOM numbers indicate good performance of devices. One such metric is pro- posed by Baliga, is the Baliga figure of merit (BFOM) which indicates minimizing conduction losses. Higher the value less will be the losses

3.2 Ga_2O_3 compared to other semiconductors:

Other large band gap semiconductors such as GaN and SiC are currently in use. However, how do we decide the right technology to invest in? We're particularly interested in Ga_2O_3 because of its large band gap and high electric breakdown field strength as compared to other materials as seen from Table 2.2

Material Parameter	Si	GaAs	4H-SiC	GaN	Diamond	β-Ga_2O_3
Bandgap E_g (eV)	1.14	1.43	3.25	3.4	5.5	4.8
Dielectric constant ε	12	13	10	9	5.5	11
Breakdown field E_C (MV/cm)	0.3	0.4	2.5	3.3	10	8
Carrier mobility μ (cm^2/(V s))	1450	8400	1000	1200	2000	300
Saturation velocity v_{sat} (10^7 cm/s)	1	1.2	2	2.5	1	2
Thermal conductivity κ (W/cmK)	150	50	370	250	2000	10–30
FOM relative to Si						
Baliga FOM = $\varepsilon\mu E_c^3$	1	14.7	317	846	24 660	3200
Johnson FOM = $E_c^2 v_{sat}^2/4\pi^2$	1	1.8	278	1089	1110	2844
Baliga High Frequency FOM = μE_c^2	1	10	46	100	1500	142
Keyes FOM = $\kappa[(cv_{sat})/(4\pi\varepsilon)]^{1/2}$	1	0.3	3.6	1.8	41.5	0.2

Figure 2.2: Properties of Ga_2O_3 relative to some other major semiconductors considering their different kinds of FOM

The high breakdown field of gallium oxide as discussed in Section 2.1 com- pared to others, shows its applications in high voltage and high-power devices like aircrafts, solar cells etc. High BFOM indicating minimal losses as discussed in Section 2.1. Seeing from the table Diamond and AlN are better than gallium oxide but gallium oxide is advantageous from them in terms of low cost. All other FOMs except Keyes of Ga_2O_3 is significantly higher than that of SiC and GaN because of its very low thermal conductivity. So, gallium oxide has been in interest for high voltage applications.

4. Results

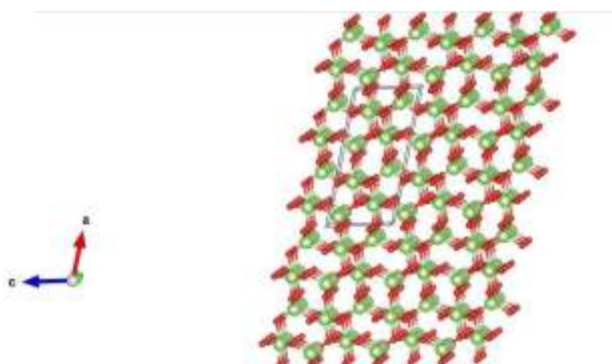


Figure 4.1: Crystal Structure of $\beta - Ga_2O_3$

A unit cell when repeated in all the three dimensions gives us a crystalline solid. The above Fig 4.1 is the crystal lattice structure of $\beta - Ga_2O_3$. The box representing in the lattice is the unit cell of $\beta - Ga_2O_3$ as shown in Fig 4.2. Aunit cell possesses same properties as of bulk since it is the repeating unit. So whenwe give a unit cell of a material, what the DFT engine solves is a repetition of the unit cell in all the three directions, which basically means that it simulates bulk Fig 4.1. So we can simulate a unit cell for the finding electronic properties or create super cells for more improved accuracy. As discussed in the modelling layers section, the crystal structure is cleaved along (100) surface plane for getting 2D materials which are shown in Fig4.3.

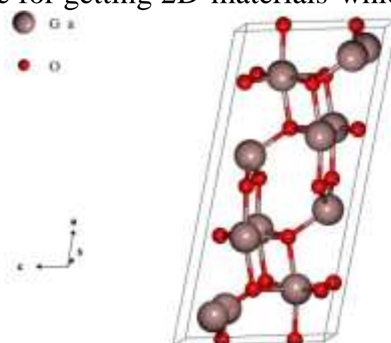


Figure 4.2: Unit cell of $\beta - Ga_2O_3$

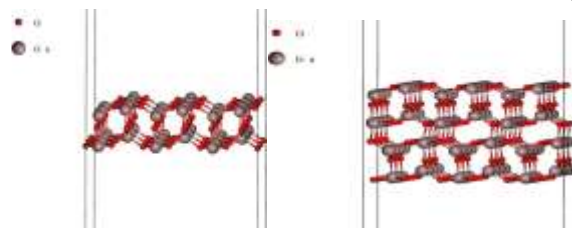


Figure 4.3: Crystal structures of Monolayer and Bilayer of $\beta - Ga_2O_3$

Monolayer as mentioned, is reduced to half of the unit cell size with mini- mum possible layer thickness. When moving from mono to bi means placing a monolayer on top of other gives bilayer similarly placing another layer on bilayer gives Tri layer and so on to get the bulk as shown in Fig 5.4. Defining a primitive lattice in reciprocal gives Brillouin zone. k-points are the sampling points in the first Brillouin zone. Brillouin zones are used to describe and analyze the electron energy in energy band structure of crystals.By the DFT calculations, the obtained electronic Band structure of $\beta - Ga_2O_3$ the E vs k along the high symmetric points Z-Γ- A-M-L[4] are From Figure we can observe the conduction band minimum and valence band maximum are at different momentum indicating a gallium oxide as an indirect semiconductor of band gap 4.8453eV with Γ cen- tered origin in the band structure. From the band structure of bulk $\beta - Ga_2O_3$, the conduction-band minimum is located at the Γ point, while the valence-band max-imum is located off Γ, we can say it is an indirect semiconductor whose calculatedvalue of B.G = 4.84eV in acceptance with the theoretical value.

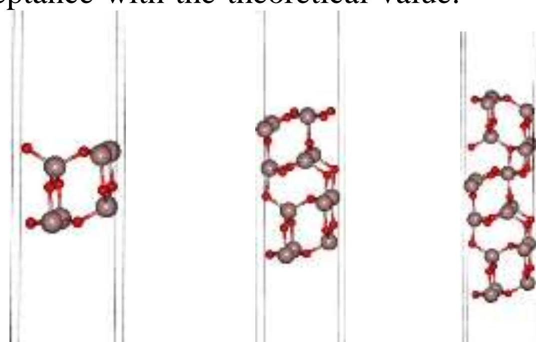


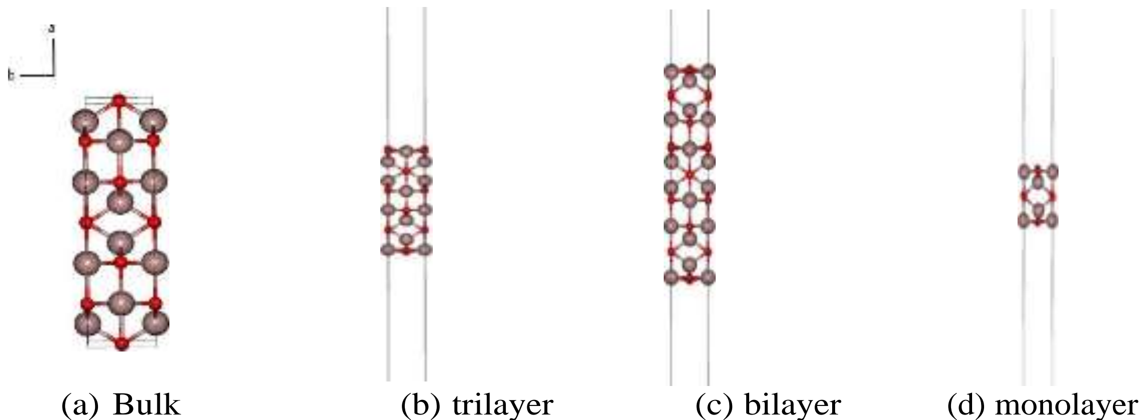
Figure 4.4: Geometrical structures of layers of $\beta - Ga_2O_3$

The accuracy in the value of band gap is obtained by hybrid functional HSE06, giving a value of 4.8453eV of $\beta - Ga_2O_3$ in acceptance with the experimental values. The side view of bulk and layers along a and b directions are shown in Fig 5.5.

Table 4.1: Band gaps

	Band gap by DFT (eV)	Band gap by using HSE06 (eV)
Bulk $\beta - Ga_2O_3$	2.027	4.8453
monolayer	3.1256	5.6241
bilayer	2.678	5.238
trilayer	2.1207	5.128

The effective mass of electrons and holes in terms of mass of electron m_o obtained from the band structure as given by Eq 4.1.



(a) Bulk (b) trilayer (c) bilayer (d) monolayer

Figure 4.5: Side view of layers

The bulk gallium oxide is isotropic. But the asymmetric positions of Ga and O atoms in 2D layers, it exhibits anisotropic nature. The Z-Γ, Γ- A of reciprocal lattice actually indicatethe 2 different directions of crystal with k = 0 as origin at the Γ point in the reciprocal plane. Since the cleavage is along (100) plane, when indicated in the reciprocal lattice the Γ- A direction in corresponds to axis c and Z-Γ direction corresponds to axis b [29] and the calculated effective mass along these directions shown in below Table 5.2. The effective masses along Γ- A are significantly larger than that along Z-Γ because of asymmetric parabola for conduction band and theflatness of band near the valence band.

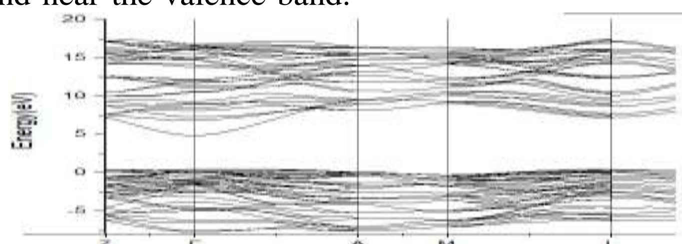
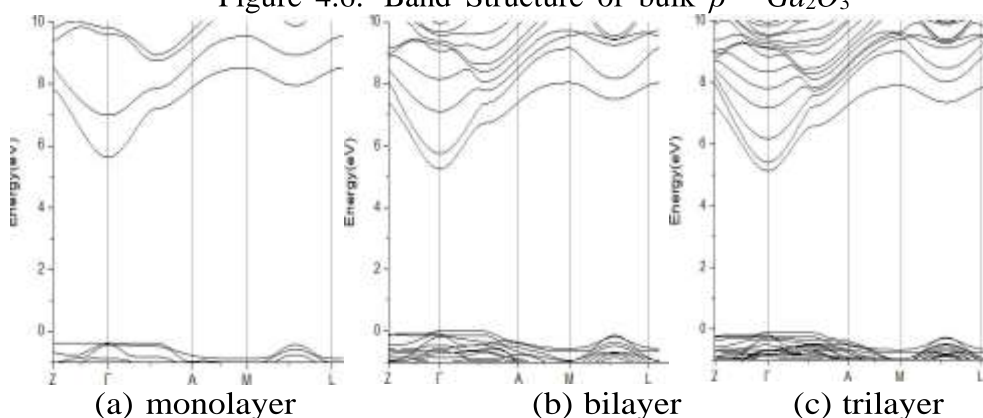


Figure 4.6: Band Structure of bulk $\beta - Ga_2O_3$



(a) monolayer (b) bilayer (c) trilayer

Figure 4.7: Band structures of layers

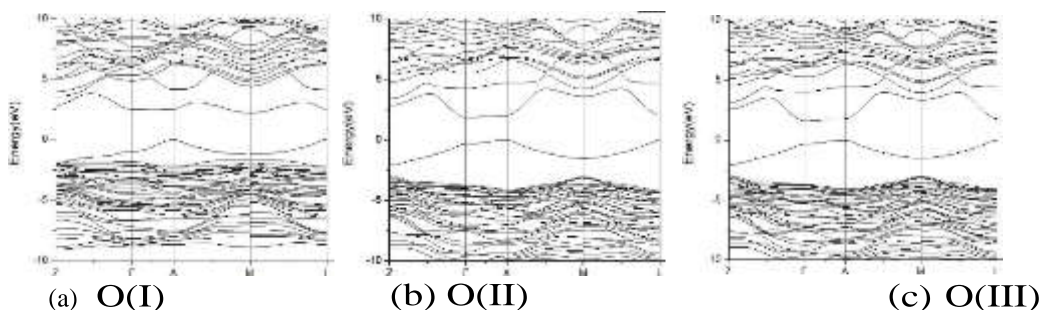
We can observe the band gap variation of 2D materials with bulk crystal[7].The layer dependent band gap can is due to quantum confinement in gallium oxide[15]. Gallium oxide is advantageous in terms of this layer dependent band gap which are stable also compared to other semiconductor materials. Monolayer has higher band gap compared to others because of quantum confinement effect and since the thickness is small the atoms are tightly packed and it becomes difficult to excitean electron into the conduction band, so large energy is required. So, it is difficult to dope the 2D material practically.

Table 4.2: Comparison Table

	direction	Effective mass of electron(m^*/m_o)	Effective mass of holes(m^*/m_o)
Bulk $\beta - Ga_2O_3$		0.2895	17.04
monolayer	b	0.514	3.52
	c	0.551	55.32
bilayer	b	0.356	3.26
	c	0.258	62.23
trilayer	b	0.291	3.24
	c	0.236	50.82

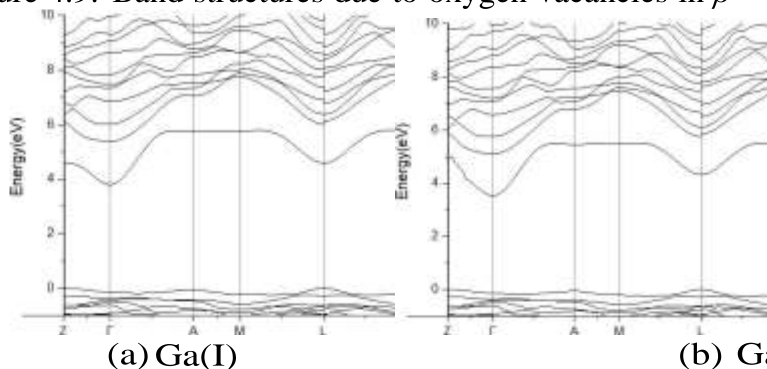
The anisotropy of layers is observed from the above table indicating different effective mass along different directions. We can observe the valence band is almost flat indicating large effective mass for bulk and 2D layers of $\beta - Ga_2O_3$. Large effective mass of valence band gives us low hole mobility indicating the problemof p-type conductivity in $\beta - Ga_2O_3$.

We have oxygen and gallium oxygen vacancies in the bulk crystal $\beta - Ga_2O_3$. Since there are 3 different sites for O vacancy and 2 different sites for Ga as shownin Fig 2.4. This unit cell consists of 20 atoms of 8 gallium and 12 oxygen atoms. One gallium atom and one oxygen atom is removed to create a vacancy at different sites respectively. The single vacancy have been created at different sites of oxygenin the unit cell Fig 5.8 and similarly done for gallium vacancy and the observed band structures are shown in Fig 5.9 and 5.10. It has been observed that O(III) site is the most stable site[31] and Ga(I) has lower formation energy[2], lower theformation energy more can be the concentration. From the band structures we can observe the oxygen and gallium vacancies induce new levels in the valence band and conduction respectively. Gallium vacancies act as deep acceptors and oxygen vacancies act as deep donors as seen from the band structures.



(a) O(I) (b) O(II) (c) O(III)

Figure 4.9: Band structures due to oxygen vacancies in $\beta - Ga_2O_3$



(a) Ga(I) (b) Ga(II)

Figure 4.10: Band structures due to gallium vacancies in $\beta - Ga_2O_3$

Group-IV elements which have extra valence electron than Gallium for n-type conductivity. We can observe here also new donor energy levels are induced below the conduction band edge

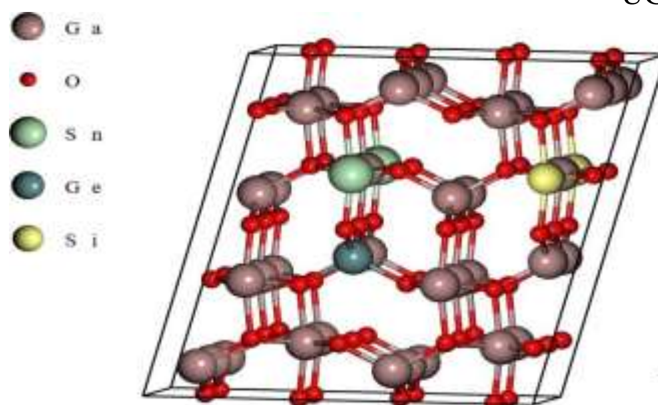
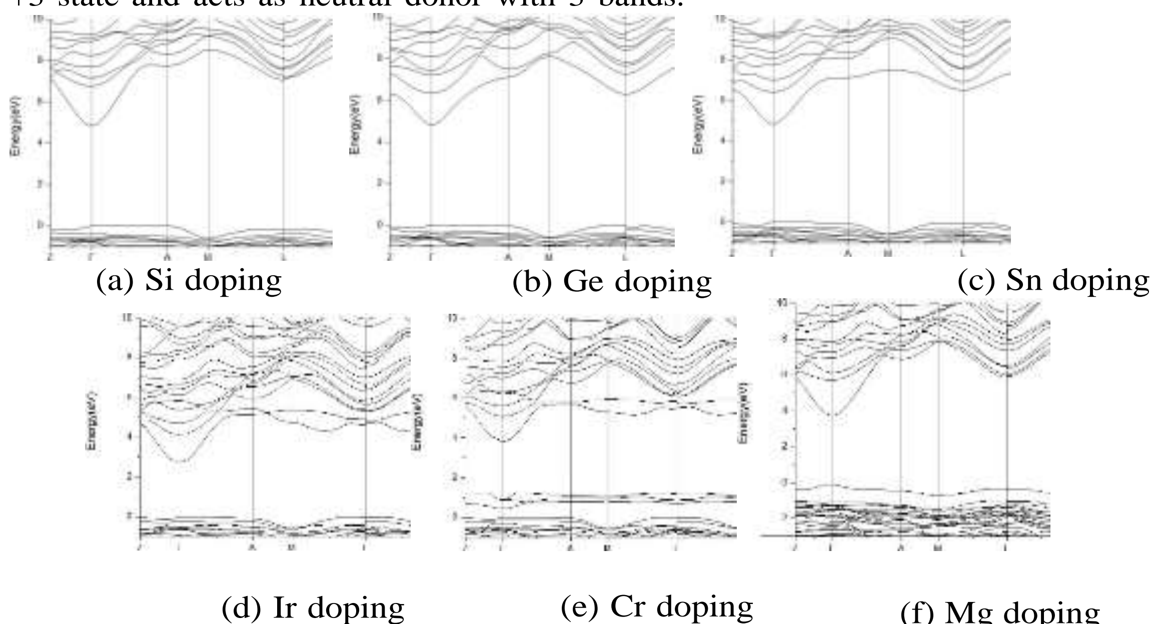


Figure 4.11: Doping in $\beta - Ga_2O_3$

Table 4.4: Band gap

	Band gap by DFT (eV)	Band gap by using HSE06 (eV)	effective mass m^*/m_o
Si	2.112	4.8412	0.32
Ge	2.014	4.8361	0.278
Sn	2.009	4.8356	0.257
Ir	1.52	2.7453	0.268
Cr	1.478	2.212	0.221

The minimum amount of energy required to remove a loosely bound electronis called Binding energy E_d [3] or ionization energy. It is defined as the difference between the conduction band edge and the new level below the conduction bandedge which should be less than 1eV to be a shallow donor. From Fig 4.12 wecan observe Iridium and Chromium have deep donor levels in the band structure which sit on the Ga(II) site. Ir and Cr are transition elements so are capableof exhibiting variable valency. Iridium impurity incorporation occurs when bulk Ga_2O_3 crystals are grown in an iridium crucible. From the band structure we observe that Chromium is in +3 state and acts as neutral donor with 3 bands.



(a) Si doping (b) Ge doping (c) Sn doping

(d) Ir doping (e) Cr doping (f) Mg doping

Figure 4.12: Band structures of different dopants in $\beta - Ga_2O_3$

in between the band gap indicating we have filled mid-gap states of the neutral cell. There are new levels in both conduction and valence band of Cr. Ir in +4 valence will act as deep donor and +3 state as neutral donor. Since Ir and Cr have $E_d = 2.09$eV and 1.04eV indicating which require high ionization energy to ionize all the dopants, hence treated as deep donors for $\beta - Ga_2O_3$. Since deep donors does not contribute much for conduction and more concentration of dopants is required [36] since these act as active recombination sites and suitable at high temperature as dopants. Whereas the E_d values for Si, Ge, Sn are 41meV, 92meV, 97meV respectively indicating these all dopants behave like shallow donors for $\beta - Ga_2O_3$.We can observe that Si behaves like a shallower donor. It was observed that with moderate doping it generates free carrier concentration in ~ 10^{19} [3] and various experiments have shown Si is an unintentional source of n-type conductivity[2].

Mg doping on the Ga(II) is done for having p-type conductivity as it has one electron less than Gallium so can act as acceptor which shows a deep level inthe valence band indicating it as a deep level acceptor with $E_d = 1.1$eV.

Many researchers have shown that various doping in $\beta - Ga_2O_3$ has this type of deep

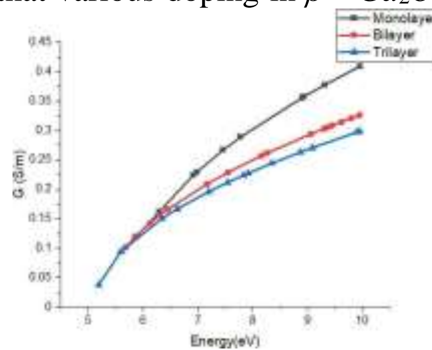


Figure 4.13: Conductance variation with energy in $\beta - Ga_2O_3$ layers

level traps in the valence band, which require high concentrations of dopants and with flat valence band of holes the difficulty of getting p-type conductivity.

The Fig 4.13 shows the variation of conductance as a function energy which has a parabolic relation for 2D $\beta - Ga_2O_3$ layers. The conductance is calculated by using Eq 4.22 and the number of sub bands by Eq 4.18, Eq 4.20 for the 2D and thebulk materials. The unit of conductance is V or Siemens(S). The number of modes M(E) is expressed as $M_{2D}(E)/\mu m$, $M_{2D}(E)/\mu m^2$ and conductance has the units $S/\mu m$ and $S/\mu m^2$ for 2D and the 3D bulk materials of $\beta - Ga_2O_3$ respectively.To get the exact the number of modes we can multiply the M(E) with the width of 2D conductor or cross -sectional area of 3D conductor. From the Fig 5.13 for monolayer for a energy at 7eV calculated using Eq 4.18 is $M_{2D}(E) = 2558.5/\mu m$if the width of the conductor is 1nm then the number of channels for conductionare $M_{2D}(E)$~ 2. Similarly, we can find the channels contributing for conduction when the width or cross-sectional area of conductors is known. The Fig 5.14 shows variation of conductance for different doping concentrations with 3%, 15%, 25% (in atoms) for shallow donors Si, Ge, Sn and the deep donors Ir and Cr. In case of Si, Ge, Sn when the doping concentration increases there is not much significant change in the band structure except in the concentration of free charge carriers inthe conductance but in Ir and Cr have more deep levels and the binding energy changes significantly not like in the case of shallow donors. Doping is done in the 1x2x2 super cell bulk $\beta - Ga_2O_3$ and the conductance as function of energy has a linear relationship not like in 2D materials. This is true because as the size of the device increases it can accommodate more channels for conduction.

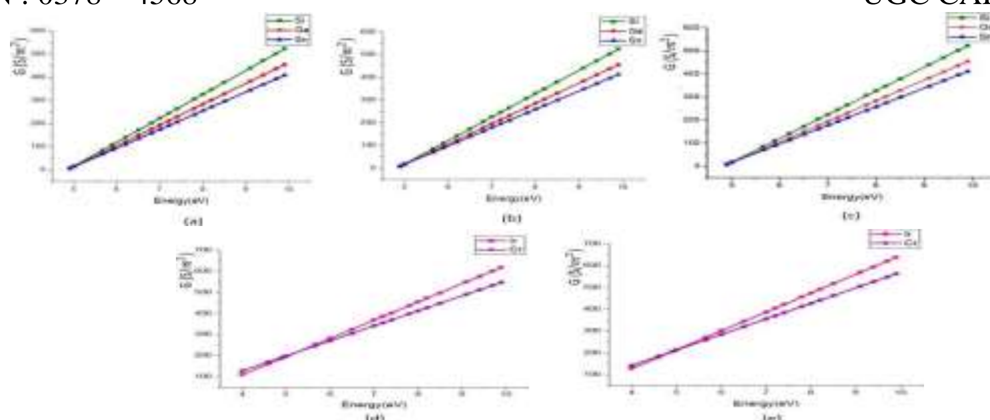


Figure 4.14: G variation with Energy for different concentration of doping in$\beta - Ga_2O_3$. For (a) 3% (b) 15% (c) 25% doping concentration in Si, Ge, Sn and (d)3% (e)15% doping concentration for deep donors Ir and Cr.

For each doping concentration the band gap and effective mass are calculated and the graphs are plotted for using Eq 4.22, Eq 4.20. The conductance unit of 3D materials is S/μm^2 and similarly the number of channels can be found if we know the cross-sectional area of device.

5. CONCLUSION

We know that the performance of 2D materials depends on the thickness hence, we observed thickness dependent band gap and effective mass variation due to the quantum confinement effect. From bulk 3D material by moving to 2D monolayerwe have an increased band gap and monolayer possess highest band gap among all.It was also observed the low mobility issues had improved when moved to thin atomic layers [7] than the bulk. The advantages of 2D materials is these layers are only few atoms thick, so are lighter and have very strong bonds so are difficultto break and can handle high voltages and high power without damaging the devices. From ballistic conduction we can observe that the current density is not dependent on the length of semiconductor. We can get higher values of current density even if the channel length is made very very small by moving from bulk to 2D layers of $\beta - Ga_2O_3$. Also, from the Fig 4.2 we can observe monolayer showing the maximum ballistic conductance, yielding a high current density with the minimum dimensions of the 2D $\beta - Ga_2O_3$.

The wide band gap semiconductors behave like an insulator. The calculated conductivity and mobility values are very less[7]. The large n-type conductivityvalues for gallium oxide were thought to be because of oxygen vacancies, but which is not true because the act as deep donors as seen from the band structure in Fig 5.9. Gallium vacancies also do not contribute any n-type conductivity because they acts as deep acceptors. As observed Si has lower ionization energy than Ge,Sn, Ir, Cr, Mg and has the the highest ballistic current density with and can givehigh carrier concentration so, can be the best source for n-type conductivity of$\beta - Ga_2O_3$. Materials doped with shallow level all the donors are nearly ionized ata moderate temperature on the other hand high ionization energy require higher temperatures to ionize the impurities so, deep donors may be suitable at higher temperatures but produce a smaller number of carriers compared to shallow donors ata given concentration. From the valence band of band structures, we can say the effective mass is very high for p-type conductivity which is indirectly related tomobility of holes so, it is difficult to have p type conductivity in gallium oxide. Many theoretical calculations have shown the p-type conductivity with differentdopants like Mg, N ,Fe have introduced deep acceptor levels and even with high concentrations of dopant it is impossible to get high mobility because of strong self- localisation of holes[30] and research is going on this.

Gallium oxide is a vast research topic and has good progress theoretically recently, because of the advantages of high band gap and high breakdown field strength for high voltage devices. More progress can be done on improving the p- type conductivity of holes by observing it in different crystal orientations. Since the optical band gap value is nearly the electrical band gap and when

doped with different materials give rise to new levels can be used for detection of various wavelengths. So gallium oxide in the field of opto-electronics is a vast and ongoing topic for future direction [37]. Deep levels are useful when operated at higher temperatures so, more study can be done on deep donors when operated under suitable conditions. $\alpha - Ga_2O_3$ has higher band gap than $\beta - Ga_2O_3$ so further developments on this phase can be useful. More research can be done to investigate the use of other transition metal dopants like Cr and Ir which have a greater number of valence electrons so, can give high concentration of free carriers thereby increasing conductivity.

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