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Study of band structures of GaAs and InAs grown on different substrates

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Abstract

In the early studies, thorough calculations for the band structures of binary and ternary semiconductor compounds have been performed. But in those studies the role of substrate, on which the studied compound is grown, has not been accounted. In this paper, the calculations for the band structures of technologically important binary semiconductors i.e. GaAs and InAs considering the effect of substrate have been performed and the results have been analysed successfully. In results, it has been shown that considering the lattice matched substrate with the grown semiconductor layers is very important for better device performance.

Keywords: *GaAs, InAs, band structures, k.p theory, substrate.*

1.0 Introduction

In general, the study of band structure is always needed to understand the working mechanism of all the semiconductor based electronic or optoelectronic devices in terms of electronic transportation. Earlier, the band structure theory has been fruitfully used to describe many physical properties of solids, such as optical, electronic, mechanical and electrical properties[1,2]. But, in optoelectronics point of view, the study of band structure at the Γ point is of great interest. Because, at the Γ point, the study of nature of compound semiconducting material is very easy. In other language, one can easily determine the direct or indirect nature of the compound semiconducting materials the Γ point[3-6]. For the study of band structure at the Γ point, the k.p model plays an important role[7,8]. In fact, k.p method provides an approximate demonstration of the energy bands in excess of the full Brillouin Zone[9,10]. In reference[9], Vurgaftman et al. have reported band structures of various binary compounds such as GaN, InN, GaAs, InAs, AlAs, GaP, InP and GaSb etc. However, in their study they have not considered the substrate effect on the reported band structures of abovementioned some binary semiconductor compounds.

In this article, authors have taken into account the substrate effect on the band structures of some technologically important binary semiconductors such as GaAs and InAs and an effort has been made to study the effect on different substrates (such as GaAs, AlAs and InAs) on the band structures of GaAs and InAs binary semiconductors. The effect has been analysed in brief.

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2.0 Theoretical Detail and Results Analysis

In order to investigate the optical response of the planned layered heterostructure, the foremost task is to study the band diagram along with offset values of QW and barrier regions. Once the band diagram is planned, one can study the structure with the help of fundamental quantum mechanics.

The k.p model can be derived from the one-electron general Schrodinger equation. Using the Bloch theorem (theorem for moving particle in periodic potential or crystalline soilds) the solutions of general Schrodinger equation can be expressed, in the reduced zone scheme, as follows:

$\Phi_{nk} = \exp(ik.r)\, u_{nk}(r)$,

where n is the band index, k lies within the first Brillouin zone, and u_{nk} has the periodicity of the lattice. When Φ_{nk} is substituted into the general Schrodinger equation, one can obtain an equation in u_{nk} of the form:

$$\left(\frac{p^2}{2m}+\frac{hk.p}{m}+\frac{h^2k^2}{2m}+V\right)u_{nk} = E_{nk}u_{nk}.$$

The above equation is referred to as k.p model for calculating the energies of different bands.

Here, the chosen binary semiconducting materials for band structure study are GaAs and InAs with different substrates such as GaAs, AlAs and InAs. In Figure 1, the band structures of GaAs grown pseudomorphically on the substrates GaAs, AlAs and InAs have been shown. In Figure 1 (a&b), it can be seen that at the Γ point (k_z=0) the LHB (Light Holes Band) and HHB (Heavy Holes Band) are aligned or overlapped. This overlapping of LHB and HHB shows that there is no strain or stress in the grown material (i.e GaAs). This is due to lattice matched situation between GaAs and the substrates (GaAs and AlAs). Refer to Figure 1 (c), at the Γ point (k_z=0), LHB and HHB are not overlapped which shows that there is little bit internal strain which exist between GaAs and InAs. This confirms that the lattices of GaAs and InAs materials are not in match. All these band structure have been calculated at 300K.

Similarly, refer to Figure 2, the band structures of InAs grown pseudomorphically on the substrates InAs, AlAs and GaAs has been shown. On carefully observation of Figure 2 (a), it can be examine that at the Γ point (k_z=0) the LHB (Light Holes Band) and HHB (Heavy Holes Band) are aligned or overlapped. This overlapping of LHB and HHB shows that there is no strain or stress in the grown material (i.e InAs) because of lattice matched parameters of InAs and the substrates (InAs) i.e. the same materials: grown material and the substrate. Refer to Figure 2 (b&c), at the Γ point (k_z=0), the LHB and HHB are not overlapped which prove the existence of internal strain which occurs between grown

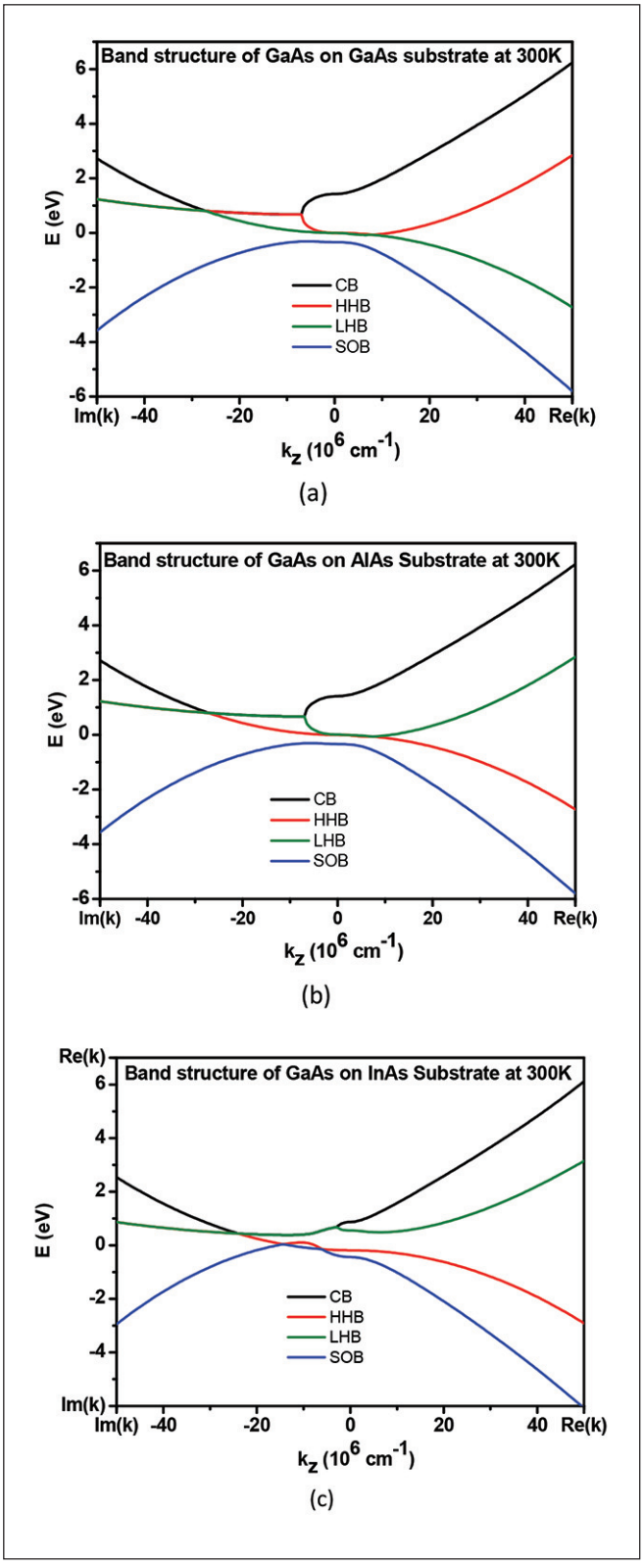

Figure 1: Band structure of GaAs grown on (a) GaAs (b) AlAs (c) InAs substrate

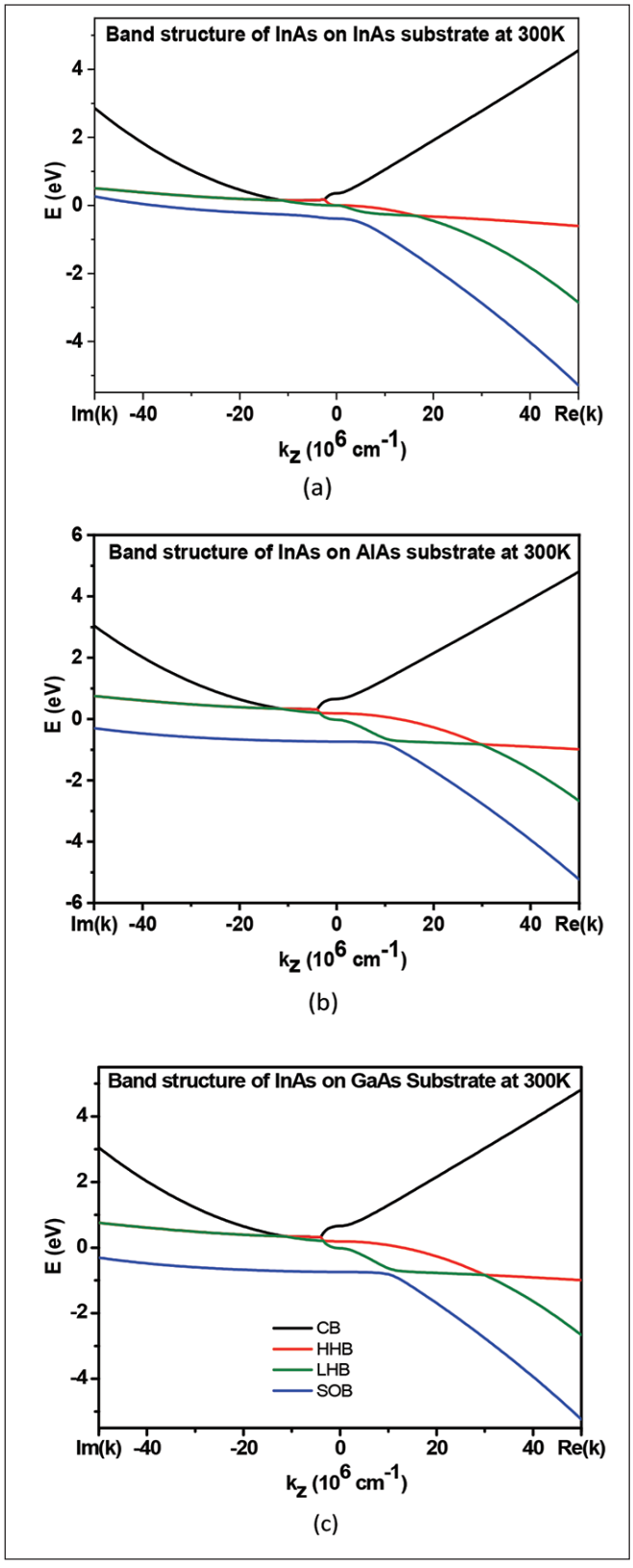

Figure 2: Band structure of InAs grown on (a) InAs (b) AlAs (c) GaAs substrate

material (i.e InAs) and the substrates (AlAs and GaAs). This confirms that the lattice parameters of InAs are not in match with those of GaAs and AlAs materials. The lattice match study of the growing layers i.e. InAs, GaAs and GaSb on the different substrates has been done to know the device performance[11-14].

4.0 Conclusion

The band structures calculations for the binary and ternary semiconductor compounds have been performed with the consideration of substrate effect. In this paper, the calculations for the band structures of technologically important binary semiconductors i.e. GaAs and InAs considering the effect of substrate have been performed and the results have been analysed successfully. In results, it has been shown that the consideration of the lattice matched substrate with the grown semiconductor layers is very important for better device performance.

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6.0 References

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