Journal of Mines, Metals and Fuels, *71(10): 1394-1400; 2023. DOI: 10.18311/jmmf/2023/34871*

Print ISSN : 0022-2755

Journal of Mines, Metals and Fuels

Contents available at: *www.informaticsjournals.com/index.php/jmmf*

Temperature Dependant Bandgap Tuning of GaAs, AlAs, InAs, and InP Binaries Grown on different Substrates

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Abstract

This article carries out the temperature-dependent study of the band structures of bulk binaries such as AlAs, GaAs, InAs, and InP grown on different substrates thus showing the combined effect of substrate and temperature on the bandgaps of the binary systems under study. For the calculations of the band structures of the binary systems grown on different substrates, the k.p technique has been used. The results have been analyzed successfully. For all the binaries, it has been found that the bandgap is reduced with increasing temperature but the rate of reduction with temperature is different for dissimilar substrates. The outcomes of the calculations for the band structures of binaries grown on lattice-matched and unmatched substrates are very useful for understanding of device performance.

Keywords: *AlAs, Band Structures, GaAs, InAs, K.P Theory, Substrate Effects*

1.0 Introduction

From photonics and energy harvesting to electronics and many other technical uses, tuning the bandgap of materials is essential[1-3]. The energy range between a material's valence and conduction bands, or bandgap, controls both its electrical and optical characteristics. Engineers and scientists may tailor the behavior of materials to meet certain requirements by adjusting the bandgap[4-7]. Bandgap engineering, for instance, enables the development of transistors with changing energy gaps in the field of semiconductor electronics, simplifying the construction of devices that can function well at various wavelengths and energy levels. This is especially important for creating sophisticated integrated circuits, sensors, and optoelectronic gadgets that meet the requirements of contemporary technology.

The efficiency of solar cells and other energy conversion technologies may also be optimized by bandgap adjustment[8,9]. Researchers can optimize the absorption and utilization of incoming photons, leading to higher energy conversion efficiencies, by adjusting the bandgap to match the solar spectrum or other pertinent energy sources. This is especially useful for utilizing renewable energy sources like solar and thermoelectric power as well as for developing technologies like Light-

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Emitting Diodes (LEDs) and lasers, where the emission and absorption characteristics are closely related to the bandgap of the materials involved[10,11]. Fundamentally, manipulating the bandgap of materials enables scientists and engineers to open up new avenues for improving the functionality of devices, energy effectiveness, and technological innovation in general.

In this article, authors have taken into account the variable temperature considering the different substrates to study the effect of temperature and the substrates simultaneously on the band structures and band gaps of some technologically important binary materials such as AlAs, GaAs, InAs, and InP. The effect has been analyzed in brief. Such a study may be very useful in understanding the tunability of the band gaps of the concerned materials for the purposes of designing tunable devices.

2.0 Theoretical Background

In order to examine the substrate effects on the band structures of III-V semiconducting materials, particularly GaAs, InAs, AlAs, and InP binaries, a k.p method leading to fundamental quantum mechanics can be very helpful. The k.p model can be derived from the one-electron general Schrodinger equation. Using the Bloch theorem (theorem for moving particles in periodic potential or crystalline solids) the solutions of the general Schrodinger equation can be expressed, in the reduced zone scheme, as follows:

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

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:

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

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

Further, the calculations for studying the temperature dependant bandgap tuning may be

performed using the following expression:

$$E_g(T) = E_g(0) - \frac{\alpha T^2}{T + \beta}$$

The above relationship between band gap energy and temperature is called Varshni's empirical expression[12].

3.0 Simulation Results and their Analysis

Initially, considering the effective mass approximations, a 6 × 6 K-L (Kohn-Luttinger) Hamiltonian is solved to find out the energy band structure of the desired bulk materials. The 6 × 6 K-L Hamiltonian typically consists of several terms, including the kinetic energy of the electrons, the electron-electron Coulomb interaction, and the electron-phonon interaction[13,14]. The specific form of the Hamiltonian depends on the level of approximation being used and the details of the system being studied. Solving the K-L Hamiltonian involves finding the quantum mechanical states and energies of the electrons within the given solid. This is a complex task that often requires approximation methods due to the large number of particles involved and the interactions between them.

In order to study the effect of temperature on the bandgap, Varshni's empirical expression has been utilized and the corresponding changes in the bandgap have been displayed in Figures 1-8. Generally, with increasing the temperature, the bandgap of all the binaries is reduced, as expected. In Figures 1 (a), (b), and (c), the temperature-dependent bandgap of the AlAs binary assumed to be grown on AlAs, GaAs, and InAs substrates have been shown. Considering AlAs and GaAs substrates, the bandgap is reduced from 3.10 eV to 2.92 eV on increasing the temperature from 150K to 400K (Figures 1 (a) and (b)); while with the InAs substrate the bandgap is reduced from 1.92 to 1.76 eV on increasing the temperature from 150K to 400K (Figure 1 (c)). The bandgap reduction of AlAs bulk material with different substrates on increasing the temperature has been summarized in Figure 2.

Refer to Figures 3 ((a), (b), and (c)) in which the temperature-dependent bandgap of GaAs binary supposed to be grown on AlAs, GaAs, and InAs substrates have been shown. For AlAs and GaAs substrates, the bandgap of GaAs is reduced from ~1.48 eV to ~1.36 eV on increasing the temperature from 150K to 400K (Figures 3 (a) and (b)); while with the InAs substrate, the bandgap

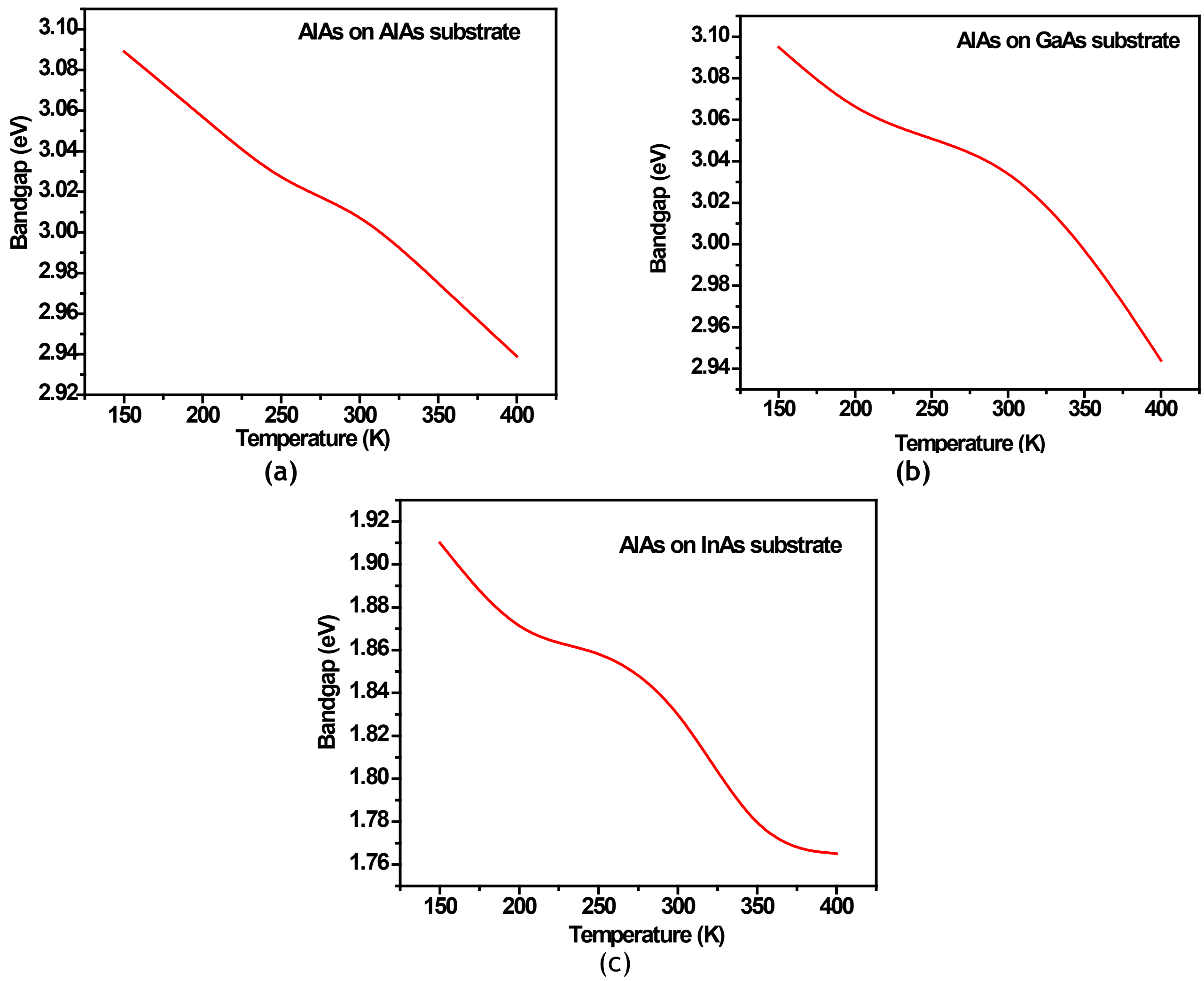

Figure 1. Temperature dependant bandgap of AlAs binary grown on **(a)** AlAs **(b)** GaAs **(c)** InAs substrates.

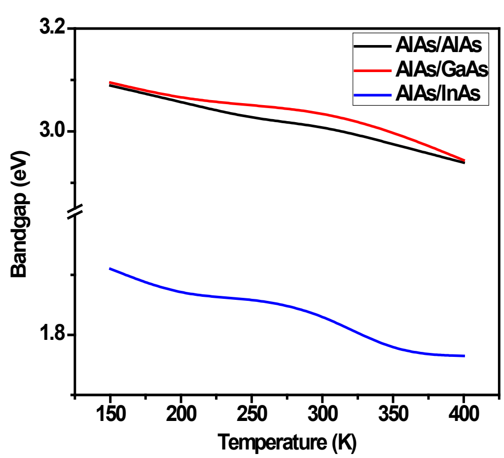

Figure 2. Summary of effects of substrates and temperature on the bandgap of AlAs binary.

of GaAs is reduced from 0.38 to 0.28 eV on increasing the temperature from 150K to 400K (Figure 3 (c)). The overall reduction in bandgap of bulk GaAs material with different substrates for increasing the temperature have been reviewed in Figure 4.

In Figures 5 ((a), (b), and (c)), emphasis has been given on the reduction in bandgap of InAs grown on AlAs, GaAs and InAs substrates kept on increasing temperature. For AlAs and GaAs substrates, the bandgap of InAs is reduced from ~0.51 eV to ~0.45 eV on increasing the temperature from 150K to 400K (Figures 5 (a) and (b)); while with the InAs substrate (with the lattice matched system) the bandgap is reduced from 0.40 to 0.33 eV on increasing the temperature (Figure 5 (c)). The diminution

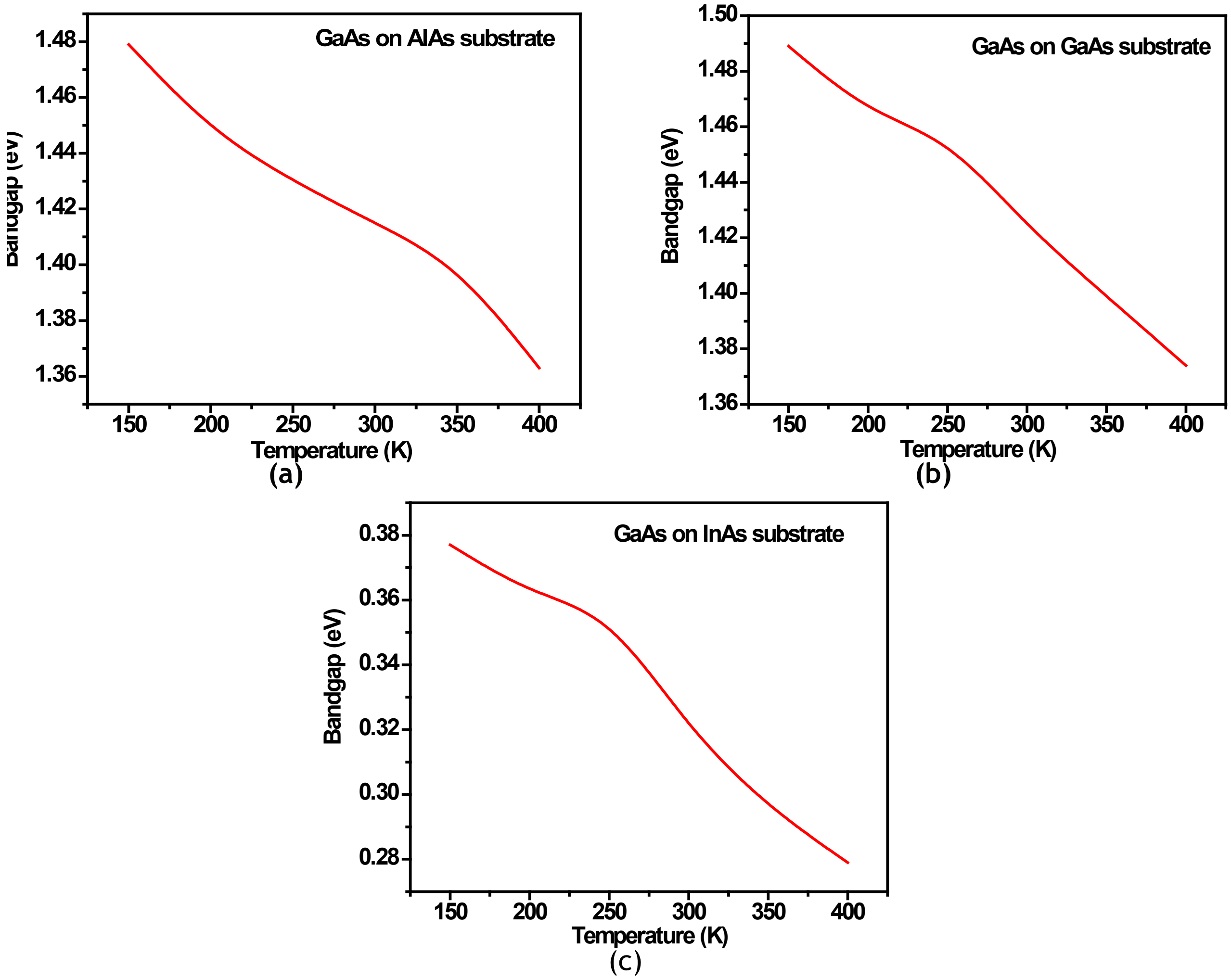

Figure 3. Temperature dependant bandgap of GaAs binary grown on **(a)** AlAs **(b)** GaAs **(c)** InAs substrates.

in bandgap of bulk InAs material with different substrates on growing the temperature has been analyzed in Figure 6. Similarly, the temperature-dependent behavior of InP has been studied in Figures 7 ((a), (b), and (c)) and Figure 8.

Refer to Figures 7 ((a), (b), and (c)), for AlP and GaP substrates, the bandgap of InP is reduced from ~1.52 eV to ~1.43 eV on increasing the temperature from 150K to 400K; while with the InP substrate (lattice matched substrate) the bandgap of InP is reduced from 1.41 to 1.32 eV on increasing the temperature from 150K to 400K (Figure 3 (c)). These reductions of bandgap with increasing temperature have been summarized in Figure 8.

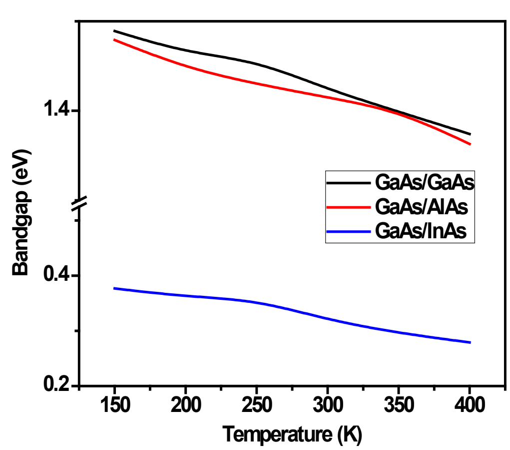

Figure 4. Summary of effects of substrates and temperature on the bandgap of GaAs binary.

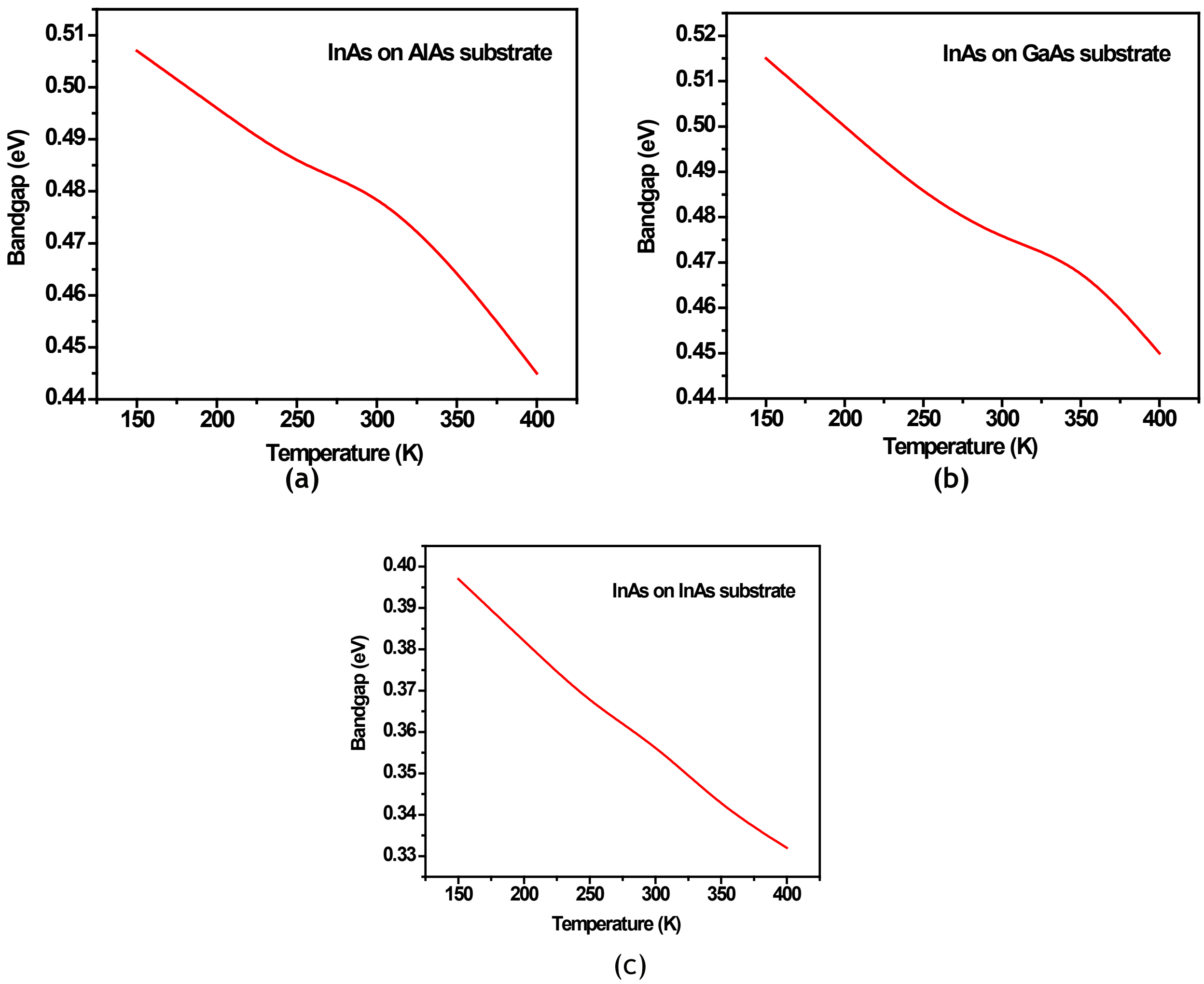

Figure 5. Temperature dependant bandgap of InAs binary grown on **(a)** AlAs **(b)** GaAs **(c)** InAs substrates.

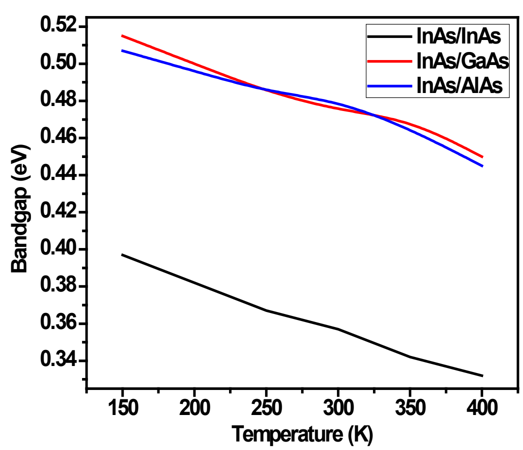

Figure 6. Summary of effects of substrates and temperature on the bandgap of InAs binary.

4.0 Conclusion

The temperature dependence of the band structures of bulk binaries grown on several substrates, including AlAs, GaAs, InAs, and InP, demonstrating the combined influence of substrate and temperature has been studied successfully. The k.p approach has been used to the computations of the band structures of binary systems grown on various substrates. The findings have been successfully analyzed. It has been discovered that the bandgap decreases with temperature for all binaries, although the rate of decrease with temperature varies for diverse substrates. For the knowledge of device performance, the results of simulations for the band

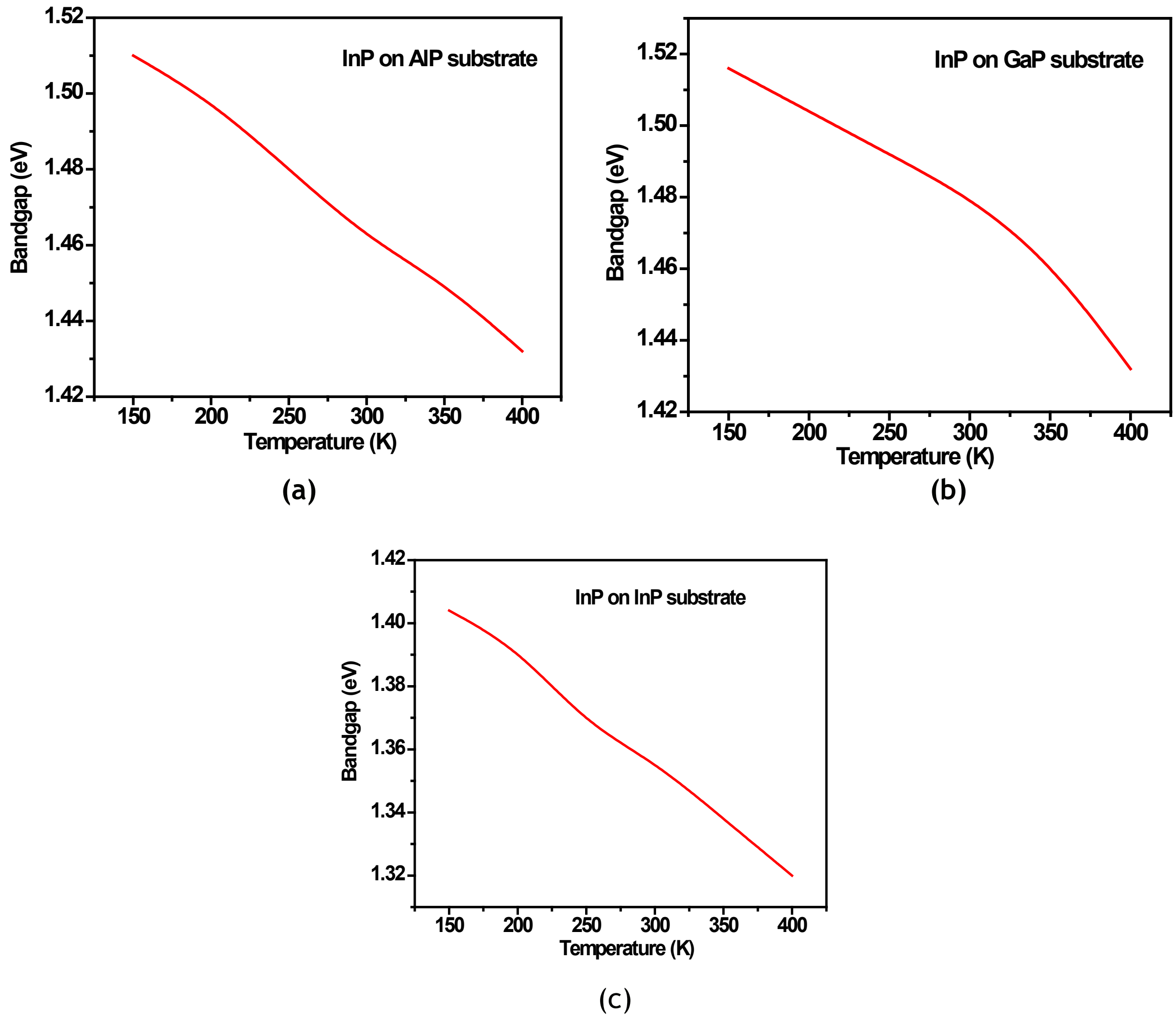

Figure 7. Temperature dependant bandgap of InP binary grown on **(a)** AlP **(b)** GaP **(c)** InP substrates

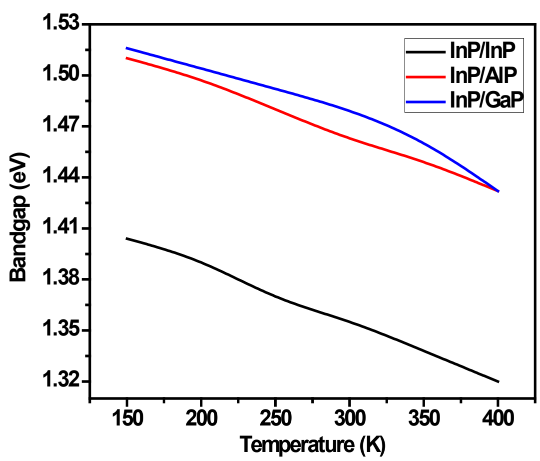

Figure 8. Summary of effects of substrates and temperature on the bandgap of InP binary.

structures of binaries grown on substrates with and without matching lattices are highly helpful.

5.0 Acknowledgement

P. A. Alvi acknowledges to DST govt. of India for supporting the research in terms of research facilities provided to Banasthali Vidyapith under CURIE and STUTI schemes.

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