Structural and Optical Properties of $AlAs_xSb_{1-x}$

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Abstract

We present a theoretical investigation of the structural and optical properties of $AlAs_xSb_{1-x}$ semiconducting alloys in zinc-blende structure based on the empirical pseudopotential method within the virtual crystal approximation combined with the Harrison bond-orbital model. The Elastic Constant, bulk modulus, refractive index, high frequency dielectric constant, static dielectric constant are calculated for $AlAs_xSb_{1-x}$. Our results for $AlAs_xSb_{1-x}$ ($0<x<1$) are predictions.

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Introduction

Semiconductor alloys based on III-V compounds have opened up new generation of device application during the last few decades [1]. Ternary alloys have the advantage that a considerably wide range of band gaps can be obtained by changing the alloy composition. Because of the wide range of its physical properties ternary alloys are an important material for many applications in microelectronics [2].

Computational Detail

The calculation of various properties of semiconductor alloys using DFT require large computational power. it is hard to model semiconductor alloys using DFT as it can only be used by means of supercells which increase the number of atoms. On contrary the EPM use the virtual crystal approximation to model the alloys which is easy to simulate. The band gap of $AlAs_xSb_{1-x}$ is calculated using empirical pseudopotential method (EPM) Considering the Zink blende structure. EPM is an approach to calculate the electronic band structure and optical properties. WE consider the disordered effects of alloys via modified virtual crystal approximation implemented in EPM [3-5]. The Value of elastic constants C_{11}, C_{12} and C_{44} are calculated using the method proposed by Baranowski [6] and Bouarissa and Kassali [7]. The Elastic Constants C_{11}, C_{12} and C_{44} for cubic Structure are Defined as:

$$C_{11} = \frac{(\sqrt{3})}{4d^5}\left[4.37\,\frac{\hbar^2}{m}\,(5+\lambda)\left(1-\alpha_p^2\right)^{\frac{3}{2}} - 0.6075\frac{\hbar^2}{m}\left(1-\alpha_p^2\right)^{\frac{1}{2}}\right] \quad (1)$$

Table 1: Various elastic constants for different alloy composition

X	Alloys	C_{11}	C_{12}	C_{44}
0.0	AlSb	97.57506	41.84139	39.52807
0.1	$AlAs_{0.1}Sb_{0.9}$	101.0197	43.32816	40.91984
0.2	$AlAs_{0.2}Sb_{0.8}$	104.3296	44.76459	42.25428
0.3	$AlAs_{0.3}Sb_{0.7}$	107.4667	46.13538	43.51549
0.4	$AlAs_{0.4}Sb_{0.6}$	110.3884	47.42344	44.68581
0.5	$AlAs_{0.5}Sb_{0.5}$	113.0475	48.60982	45.74566
0.6	$AlAs_{0.6}Sb_{0.4}$	115.3923	49.67353	46.67348
0.7	$AlAs_{0.7}Sb_{0.3}$	117.3654	50.59149	47.44562
0.8	$AlAs_{0.8}Sb_{0.2}$	118.9048	51.33841	48.03627
0.9	$AlAs_{0.9}Sb_{0.1}$	119.9428	51.88674	48.41747
1.0	AlAs	120.4065	52.20667	48.55911

$$C_{12} = \frac{(\sqrt{3})}{4d^5}\left[4.37\,\frac{\hbar^2}{m}\,(3-\lambda)\left(1-\alpha_p^2\right)^{\frac{3}{2}} + 0.6075\frac{\hbar^2}{m}\left(1-\alpha_p^2\right)^{\frac{1}{2}}\right] \quad (2)$$

$$C_{44} = \frac{3(\,C_{11}+2C_{12}\,)(C_{11}-C_{12}\,)}{(7C_{11}+2C_{12}\,)} \quad (3)$$

Table 2: Various elastic constants for different alloy composition

X	Alloys	B_S	C_S
0.0	AlSb	60.41928	27.86684
0.1	$AlAs_{0.1}Sb_{0.9}$	62.55866	28.84575
0.2	$AlAs_{0.2}Sb_{0.8}$	64.61959	29.7825
0.3	$AlAs_{0.3}Sb_{0.7}$	66.57914	30.66564
0.4	$AlAs_{0.4}Sb_{0.6}$	68.41175	31.48246
0.5	$AlAs_{0.5}Sb_{0.5}$	70.08906	32.21886
0.6	$AlAs_{0.6}Sb_{0.4}$	71.57977	32.85936
0.7	$AlAs_{0.7}Sb_{0.3}$	72.84947	33.38697
0.8	$AlAs_{0.8}Sb_{0.2}$	73.86054	33.7832
0.9	$AlAs_{0.9}Sb_{0.1}$	74.57209	34.02803
1.0	AlAs	74.93996	34.09994

Table 3: Various refractive index values for different composition.

X	Alloys	n	ε_∞	ε_0
0.0	AlSb	2.59869765	6.7532290	6.758950997
0.1	$AlAs_{0.1}Sb_{0.9}$	2.57671772	6.6394744	6.660381224
0.2	$AlAs_{0.2}Sb_{0.8}$	2.54633767	6.4838356	6.529181622
0.3	$AlAs_{0.3}Sb_{0.7}$	2.50832385	6.2916883	6.370223121
0.4	$AlAs_{0.4}Sb_{0.6}$	2.46359120	6.0692812	6.189077591
0.5	$AlAs_{0.5}Sb_{0.5}$	2.41315494	5.8233168	5.991684468
0.6	$AlAs_{0.6}Sb_{0.4}$	2.35808168	5.5605494	5.78404425
0.7	$AlAs_{0.7}Sb_{0.3}$	2.29944394	5.2874425	5.571965674
0.8	$AlAs_{0.8}Sb_{0.2}$	2.23828074	5.0099009	5.360885644
0.9	$AlAs_{0.9}Sb_{0.1}$	2.17556613	4.7330878	5.155770962
1.0	AlAs	2.11218617	4.4613304	4.961103352

The bulk and Shear Moduli can be computed applying the following relations [8].

$$B_S = \frac{(C_{11} + 2C_{12})}{3} \quad (4)$$

$$C_S = \frac{(C_{11} - C_{12})}{2} \quad (5)$$

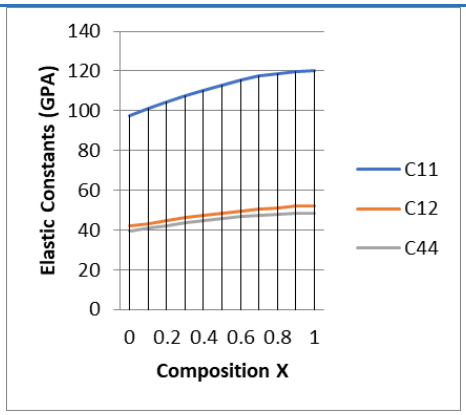

Figure 1: Elastic Constants C_{11}, C_{12}, C_{44} of $AlAs_xSb_{1-x}$ as a function of composition x.

Table 2 shows Elastic Constants Bs and Cs that are calculated by equation (4), (5) and table 3 shows refractive index values for different composition calculated by equation (6), (7), (8) using empirical pseudopotential method.

The Wavelength independent refractive index (n) is Calculated by Band gap (E_g) using Moss's Formula [9] given as

$$n^4 = \frac{E_g(E_v)}{95} \quad (6)$$

The high frequency dielectric constant ε_∞ can be obtained using the following relation:

$$\varepsilon_\infty = n^2 \quad (7)$$

According to the Harrison bond orbital model the static dielectric constant is directly related to ε_∞ as [10].

$$\varepsilon_0 = 1 + (\varepsilon_\infty - 1)\left(1 + \frac{\alpha_p^2(1+\alpha_c^2)}{2\alpha_c^2}\right) \quad (8)$$

Figure 1 Compared different Elastic Constants for composition 0<x<1 of alloy $AlAsxSb_{1-x}$.

Conclusion and Future Prospective

The structural property (Elastic Constant, bulk modulus) and optical property (refractive index, high frequency dielectric constant, static dielectric constant) are calculated for alloy ZnS_xTe_{1-x} for 10 compositions in table 1 using EPM The experimental value is given in binary numbers. It has been observed that the static and high frequency dielectric constants increase when the antimony concentration is increase. Our results are predictions.

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