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Elastic properties of $Ga_xIn_{1-x}P$ semiconductor

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ABSTRACT

A theoretical procedure is presented for the study of elastic properties of the ternary alloy $Ga_xIn_{1-x}P$. The calculations are based on the pseudopotential formalism in which local potential coupled with the virtual crystal approximation (VCA) is applied to evaluate elastic constants c_{11}, c_{12} and c_{44}, bulk modulus, shear modulus, Young's modulus and Poisson's ratio for the entire range of the alloy composition x of the ternary alloy $Ga_xIn_{1-x}P$. The effect of compositional disorder is included. Our results for parent compounds are compared to experimental and other theoretical calculations and showed generally good agreement. The inclusion of compositional disorder increases values of all elastic constants. During the present study it is found that elastic constant c_{11} is largely influenced by compositional disorder.

1. Introduction

In searching for the desired material parameters like lattice parameter, band gap, lattice matching to substrate, dielectric constant, refractive index and carrier mobility scientists have investigated a large number of materials. Recently there has been increasing interest in the group II–VI and III–V semiconductor ternary alloys as their lattice parameter and energy band gap can be changed and fabricated independently, which make them suitable materials for optical spectroscopy and optoelectronic applications. The wide energy gap ternary alloys of groups II–VI are useful to optical devices in the blue–near-ultraviolet region [1]. While group III–V ternary alloys are useful to fabricate high speed switching devices, communication devices such as emitters, wave guides, optoelectronic devices like light emitting diodes, infrared detectors and infrared diode lasers in the visible–infrared regions [2,3]. Ternary alloy $Ga_xIn_{1-x}P$ is used in high-power and high-frequency electronics. It is used mainly in high electron mobility transistor (HEMT) [4], heterojunction bipolar transistor (HBT) [5–7], for the fabrication of high efficiency solar cells used for space applications [8,9] and in combination with aluminum (AlGaInP alloy) to make high brightness LEDs with orange-red, orange, yellow and green colors [10,11]. Specially important is the alloy $Ga_{0.5}In_{0.5}P$, which is almost lattice matched to GaAs [12]. This allows, in combination with $(Al_xGa_{1-x})_{0.5}In_{0.5}$, the growth lattice matched quantum wells for red emitting semiconductor lasers (650 nm) or vertical cavity surface emitting lasers (VCSELs) for plastic optical fibers [13]. $Ga_{0.5}In_{0.5}P$ is used as the high energy junction on double and triple junction photovoltaic cells grown on GaAs. The alloy of GaInP, lattice matched to GaInAs, is utilized as the high energy junction of GaInP/GaInAs/Ge triple junction photovoltaic cells [14]. These ternary alloys are strong candidates for sensors because they are very sensitive to external influences such as temperature, external fields and strains. Predicting the effect of strain on the electronic properties requires knowledge of elastic properties and elastic constants of materials. As elastic constants describe the response to an applied stress, study of the dependence of the elastic constants and their related elastic properties on the composition x of $Ga_xIn_{1-x}P$ is very important. The compounds GaP and InP crystallize in zinc-blende phase, making a continuous series of alloys $Ga_xIn_{1-x}P$, over the entire range in x from 0 to 1. Traditionally, because of simplicity, the virtual crystal approximation (VCA) is used to study various electronic properties of semiconductor ternary systems in which the effective potential is made up of the linear interpolated potentials of their constituent elements. But experimentally, band gap and refractive index variations show a non-linear bowing behavior regarding disorder [15,16]. The all electron mixed basis approach [17] and the coherent potential approximation (CPA) [18] have been proposed so far to study this disorder effect on the band structure of the material. But these methods require too much computational efforts. Bourissa [2] used an empirical pseudopotential method (EPM) within the improved virtual crystal approximation (VCA), which included the disorder effect. In the present paper we have used our novel model potential bearing a single parameter, using the improved VCA to study the composition effect on the elastic constants c_{11}, c_{12} and c_{44},

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bulk modulus, shear modulus, Young's modulus and Poisson's ratio of semiconductor ternary alloy $Ga_xIn_{1-x}P$. The paper is organized as follows. In Section 1 we give a brief introduction. Section 2 contains a theoretical background for the calculation procedure. Section 3 covers discussion of the results. A summary of our conclusions is narrated in Section 4.

2. Theory

The bare-ion potential used in the present investigations proposed in **r**-space [19] is

$$W^{\text{ion}}(r) = -\frac{Ze^2}{2R_c}\left[2-\left(2-\frac{r}{R_c}-\frac{r^2}{R_c^2}\right)\exp\left(\frac{-r}{R_c}\right)\right] \text{ for } r \le R_c$$

$$W^{\text{ion}}(r) = -\frac{Ze^2}{r} \text{ for } r \ge R_c \quad (1)$$

It is to be noted that to represent core–core repulsion usually the Born–Mayer term is employed. We have also incorporated this feature in our potential through exponential factor. Inside the core, it is represented as the combination of linear and quadratic terms modulated by repulsive exponential factor, which tends to cancel the Coulomb potential inside the core, while outside the core, it has the Coulombian tail. It becomes analytic at $r=0$ and smoothness of the bare-ion potential due to exponential term results in faster conversions in **r**-space. In addition this bare-ion potential is continuous at the core. Its form factor becomes

$$W_B(q) = \frac{-2\pi Ze^2}{\Omega_0 q^2}\left[\frac{2\sin u}{u} + \frac{1}{(1+u^2)^4}\left\{\begin{array}{l}(26u^2-28u^4-6u^6) \\ +e^{-1}\left(\begin{array}{l}\begin{pmatrix}3u^7+21u^5+\\ 49u^3-17u\end{pmatrix}\sin u \\ +\begin{pmatrix}2u^6-4u^4\\ -54u^2\end{pmatrix}\cos u\end{array}\right)\end{array}\right\}\right] \quad (2)$$

where Z, e, Ω_0, q and R_c are valency, electronic charge, atomic volume, reciprocal lattice vector and pseudo-core radius, respectively, and $u=qR_c$. Here R_c is estimated through the zero pressure condition.

For ternary semiconductor $Ga_xIn_{1-x}P$, the total form factor and lattice constant of the system are given by Vegard's law [2] as

$$V_{S,A}^{GaInP}(q) = xV_{S,A}^{GaP}(q) + (1-x)V_{S,A}^{InP}(q) \quad (3)$$

$$a^{GaInP} = xa^{GaP} + (1-x)a^{InP} \quad (4)$$

While considering the disorder effect the total form factor becomes

$$V_{S,A}^{GaInP}(q) = xV_{S,A}^{GaP}(q) + (1-x)V_{S,A}^{InP}(q) - p[x(1-x)]^{1/2}(V_{S,A}^{GaP}(q) - V_{S,A}^{InP}(q)) \quad (5)$$

Here $V_S(q)$ and $V_A(q)$ are symmetric and asymmetric part of the form factor, respectively. The value of adjustable disorder parameter is taken as $p=0.2$ to match the energy band gap. Vogl's polarity α_p [20] becomes

$$\alpha_p = -\frac{V_A(3)}{V_S(3)} \quad (6)$$

where $V_S(3)$ and $V_A(3)$ are the symmetric and asymmetric pseudopotential form factor at G(1 1 1), respectively. The transverse effective charge e_T^* is computed from the relation

$$e_T^* = \frac{1}{2}\left(-\Delta Z + \frac{8\alpha_p}{1+\alpha_p^2}\right) \quad (7)$$

$$\Delta Z = xZ_{Ga} + (1-x)Z_{In} - Z_P \quad (8)$$

Here Z_{Ga}, Z_{In} and Z_P are valences of Ga, In and P, respectively.

The elastic constants are calculated using the covalent and overlap interactions within the bond in tetrahedral compounds and improved the description by Baranowski [21]. After simplifications they are written as

$$c_{11} = \frac{\sqrt{3}\hbar^2}{4d^5 m}(1-\alpha_p^2)^{1/2}\left[4.37(5+\lambda)(1-\alpha_p^2) - 0.6075\right] \quad (9)$$

$$c_{12} = \frac{\sqrt{3}\hbar^2}{4d^5 m}(1-\alpha_p^2)^{1/2}\left[4.37(3-\lambda)(1-\alpha_p^2) + 0.6075\right] \quad (10)$$

$$c_{44} = \frac{\sqrt{3}}{4d}(\alpha+\beta) - 0.136SC_0 - C\zeta^2 \quad (11)$$

In the above equation, $d=\sqrt{3}a/4$ is the nearest neighbor distance and λ is a dimensionless parameter with constant value 0.738 [2]; α, β and ζ represent the bond-stretching force constants, bond-bending force constants and the internal-strain parameter, respectively [22], which are expressed as

$$\alpha = \frac{d}{\sqrt{3}}(c_{11}+3c_{12}) + \frac{d}{3\sqrt{3}}(1.473SC_0) \quad (12)$$

$$\beta = \frac{d}{\sqrt{3}}[(c_{11}-c_{12}) - 0.053SC_0] \quad (13)$$

$$\zeta = \frac{(2c_{12}-0.314SC_0)}{(c_{11}+c_{12}-0.314SC_0)} \quad (14)$$

Here

$$S = \frac{Z^{*2}}{\varepsilon} \quad (15)$$

$$Z^* = e_T^* - \frac{8}{3}\alpha_p(1-\alpha_p^2) \quad (16)$$

$$C_0 = \frac{e^2}{d^4} \quad (17)$$

$$C = \frac{\sqrt{3}}{4d}(\alpha+\beta) - 0.2666SC_0 \quad (18)$$

The values of static dielectric constant (ε) are 11.11 and 12.56 for GaP and InP [23], respectively, and Z^* is the effective charge.

Bulk modulus, shear modulus, Poisson's ratio and Young's modulus are, respectively, given by

$$B = \frac{c_{11}+2c_{12}}{3} \quad (19)$$

$$c' = \frac{c_{11}-c_{12}}{2} \quad (20)$$

$$\sigma = \frac{c_{12}}{(c_{11}+c_{12})} \quad (21)$$

$$Y = 3B(1-2\sigma) \quad (22)$$

3. Results and discussions

The input parameters are given in Table 1. In the present study we have considered only zinc-blende structures of GaP and InP. The elastic constants, for parent compounds computed using the

Table 1
Input parameters used in calculations.

Material	Structure	a (a.u.)	Ω_0 (a.u.)^3	k_F (a.u.)	ε [22]
GaP	Zinc-blend	10.30	136.70	0.9533	11.11
InP	Zinc-blend	11.09	170.50	0.8856	12.56