Available online at www.sciencedirect.com

ScienceDirect

ELSEVIER

Materials Chemistry and Physics 100 (2006) 41–47

MATERIALS CHEMISTRY AND PHYSICS

www.elsevier.com/locate/matchemphys

Elastic constants and acoustical phonon properties of $GaAs_xSb_{1-x}$

Nadir Bouarissa *

Department of Physics, Faculty of Science, King Khalid University, Abha, P.O. Box 9004, Saudi Arabia

Received 30 March 2005; received in revised form 20 November 2005; accepted 5 December 2005

Abstract

Elastic constants of zinc-blende $GaAs_xSb_{1-x}$ are calculated from the framework of the pseudopotential method within the virtual crystal approximation combined with the bond-orbital model of Harrison. These constants are used to calculate the sound wave velocities propagating in different directions in the material of interest. A particular attention has been devoted to the effect of compositional disorder. For this purpose, a correction to the alloy potential has been introduced. Numerically calculated values show reasonable agreement with known data. Comparisons between our results and those of interpolation schemes reported in previous studies suggest that the applicability of the linear interpolation approaches for the properties being studied for the alloy under consideration is possible.

PACS: 71.20.Nr

Keywords: III–V Semiconductor alloys; Elastic constants; Phonon properties; Pseudopotentials

1. Introduction

Ternary semiconducting alloys of III–V compounds are of continuing great interest owing to their vast technical applications, namely lasers, light-emitting diodes (LED), optical amplifiers, electro-optic modulators, detectors and frequency-mixing components [1]. The importance of these materials lies in the fact that their energy band structure and lattice parameters can be tailored independently which can lead to new semiconductor materials that may provide more diverse opportunities to achieve desired band gaps over a continuous broad spectrum of energies. $GaAs_xSb_{1-x}$ is one of the III–V ternary semiconductor alloys that is particularly important for the fabrication of electronic and opto-electronic devices covering the wavelength range between 0.9 and 1.7 μm. Despite the existence of an extensive miscibility gap, this alloy has been grown across the entire composition range by molecular beam epitaxy [2,3], organo-metallic vapor phase epitaxy [4], multi target sputter deposition [5,6] and liquid phase epitaxy [6,7]. Photoluminescence results on $GaAs_xSb_{1-x}$ epilayers with the composition ranging from 0 to 0.5 were reported in ref. [6]. A wide variety of III–V heterostructure devices is achieved by incorporating $GaAs_xSb_{1-x}$ epilayers with InAlAs for heterojunction field-effect transistors [8,9], with AlAsSb for distributed Bragg reflectors [9,10] and with AlGaSb for double heterostructure lasers [9,11]. It may serve as a model system for the investigation of the spontaneous ordering expected in III–V–V alloys [9,12].

Accurate modeling of device designs requires knowledge of the fundamental properties of the devices. Furthermore, information on the compositional dependence of these properties in semiconductor alloys is very important for the application. In spite of the importance of the knowledge of these properties and their compositional dependence, only limited experimental and theoretical investigations have been reported on them, while to the best of our knowledge there is no report up to date for the elastic and acoustical properties of $GaAs_xSb_{1-x}$ alloy unless linear interpolation schemes which are based on known values of the physical constants for the related end compounds (binaries) [13]. So, the aim of this work is to focus on the theoretical calculations of the compositional dependence of the elastic constants and acoustic wave velocities in $GaAs_xSb_{1-x}$. The calculations are based on the empirical pseudopotential method (EPM) under the virtual crystal approximation (VCA) combined with the bond-orbital model of Harrison. To take into account the compositional disorder effect, a correction to the alloy potential has been introduced. Our numerically calculated results over the full compositional range of the zinc-blende structure alloy are

---

* Tel.: +966 72269326; fax: +966 72269326.
E-mail address: N_Bouarissa@yahoo.fr.

0254-0584/$ – see front matter © 2005 Elsevier B.V. All rights reserved.
doi:10.1016/j.matchemphys.2005.12.004

Table 1
Experimental band-gap energies of GaSb and GaAs fixed in the fits

Material	Band-gap energy (eV)		
	E_{Γ}^{Γ}	E_{Γ}^{X}	E_{Γ}^{L}
GaSb	0.725[a,b]	1.03[b]	0.761[b]
GaAs	1.42[c]	1.81[c]	1.72[c]

[a] Ref. [16].
[b] Ref. [17].
[c] Ref. [18].

reported. The obtained results compare reasonably well with the known data in the literature.

2. Computational method

The calculations are based on the EPM under the VCA. Particular attention has been given to the effect of the alloy disorder. For this purpose, the compositional disorder effect is included as an effective potential [14,15]. In the EPM, the crystal potential is represented by a linear superposition of atomic potentials, which are obtained for parent compound semiconductors (i.e. GaSb and GaAs in the present work) 'empirically' requiring that the calculation reproduces the observed gaps at selected points in the Brillouin zone as accurate as possible. Table 1 gives the input experimental band-gap energies for GaSb and GaAs used in the fitting procedure. The procedure is based on the non-linear least-squares method [19] for the optimization of the empirical pseudopotential parameters. The dimension of our eigenvalue problem is a (136 × 136) matrix. However, 59 plane waves have given a good convergence in our case. Table 2 lists the final adjusted symmetric ($V_S(G)$) and antisymmetric ($V_A(G)$) pseudopotential form factors for GaSb and GaAs. Used lattice constants for these compounds are also shown in the table, while those of the alloy under study are calculated using Vegard's rule [20]. The adjusted pseudopotential form factors at $G(1\,1\,1)$ (where G is a reciprocal lattice vector) are used in the determination of the polarity (α_P) using the Vogl definition [21],

$$\alpha_P = -\frac{V_A(3)}{V_S(3)} \tag{1}$$

which in turn is used for the estimation of the transverse effective charge (e_T^*) using the expression reported in ref. [15] as,

$$2e_T^* = \Delta z + \frac{8\alpha_P}{1+\alpha_P^2} \tag{2}$$

with

$$\Delta z = -z_{Ga} + (1-x)z_{Sb} + x z_{As} \tag{3}$$

where z_{Ga}, z_{Sb} and z_{As} are the valency (number of the valence electrons) of Ga, Sb and As elements, respectively.

The pseudopotential form factors for the alloy under study are obtained using the approximation of Lee et al. [14], in which the potential of the alloy $A_xB_{1-x}C$ is represented by,

$$V(r) = V_{VCA}(r) + V_{dis}(r) \tag{4}$$

where $V_{VCA}(r)$ is the periodic virtual crystal potential and $V_{dis}(r)$ is the non-periodic potential due to the compositional disorder. For a particular distribution $V_{dis}(r)$ is given by [14,22],

$$V_{dis}(r) = (1-x)\sum_{j_A}\Delta(r-R_j) - x\sum_{j_B}\Delta(r-R_j) \tag{5}$$

where $\Delta(r) = V_{AC}(r) - V_{BC}(r)$. Here, j_A indicates that the summation on j is carried out on the AC molecular sites only, and j_B on BC molecular sites only. Lee et al. [14] introduced the disorder effect by assuming that $\sum_{j_A}\Delta(r-R_j) = \alpha x\sum_{j}\Delta(r-R_j)$ and $\sum_{j_B}\Delta(r-R_j) = \beta(1-x)\sum_{j}\Delta(r-R_j)$ where α and β are disorder functions dependent on the concentration x and the potential energy. With this approximation, the disorder potential becomes,

$$V_{dis}(r) = (\alpha-\beta)x(1-x)\sum_{j}\Delta(r-R_j) \tag{6}$$

The concentration dependence of $\alpha - \beta$ is evaluated by considering an ensemble average of the potential energy deviation from the VCA value. More details are given in ref. [14]. By simplification, the authors of ref. [14] found that,

$$\alpha - \beta = \pm[x(1-x)N]^{-\frac{1}{2}} \tag{7}$$

By assuming that the disorder lowers the effective potential and hence choosing the negative sign for $\alpha - \beta$, the effective disorder potential was given by,

$$V_{dis}(r) = -\left(\frac{x(1-x)}{N}\right)^{\frac{1}{2}}\sum_{j}\Delta(r-R_j) \tag{8}$$

Here, N is 12 for the face-centered cubic structure. By including the whole crystal in the contribution, $V_{dis}(r)$ could be written as,

$$V_{dis}(r) = -p[x(1-x)]^{1/2}\sum_{j}\Delta(r-R_j) \tag{9}$$

Table 2
Pseudopotential form factors and lattice constants for GaSb and GaAs

Material	Form factors (Ryd)						Lattice constant (Å)
	V_S (3)	V_S (8)	V_S (11)	V_A (3)	V_A (4)	V_A (11)	
GaSb	−0.191206	0.005	0.043533	0.045340	0.03	0.00	6.118
GaAs	−0.239833	0.0126	0.059625	0.060536	0.05	0.01	5.653