Materials Science in Semiconductor Processing 31 (2015) 493–500

Contents lists available at ScienceDirect

Materials Science in Semiconductor Processing

journal homepage: www.elsevier.com/locate/mssp

Band gap behavior of scandium aluminum phosphide and scandium gallium phosphide ternary alloys and superlattices

S. Benalia [a], M. Merabet [a], D. Rached [a,*], Y. Al-Douri [b], B. Abidri [a], R. Khenata [c], M. Labair [a]

[a] Laboratoire des Matériaux Magnétiques, Faculté des Sciences, Université Djillali Liabès de Sidi Bel-Abbès, Sidi Bel-Abbès 22000, Algérie
[b] Institute of Nano Electronic Engineering, University Malaysia Perlis, 01000 Kangar, Perlis, Malaysia
[c] Laboratoire de Physique Quantique et de Modélisation Mathématique de la Matière, (LPQ3M), Université de Mascara, Mascara 29000, Algérie

ARTICLE INFO

Available online 8 January 2015

Keywords:
Ab intio method
Ternary alloy
Energetic transition

ABSTRACT

Full-potential linear muffin-tin (FP-LMTO) has been implanted within density functional theory (DFT) and within local density approximation. The structural and electronic properties of GaP, AlP and ScP binary compounds and their ternary alloys $Sc_xAl_{1-x}P$ and $Sc_xGa_{1-x}P$ over a whole range of compositions ($0 \leq x \leq 1$) and the superlattices $Sc_{0.25}Ga_{0.75}P/Sc_{0.5}Ga_{0.5}P$ and $Sc_{0.25}Al_{0.75}P/Sc_{0.5}Ga_{0.5}P$ in the zinc-blende structure are investigated. The calculated resulted gave reasonable agreements with other published data.

1. Introduction

III–V compounds have been extensively studied theoretically and experimentally during the last decades. This family of semiconductors has demonstrated possibilities in terms of applications in optoelectronics; light-emitting diodes, laser diode, gas captors, solar cells and devices in hostile environments; high temperatures and high frequency with high-performance [1–17].

The III–phosphide binary compounds appear; at ambient conditions, these compounds crystallize in the zinc-blende structure and have indirect band gap [18–32], with exceptional cases of InP [33]. The weak optical transition in indirect gap materials GaP and AlP is a major limitation for their use in optical devices. The radiative transition in these materials is accompanied by phonon emission and the oscillator strength of such transitions is smaller compared to direct band-gap semiconductors like GaAs [34].

The search of new materials which allows the design and construction of new optoelectronics, takes us to propose new materials. These new ones exhibit a range of unexpected characteristics. Particularly, we have aimed to combine AlP to ScP and GaP to ScP with different structural and electronic properties in order to obtain new materials $Sc_xAl_{1-x}P$ and $Sc_xGa_{1-x}P$ ternary alloys with intermediate properties. It is also expected to give a good opportunity for superlattices (SLs) applications.

Recent investigations have showed that ScP crystallizes in the rocksalt (B1) phase with the possibility of transition to CsCl (B2) phase at high pressures, with a semi-metallic behavior in both phases. However, ScP has wide and direct band gap in the zinc blende (B3) phase [35]. We note that ScP has started to attract more attention [36,37], but there is still a lack of experimental investigations on it.

In order to take advantageous properties of these compounds for eventual technological applications, a theoretical investigation of structural and electronic properties is necessary. For this purpose we used the first-principle calculations to investigate the structural and electronic properties of the binary compounds GaP, AlP and ScP, the

* Corresponding author.

http://dx.doi.org/10.1016/j.mssp.2014.12.021
1369-8001/

ternary alloys; $Sc_xAl_{1-x}P$ and $Sc_xGa_{1-x}P$ over a whole range of compositions ($0 \le x \le 1$) and the superlattices $Sc_{0.25}Ga_{0.75}P/Sc_{0.5}Ga_{0.5}P$ and $Sc_{0.25}Al_{0.75}P/Sc_{0.5}Ga_{0.5}P$ in the zinc-blend structure, using the state of the art full-potential linear muffin-tin orbital (FP-LMTO) method, in the framework of density functional theory (DFT) within the local density approximation (LDA) for the exchange correlation functional.

The organization of the paper is as follows. In Section 2, we briefly described the employed method and the detailed calculations. Results and discussions of structural and electronic properties of binary, ternary and SLs presented in Section 3. In Section 4, a brief conclusion is presented.

2. Calculations

The calculations reported in this work were carried out using the full potential linear muffin-tin (FP-LMTO) [38,39]. This is an implementation of the density functional theory (DFT) which is a universal quantum mechanical approach for many body problems. In this theory, the quantum many body problems of interacting electrons and nuclei can mapped onto a system of one electron equations called Kohn–Sham equations [40,41]. In the FP-LMTO method the space is divided into an interstitial region (IR) and non-overlapping muffin-tin (MT) spheres centered at the atomic sites. In the IR region, the basis set consists of plane waves. Inside the MT spheres, the basis sets are described by radical solutions of the one particle Schrodinger equation (at fixed energy) and their energy derivatives multiplied by spherical harmonics.

In order to achieve energy eigenvalues convergence, the charge density and potential inside the MT spheres are represented by spherical harmonics up to $l_{max}=6$. The exchange–correlation potential is treated within the local density approximation developed by Perdew–Wang [42]. The self-consistent calculations are considered to be converged when the total energy of the system is stable within 10^{-5} Ry. The k integration over the Brillouin zone is performed on method using the tetrahedron method [43].

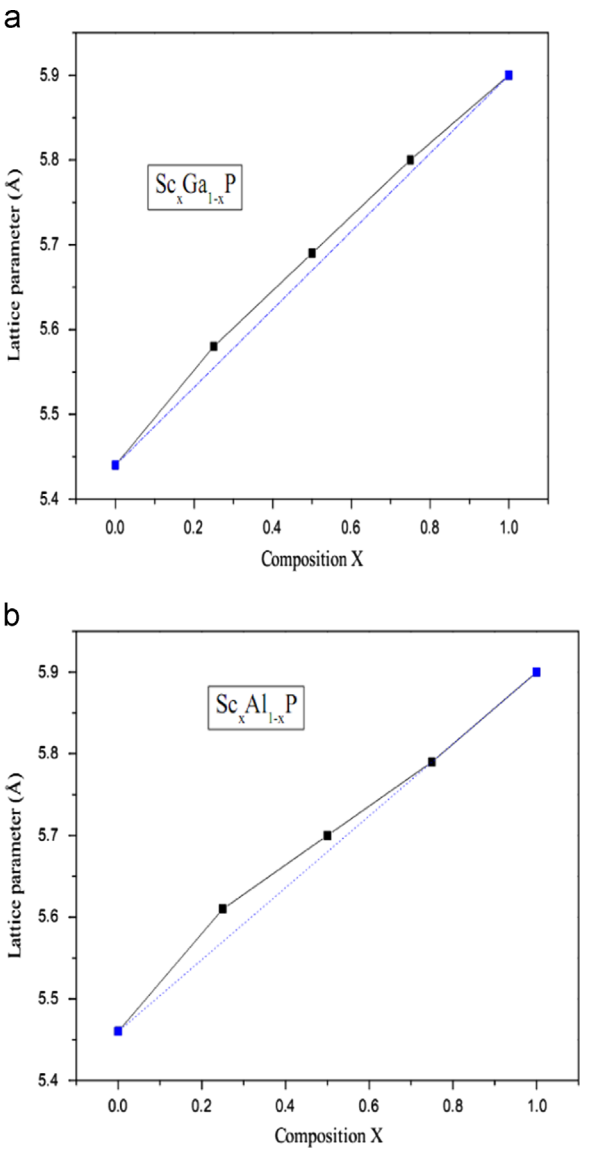

Fig. 1. Composition dependence of the calculated lattice constant (solid squares) of (a) $Sc_xGa_{1-x}P$ alloy and (b) $Sc_xAl_{1-x}P$ alloy; compared with Vegard's law (dotted line).

Table 1
Calculated lattice parameter (a), bulk modulus (B_0) and its pressure derivatives (B_0') for Sc_x $Al_{1-x}P$ and Sc_x $Ga_{1-x}P$ alloys and its binary compounds.

	x	a_0 (A)	B_0 (GPa)	B_0'
Sc_x $Al_{1-x}P$	0	5.46, 5.451[a], 5.511[b]	86.3, 86[a], 89[b]	4.144, 4.14[b]
	0.25	5.62	68.66	3.42
	0.5	5.7	69.25	3.33
	0.75	5.8	68	3.08
	1	5.9, 5.898[c]	66.45, 65.49[c]	3.45, 3.24[c]
Sc_x $Ga_{1-x}P$	0	5.44, 5.45[a], 5.512[b]	91.15, 91[a], 91[b]	3.6, 4.6[b], 4.76[b]
	0.25	5.57	67	4.18
	0.5	5.69	65.42	4.13
	0.75	5.8	63.8	3.31
	1	5.9, 5.898[c]	66.45, 65.49[c]	3.45, 3.24[c]

[a] Ref. [18].
[b] Ref. [29].
[c] Ref. [35].