Emerging Materials Research
Volume 2 Issue EMR2
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Pages 109–113 http://dx.doi.org/10.1680/emr.13.00004
Themed Issue Research Paper
Received 03/02/2013 Accepted 12/03/2013
Published online 15/03/2013
Keywords: electronic property/first-principles calculation/formation enthalpy/GaPxSb1-x/InPxSb1-x/structure

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Structural, thermodynamic and electronic properties of GaP_xSb_{1-x} and InP_xSb_{1-x} alloys

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In this study, the authors have investigated the properties of GaP_xSb_{1-x} and InP_xSb_{1-x} for various structures and compositions using first-principles method. The authors found that GaP_xSb_{1-x} is less relaxed than InP_xSb_{1-x} compounds, with respect to their respective binary compounds, due to the larger lattice mismatch. The formation enthalpy decreases from Ga to In compounds and increases with the increasing degree of alloy mixture. The crystal field splitting and band gap are larger in GaP_xSb_{1-x} than in InP_xSb_{1-x}. All the properties, investigated in this study, are strongly dependent on structure and composition. Good accord between the calculated results of this study and the experimental values in the literature is obtained.

1. Introduction

Group III–V ternary semiconductor alloys have been extensively studied for decades due to their technological applications in optoelectronic devices such as lasers, solar cells, optoelectronic integrated circuits and high-speed, low-power logic applications. For example, the adjustable band gap of GaP_xSb_{1-x} with composition[1] makes it a potentially useful material in fiberoptic communication systems. The expected resonance enhancement of the hole-impact ionization rate makes GaP_xSb_{1-x} a useful material for low-noise avalanche photodiodes using hole injection.[2] InP_xSb_{1-x} is an interesting material for optical devices in the mid-infrared. The first mid-infrared lasers, using InPSb layers, have been reported by some groups.[3,4]

Spontaneous ordering has been observed in both GaP_xSb_{1-x} and InP_xSb_{1-x} alloys. The types of ordering depend on the growth temperature, growth rates, III/V ratio, substrate misorientation and doping. One might expect important variations in the properties due to different ordering. For a ternary semiconductor alloy, AB_xC_{1-x}, there are five generally observed ordered structures derived from zincblende structure of the binary constituents (AB and AC) according to the Landau-Lifshitz theory,[5] that is, for composition 0·5–0·5, layered tetragonal CuAu-I-like (CA) structure, layered trigonal CuPt (CP) structure and chalcopyrite (CH) structure are derived, while for compositions 0·25–0·75 and 0·75–0·25, famatinite (FM) structure and luzonite-like (LZ) structure are derived. Details of these structures can be found in Ref. 6 and 7.

In this work, the authors study the structures, formation enthalpies and electronic properties of GaP_xSb_{1-x} and InP_xSb_{1-x} alloys for various ordering and composition, using first-principle total energy and self-consistent band structure calculations. A number of properties are addressed, including (*a*) qualitative relationship between degree of structural relaxation and lattice mismatch, (*b*) formation enthalpies, (*c*) ordering-induced crystal field splitting and (*d*) the alloy band gap and bowing coefficient. The calculated results are compared with the available experimental and theoretical data in the literature.

2. Method of calculation

The calculations of structure, total energy and electronic properties have been performed within the density functional formalism (local-density approximation [LDA]) by using the projector-augmented wave method.[8] The cut off energies and size of k points are tested to ensure that the total energies converge within 0·1 meV per atom. The authors use the Ceperley-Alder exchange correlation

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potential[9] as parameterized by Perdew and Zunger[10] as the exchange correction function. The Ga 3d and In 4d states are treated in the same manner as the other s and p valence states. Atomic and volume relaxations are performed for each unit cell. The calculated equilibrium lattice constants are 5·51, 6·22, 5·83 and 6·46 Å for GaP, GaSb, InP and InSb, respectively and are within 0·8% of the experimental values.[11]

3. Results and discussion

3.1 Structural properties

The authors have applied the first-principle total energy minimization approach to obtain the structural parameters of each ordered structure. The calculated lattice constants of the alloys are in accord with the experimental data[12,13] and follow a linear function with the alloy composition. The results of the calculations are presented in Tables 1 and 2. Some interesting features found in these calculations are discussed in the following sections.

3.1.1 Lattice relaxation

The standard zincblende structure has ideal tetragonal distortion parameter $\eta = 1$ and cell internal relaxation parameter $\mu = 0{\cdot}25$, corresponding to a fully relaxed structure. The deviations of these two parameters from their ideal values reflect the degree of structural relaxation of the alloys. The calculated results, in Tables 1 and 2, show that the deviations of these two parameters from their ideal values in GaPSb compounds are larger than those in InPSb compounds. This is due to the fact that the lattice mismatch between the binary constituents in GaPSb (11·2%) is larger than that in InPSb (9·8%). This indicates that the alloys with larger lattice mismatch between their constituents will be less relaxed.

3.1.2 Bimodal behavior

It is observed that the bond length in ordered conventional alloys such as GaAsSb and AlGaAs is not uniformly distributed. However, instead, it exhibits a bimodal behavior.[14] In this work, the authors have calculated the bond lengths in GaPSb and InPSb compounds. The results of bond lengths in In alloys are listed below (units: Å):

- ZB: R(In-P) = 2·525; R(In-Sb) = 2·795
- CA: R(In-P) = 2·576; R(In-Sb) = 2·754
- CH: R(In-P) = 2·539; R(In-Sb) = 2·773
- CP: R(In-P) = 2·500; R(In-Sb) = 2·728 (×3)
- R(In-P) = 2·611 (×3); R(In-Sb) = 2·820

Instead of average, the bond lengths exhibit a bimodal distribution. The short bonds in CA and CH structures are, in general, smaller, while the longer bonds are greater than those in the corresponding zincblende binary constituents. This local structure property indicates the importance of distortion and internal relaxation parameters in releasing the cell internal strain energy. Four different bonds (singlet and triplet) are observed in CP structure because there are more degrees of freedom to vary in that crystal relaxation. Similarly, singlet and doublet bonds are found in FM structure for composition 0·25 and 0·75.

3.2 Formation enthalpies

The formation enthalpy ΔH of alloy AB_xC_{1-x} is defined in terms of the fully relaxed total energies E of the alloy and binary components as follows:

$$\Delta H(x) = E(AB_xC_{1-x}) - xE(AB) - (1-x)E(AC) \quad (1)$$

The calculated results of ΔH are presented in Tables 1 and 2, and all the findings associated are discussed in the following sections.

3.2.1 Structure dependence

The calculated formation enthalpies show the trend $\Delta H(CP) > \Delta H(CA) > \Delta H(CH)$ for composition x = 0·5, suggesting that the alloys favor CH structure as their stable

Alloys	Structure	a (Å)	η	μ	ΔH (eV/atom)	Δ_{CF} (eV)	E_g (eV)	E_g (LDA+C) (eV)	b (eV)
$GaP_{0{\cdot}75}Sb_{0{\cdot}25}$	FM	5·554	0·998	0·268	0·039	0·042	0·832	1·56	3·306
$GaP_{0{\cdot}75}Sb_{0{\cdot}25}$	LZ	5·561	1·000	0·263	0·060	0	0·327	1·06	5·996
$GaP_{0{\cdot}5}Sb_{0{\cdot}5}$	CA	5·725	1·004	0·224	0·071	0·265	0·156	0·80	3·377
$GaP_{0{\cdot}5}Sb_{0{\cdot}5}$	CH	5·711	0·994	0·213	0·029	–0·082	0·891	1·52	0·438
$GaP_{0{\cdot}5}Sb_{0{\cdot}5}$	CP	5·735	1·002	0·234	0·084	0·523	–0·731	–0·10	6·923
$GaP_{0{\cdot}25}Sb_{0{\cdot}75}$	FM	5·882	0·998	0·231	0·027	0·012	0·365	0·90	0·98
$GaP_{0{\cdot}25}Sb_{0{\cdot}75}$	LZ	5·889	1·000	0·236	0·048	0	0·147	0·68	2·143

CA, CuAu-I; CH, chalcopyrite; CP, CuPt; FM, famatinite; LZ, luzonite; LDA, local-density approximation.

Table 1. LDA-calculated properties of GaP_xSb_{1-x} alloys.

Alloys	Structure	*a* (Å)	η	μ	ΔH (eV/atom)	Δ_{CF} (eV)	E_g (eV)	E_g (LDA+C) (eV)	*b* (eV)
$InP_{0.75}Sb_{0.25}$	FM	5·981	0·998	0·268	0·026	0·017	0·203	0·81	0·884
$InP_{0.75}Sb_{0.25}$	LZ	5·987	1·000	0·262	0·041	0	0·048	0·65	1·711
$InP_{0.5}Sb_{0.5}$	CA	6·142	1·003	0·225	0·049	0·195	–0·290	0·25	1·738
$InP_{0.5}Sb_{0.5}$	CH	6·132	0·995	0·217	0·020	–0·082	0·067	0·60	0·313
$InP_{0.5}Sb_{0.5}$	CP	6·147	1·002	0·234	0·059	0·517	–0·841	–0·31	3·946
$InP_{0.25}Sb_{0.75}$	FM	6·292	0·998	0·233	0·019	–0·001	–0·161	0·29	0·438
$InP_{0.25}Sb_{0.75}$	LZ	6·297	1·000	0·237	0·033	0	–0·291	0·16	1·129

CA, CuAu-I; CH, chalcopyrite; CP, CuPt; FM, famatinite; LZ, luzonite; LDA, local-density approximation.

Table 2. LDA-calculated properties of InP_xSb_{1-x} alloys.

ground-state structure rather than CA and CP structures. In experiments, the transmission electron diffraction pattern[15] shows a CA ordering mixed with disordered structure in GaPSb alloy. To verify this partial ordering structure, the authors calculated the formation enthalpy of disordered $GaP_{0.5}Sb_{0.5}$ alloy using special quasirandom structures (Q4) model.[16] The authors find that $\Delta H(CA) > \Delta H(Q4) > \Delta H(CH)$, indicates, as in experiments, a high possibility of finding a CA and random mixed structure. Similarly, $\Delta H(LZ) > \Delta H(FM)$ suggests that FM structure is more stable than that of LZ structure. For a given ordering, such as CA and LZ along (100) direction, the dependence of formation enthalpy on composition is also observed.

3.2.2 Trend from Ga to In cations

For a given structure, the calculated values show that the formation enthalpy decreases from GaPSb to InPSb compounds. This is due to the smaller lattice mismatch and smaller bulk modulus[17] in InPSb compounds. This smaller lattice mismatch leads to smaller strain energy and thus smaller formation enthalpy. This trend is consistent with the conclusion of lattice relaxation, in Section 3.1, that alloys with larger lattice mismatch will be less relaxed.

3.2.3 Degree of alloy mixture

The results show that the formation enthalpy does not monotonically decrease from GaP to GaSb. Instead, ΔH is smaller in $GaP_{0.25}Sb_{0.75}$ and $GaP_{0.75}Sb_{0.25}$ and larger in $GaP_{0.5}Sb_{0.5}$. The same trend is also found in In compounds. This is because large degree of alloy mixture induces more strain energy and hence larger formation enthalpy. This also explains the observation of large-range miscibility gap in experiments.

3.3 Electronic properties and bowing parameter

Tables 1 and 2 also show the LDA-calculated electronic properties (i.e. crystal field splitting and band gap) and bowing parameters. Together listed are the LDA-corrected[18] band gaps in order to compare with experimental values since LDA underestimates the band gap. The bowing parameters are calculated using the uncorrected band gaps.

3.3.1 Crystal field splitting

According to the perturbation theory, for a given structure, an alloy with larger valence band offset between its binary components will have larger crystal field splitting. For a given alloy, the crystal field splitting induced by structure effect can be described by $\frac{(\Delta V)^2}{(\epsilon_m[k_1]-\epsilon_n[k_2])}$ where, ΔV is the coupling matrix determined by the binary constituents' potential difference and bond length mismatch.[14] The energy denominator refers to the energy difference between the unperturbed states of the binary components before folding. The details of the folding relationship can be found in Ref. 14. With these two considerations, the authors can explain the results: (*i*) Among the different structures, the following relationship holds: $\Delta_{CF}(CP) > \Delta_{CF}(CA) > \Delta_{CF}(CH)$. This is because the energy difference $\epsilon_m(k_1)-\epsilon_n(k_2)$ of these structures follows an opposite sequence. For example, the energy difference $(\Gamma_{15v} - L_{3v} = 0\cdot925\ \text{eV})$ of CP structure of alloy $GaP_{0.5}Sb_{0.5}$ is much smaller than the energy difference $(\Gamma_{15v} - X_{5v} = 2\cdot56\ \text{eV})$ of its CA structure. The authors have listed the available experimental energy levels[11] in Table 3; (*ii*) for a given structure, the authors always have $\Delta_{CF}(\text{GaPSb}) > \Delta_{CF}(\text{InPSb})$ due to the same trend in band offset: GaPSb(1·04 eV) > InPSb(0·92 eV) and (*iii*) the negative crystal field splitting in CH structure occurs because of the stronger $(\Gamma_{15v} - W_{5v})$ coupling than $\Gamma_{15v} - X_{5v}$ coupling making the Γ_{4v} above Γ_{5v} state.[19]

3.3.2 Band gap

These calculated values of direct Γ point band gaps for all four alloy compounds have the following trend: $E_g(CH) > E_g(CA) > E_g(CP)$ and $E_g(FM) > E_g(LZ)$. This structure-induced difference in band gap can also be explained

	GaP	GaSb	InP	InSb
Γ_{15v}	−0·08	−0·75	−0·11	−0·80
L_{3v}	−1·13	−1·55	−1·00	−1·40
X_{5v}	−2·85	−3·10	−2·00	−2·40
Γ_{1c}	2·90	0·81	1·43	0·24
L_{1c}	2·64	1·10	2·04	1·00
X_{1c}	2·35	1·72	2·30	1·70

Table 3. Experimental energy levels (in eV) of zincblende binary constituents, GaP, GaSb, InP and InSb.

in terms of the perturbation theory used for crystal field splitting. However, the denominator energy difference will be mainly contributed by the conduction energy levels (Table 3).[11] The energy difference in CP structure $(\Gamma_{1c} - L_{1c} = 0 \cdot 015\,\text{eV})$ in $GaP_{0\cdot5}Sb_{0\cdot5}$ is smaller than the energy difference in CA structure $(\Gamma_{1c} - X_{1c} = 0 \cdot 18\,\text{eV})$, resulting in a greater band gap narrowing and hence a smaller band gap in CP phase. Similarly, the largest band gap in CH structure is due to the greatest $(\Gamma_{1c} - W_{1c})$ difference compared with CA and CP structures. The same mechanism can also explain the band gap comparison between FM and LZ structures. Comparison between Tables 1 and 2 also shows that the band gap of GaPSb compound is always larger than that of InPSb compound.

3.3.3 Bowing parameter

The band gap $E_g(x)$ of a random AB_xC_{1-x} alloy is described by a bowing function as follows:

$$E_g(x) = xE_g(AB) + (1 - x)E_g(AC) - bx(1 - x) \quad (2)$$

where, b is the bowing parameter. $E_g(AB)$ and $E_g(AC)$ are the band gaps of binary constituents AB and AC, respectively. The results show that the bowing parameters for these two systems depend strongly on the structures, that is, $b(CP) > b(CA) > b(CH)$ and $b(LZ) > b(FM)$. This is due to the different identities of the repelling states and the different symmetry properties. The calculations of GaPSb compound ordering along (001) plane shows that the bowing parameter increases by 58% from $GaP_{0\cdot25}Sb_{0\cdot75}$ to $GaP_{0\cdot5}Sb_{0\cdot5}$ and 78% from $GaP_{0\cdot5}Sb_{0\cdot5}$ to $GaP_{0\cdot75}Sb_{0\cdot25}$. For InPSb compound, the bowing parameter increases by 54% from $InP_{0\cdot25}Sb_{0\cdot75}$ to $InP_{0\cdot5}Sb_{0\cdot5}$. The reason for this large and composition-dependent bowing parameter is attributed to the large differences between the two constituents in their lattice constants and energy levels.

4. Comparison with experiments and other calculations

For the formation enthalpy, Fedders *et al.*[20] derived a model in terms of bond distortions and macroscopic elastic properties, which predicts results that are in good accord with experiments. They find the formation enthalpies of $GaP_{0\cdot5}Sb_{0\cdot5}$ to be 0·053 eV and $InP_{0\cdot5}Sb_{0\cdot5}$ as 0·056 eV, in good agreement with our calculated values of CA structure. This comparison of formation enthalpy may suggest that the CA structure can serve as the representative structure other than CH and CP structures.

For GaPSb compounds, Stringfellow group reported[12] a low-temperature photoluminescence peak at 1·394 eV for sample $GaP_{0\cdot73}Sb_{0\cdot27}$ and a fitted bowing parameter of 3·8 eV. Absorption spectra measurements[21] from the same group observed single-line peaks at 1·14 eV for $GaP_{0\cdot53}Sb_{0\cdot47}$ and 1·625 eV for $GaP_{0\cdot76}Sb_{0\cdot24}$ with bowing parameter of 3·11 eV. The calculations for the CA and LZ structures of GaPSb compound suggest that $GaP_{0\cdot5}Sb_{0\cdot5}$ and $GaP_{0\cdot75}Sb_{0\cdot25}$ should have band gaps of 0·8 and 1·06 eV and bowing parameter of 3·377 eV. The reason that their reported band gaps are larger than the predicted values is due to the fact that the structures of their samples are CA and disorder mixture and the band gap of random structure is larger than that of the CA structure.[19] Room temperature photoluminescence and optical transmission measurements[22] observed a peak at energy 0·845 eV, which is identified as band gap transition $E_0(\Gamma_V - \Gamma_{1c})$, in agreement with the calculated data.

For InPSb compound, Jou *et al.*[23] found, via low-temperature photoluminescence measurements, a direct band gap transition at an energy of 0·62 eV for $GaP_{0\cdot69}Sb_{0\cdot31}$ compared with 0·65 eV for composition 0·75–0·25 of the predicted value. Their fitting to all the experimental data yields a band gap of 0·35 eV for compound $InP_{0\cdot5}Sb_{0\cdot5}$ and bowing parameter of 1·83 eV, in accord with the predicted value 0·25 eV for band gap and 1·738 eV for bowing parameter. Similarly, photoluminescence and absorption spectra measurements, by Reihlen *et al.*,[24] suggest a band gap of 0·445 eV for $InP_{0\cdot577}Sb_{0\cdot423}$ with bowing parameter of 1·52 eV. It is to be noted here that neglecting the spin–orbital interaction makes the calculated band gap to deviate from the experimental values.

5. Summary

In summary, the crystal relaxation, formation enthalpy and electronic properties of GaP_xSb_{1-x} and InP_xSb_{1-x} are discussed for various structures and compositions. GaP_xSb_{1-x} is found to be less relaxed than InP_xSb_{1-x} compounds. The formation enthalpy is found to decrease from Ga to In compounds and to increase with increasing degree of alloy mixture. The crystal field splitting and band gap are larger in GaP_xSb_{1-x} than in InP_xSb_{1-x}. This has been explained in terms of the energy repulsion rules. All the properties are found to be strongly structure and composition dependent. Good accord between the calculated results of this and experimental values in the literature is obtained.

Acknowledgements

The authors thank Emeritus Professor Peter Y. Yu of the Department of Physics at the University of California–Berkeley for his very helpful comments on the manuscript.

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