

PACS 62.20.Dc, 71.15.Dx, 71.15H, 71.25T, 71.45N

Some physical properties of $\text{Si}_{1-x}\text{Ge}_x$ solid solutions using pseudo-alloy atom model

A.R. Jivani, H.J. Trivedi, P.N. Gajjar, A.R. Jani

Department of Physics, Sardar Patel University, Vallabh Vidyanagar-388 120, Gujarat, India

Phone: Head: +91-2692 – 226843; office: +91-2692 - 226844, 226845, 226846 (Ext. 211);

Fax: +91-2692-236475;

E-mail: janiar@rediffmail.com; jivani_a_r@yahoo.com

Abstract. Some electronic, thermodynamical and mechanical properties of $\text{Si}_{1-x}\text{Ge}_x$ solid solution with an arbitrary (atomic) concentration (x) are studied using the pseudo-alloy atom model. This work is based on the pseudopotential theory of covalent crystals and on the higher-order perturbation scheme with the application of our proposed model potential. We have used the latest local field correction function proposed by Sarkar *et al.* along with other four local-field correction functions of Hartree, Taylor, Utsumi *et al.* and Farid *et al.* to study Si-Ge system. The total energy of the $\text{Si}_{1-x}\text{Ge}_x$ solid solutions is investigated and compared with available experimental data. The calculated numerical values of the heat of solution for Si-Ge system are small and positive. The positive sign of the heat of solution predicts that, at low temperatures, the phase mixture will be more stable than the disordered solid solution. Like the case of simple metals, it is seen that a graph of the ratio of the heat of formations and $x(1-x)$ against x is linear. The bulk modulus of $\text{Si}_{1-x}\text{Ge}_x$ is also investigated with different concentrations x of Ge. We have found in the present study that the bulk modulus decreases linearly with an increase in the concentration x .

Keywords: pseudopotential method, $\text{Si}_{1-x}\text{Ge}_x$ solid solutions, the pseudo-alloy atom model, heat of formation, bulk modulus, elastic constants.

Manuscript received 20.07.05; accepted for publication 25.10.05.

1. Introduction

Group IV semiconductor alloys like Si-Ge, Ge-Sn, Si-Sn *etc.* have the immense potential for technological applications. The main reason for this is the requirement of the direct gap materials for fabrication of optoelectronic devices. The system, for example, Si-Ge improves the transport and optical properties as compared to silicon. Due to such applications of the system in optoelectronics devices, the theoretical and experimental studies of Si-Ge system is an important task [1-3]. The number of bonding electrons does not change when the solid solution of $\text{Si}_{1-x}\text{Ge}_x$ is formed and, hence, the theoretical study of the system of Si-Ge solid solutions is also interesting.

Previously, we have reported the application of our proposed model potential [4] to investigate the total energy, equation of state and bulk modulus of Si and Ge. We have also employed the model potential [4] to investigate some properties of Group III-V and Group II-VI semiconductor compounds [5-10]. The results obtained are in a good agreement with experimental

values and other available theoretical values. The application of the model potential proposed by Jivani *et al.* [4] is extended in the present work to investigate electronic, thermodynamical and mechanical properties of the $\text{Si}_{1-x}\text{Ge}_x$ solid solutions with an arbitrary (atomic) concentration x . In this work, we have used the pseudo-alloy atom model (hereafter referred to as PAA) to investigate the total energy, heat of solutions and bulk modulus of the $\text{Si}_{1-x}\text{Ge}_x$ system.

2. Computational method

2.1 Model potential

The form of the model potential proposed by Jivani *et al.* [4] in real space is

$$W(r) = -\frac{Z e^2}{R_c} \left[\frac{3 r}{2 R_c} - \frac{r^2}{2 R_c^2} \right], \quad r \leq R_c \quad (1)$$
$$W(r) = -\frac{Z e^2}{r}, \quad r \geq R_c$$

and its momentum-space representation of the model potential [4] is

$$W_b(q) = -\frac{12\pi Ze^2}{\Omega q^3 R_c} \left[\frac{\sin(qR_c)}{2} - \frac{1}{qR_c} + \frac{\sin(qR_c)}{(qR_c)^2} \right]. \quad (2)$$

Here, Z is the ion valency, e is the electron charge, Ω is the atomic volume, q is the wave vector and R_c is the parameter of the potential. The value of model parameter R_c for a single element is determined by satisfying the zero pressure equilibrium condition. The potential has a unique feature of interaction within the core, which consist of both linear and quadratic types of interaction. Due to such type of choice, the potential becomes weaker within core because of the cancellation of attractive (linear) and repulsive (quadratic) terms.

2.2 The higher-order perturbation theory

In the higher-order perturbation theory, the total energy of the crystal per atom [4] is given by

$$E = E_i + E_0 + E_1 + E_2 + E_{\text{cov}}. \quad (3)$$

In Eq. (3), E_i is the electrostatic energy of point ions in the uniform gas of valence electrons, E_0 is the sum of the kinetic, exchange and correlation energies of the valence electron, E_1 is the first-order perturbation energy of the valence electron due to the pseudopotential, E_2 is the second-order perturbation term, and E_{cov} is the covalent correction term. The detailed expressions of the energy terms used in Eq. (3) are given in reference [4].

2.3 Pseudo-alloy atom model

In the pseudo-alloy atom model, a hypothetical monoatomic periodic lattice is replaced by the disordered alloy [11]. The screened potential form factor $W_s^{\text{PAA}}(q)$ of an electron with a single PAA in the case of solid solution $\text{Si}_{1-x}\text{Ge}_x$ is given by

$$W_s^{\text{PAA}}(q) = -\frac{12\pi Z^{\text{PAA}} e^2}{\Omega q^3 R_c^{\text{PAA}} \varepsilon(q)} \times \left[\frac{\sin(q R_c^{\text{PAA}})}{2} - \frac{1}{q R_c^{\text{PAA}}} + \frac{\sin(q R_c^{\text{PAA}})}{(q R_c^{\text{PAA}})^2} \right], \quad (4)$$

where $Z^{\text{PAA}} = Z^{\text{Si}} = Z^{\text{Ge}} = 4$ and the parameter

$$R_c^{\text{PAA}}(x) = (1-x) R_c^{\text{Si}} + x R_c^{\text{Ge}}. \quad (5)$$

In Eq. (4), $\varepsilon(q)$ is the static Hartree dielectric function which is given by

$$\varepsilon(q) = 1 - \frac{8\pi e^2}{\Omega q^2} [1 - f(q)] \chi(q). \quad (6)$$

Here $f(q)$ is the local-field correction function and $\chi(q)$ is the perturbation characteristics that is given by

$$\chi(q) = -\frac{3Z}{4k_F^2} \left[\frac{1}{2} + \frac{1-\eta^2}{2\eta} \ln \left| \frac{1+\eta}{1-\eta} \right| \right];$$

$$\eta = \frac{q}{2k_F}. \quad (7)$$

For the incorporation of exchange and correlation effects to the dielectric function $\varepsilon(q)$ through $f(q)$, we have adopted five approximations, namely: Hartree (H) [12], Taylor (T) [13], Utsumi *et al.* (UI) [14], Farid *et al.* (F) [15] and Sarkar *et al.* (S) [16].

The system $\text{Si}_{1-x}\text{Ge}_x$ is composed of a monoatomic diamond type lattice like group IV elements. The total energy per atom $E^{\text{PAA}}(x)$ of the Si-Ge solid solution is calculated using the average screened potential as defined in Eq. (4) and model parameter as defined in Eq. (5).

2.4 The heat of formation

The heats of formation $\Delta E(x)$ for $\text{Si}_{1-x}\text{Ge}_x$ is defined as the energy difference between the energy of solid solution $E^{\text{PAA}}(x)$ and the energy of phase mixture $E_{\text{mix}}(x)$ that is given by

$$\Delta E(x) = E^{\text{PAA}}(x) - E_{\text{mix}}(x), \quad (8)$$

where the total energy of the phase mixture of $\text{Si}_{1-x} + \text{Ge}_x$ is given by

$$E_{\text{mix}}(x) = (1-x) E^{\text{Si}} + x E^{\text{Ge}}. \quad (9)$$

In Eq. (9), E^{Si} and E^{Ge} are the total energy per atom of Si and Ge calculated using Eq. (3).

2. Results and discussion

In Table, we have shown the total energy $E^{\text{PAA}}(x)$ of solid solutions $\text{Si}_{1-x}\text{Ge}_x$ using PAA model investigated using five different screening functions with different concentrations x of Ge. The obtained results are compared with the available experimental data [17]. The incorporation of exchange and correlation effects through various screening functions suppresses total energy of the solid solution in comparison with the static dielectric function. The inclusion of F local-field correction function generates the lowest total energy and use of H generates the highest total energy.

A graph of the heat of formation $\Delta E(x)$ for $\text{Si}_{1-x}\text{Ge}_x$ against the concentration x is plotted in Fig. 1. The local-field correction functions F and UI generate, respectively, maximum and minimum values of the heat of formation $\Delta E(x)$ at a particular concentration x and, hence, such results due to only these two screening functions are shown in Fig. 1. The higher value of investigated $\Delta E(x)$ at a particular concentration compared to the value reported by Soma [11] is due to

Table. The total energy ($-E^{\text{PAA}}$) in Rydberg per atom of solid solutions $\text{Si}_{1-x}\text{Ge}_x$ with various concentrations (x) of Ge.

x	Screening function $f(q)$					Observed [17]
	H	T	UI	F	S	
0.0	1.9452	2.1504	2.2035	2.2107	2.0815	1.98
0.1	1.9365	2.1409	2.1945	2.2010	2.0724	
0.2	1.9279	2.1315	2.1855	2.1914	2.0635	
0.3	1.9194	2.1221	2.1767	2.1818	2.0543	
0.4	1.9109	2.1129	2.1679	2.1724	2.0458	
0.5	1.9026	2.1038	2.1592	2.1630	2.0371	
0.6	1.8943	2.0947	2.1506	2.1537	2.0285	
0.7	1.8861	2.0857	2.1420	2.1445	2.0199	
0.8	1.8780	2.0768	2.1335	2.1354	2.0114	
0.9	1.8699	2.0680	2.1251	2.1264	2.0030	
1.0	1.8619	2.0592	2.1167	2.1175	1.9947	1.978

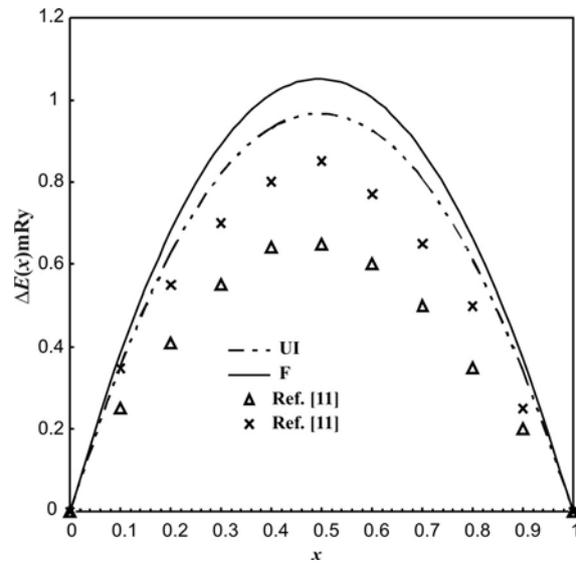
application of different exchange and correlation functions. Our investigated $\Delta E(x)$ at $x=0.5$ is deviated about 0.2 mRy to 0.4 mRy. It is also seen that $\Delta E(x)$ is small and positive. The positive sign of $\Delta E(x)$ predicts that, at low temperatures, the phase mixture will be more stable than the disordered solid solution. This favors the conclusion drawn by Soma [11] and Phillips [18].

In Fig. 2, we have shown the graph of $\Delta E(x)/[x(1-x)]$ against x . This ratio linearly varies with the atomic fraction x of Ge. The use of UI and F screening function generates maximum and minimum values of the ratio $\Delta E(x)/[x(1-x)]$ at the specific concentration x . The value of the ratio $\Delta E(x)/[x(1-x)]$ is almost constant for a particular screening function. This type of relation was studied by Soma [19] for alloys composed of alkali metal having the nearly equal atomic size. In spite of nonmetallic bonding presented in SiGe system, such linear relationship is observed and this is due to the nearly equal atomic size of Si and Ge.

We have calculated the bulk modulus by using the second derivative of the cohesive energy with respect to the atomic volume [20]. As shown in Fig. 3, the bulk modulus varies linearly with the concentration x . The bulk modulus decreases with increase in the concentration x . The linear relation between the calculated bulk modulus and the concentration x with the application of Sarkar *et al.* [16] screening function is

$$B \text{ (GPa)} = -14.8x + 91.421. \quad (10)$$

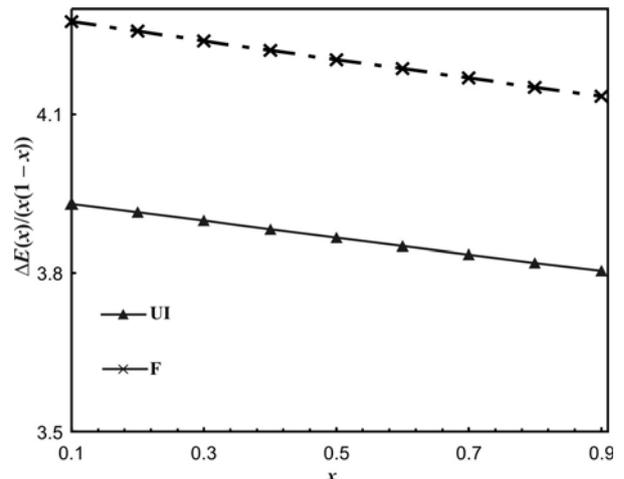
It is also seen from the graph that the bulk modulus at the concentration x due to S agrees well with the


Fig. 1. The energy difference $\Delta E(x)$ in mRy between the phase mixtures and solid solutions in PAA.

available experimental values [17] and other such reported values measured at the room temperature [21].

In conclusion, electronic, thermodynamic and mechanical properties of Si-Ge solid solutions are studied employing the present formulation of the model potential [4] with the higher order perturbation theory and the pseudo-alloys atom model. Study of physical properties is an important task due to importance of SiGe alloys system. The following conclusions can be drawn from the present studies:

1. The inclusions of screening functions in the investigations of total energy of SiGe system play an important role.


Fig. 2. The ratio $\Delta E(x)/[x(1-x)]$ as a function of the atomic fraction x of Ge.

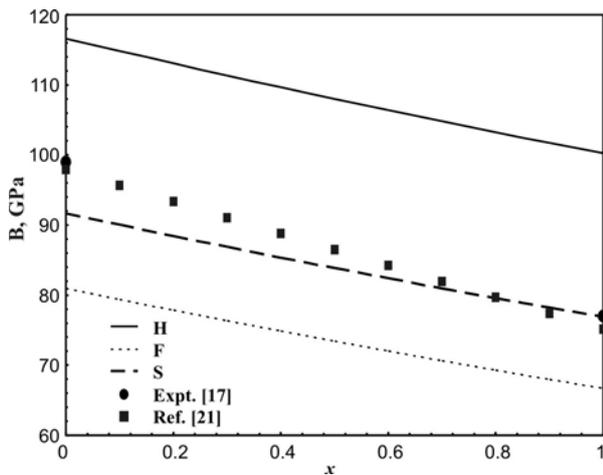


Fig. 3. Bulk modulus B (in GPa) of Si-Ge system as a function of the concentration x .

- At low temperatures, the phase mixture will be more stable than the disordered solid solution.
 - The linear relationship exists between $\Delta E(x) / [x(1-x)]$ and concentration x .
 - The relationship between the calculated bulk modulus and concentration x is also linear.
- Hence, this work will surely helpful for a better understanding of the physical properties of Si-Ge alloys.

Acknowledgements

We acknowledge the financial support of University Grand Commission, New Delhi.

References

- N. Bouarissa, F. Annane, Electronic properties and elastic constants of the $\text{Ge}_{1-x}\text{Sn}_x$ alloys // *Material Science and Engineering* **B95**, p. 100-106 (2002).
- S. Gonzalez, Empirical pseudopotential method for the band structure calculations of strained silicon germanium materials. Ph. D. Thesis, Arizona State University, Arizona, 2001.
- C.J. Williams, Impact ionization and Auger recombination in SiGe heterostructures. Ph. D. Thesis, University of Newcastle, Tyne, 1996.
- A.R. Jivani, P.N. Gajjar and A.R. Jani, Total energy, equation of states and bulk modulus of Si and Ge // *Semiconductor Physics, Quantum Electronics and Optoelectronics* **5**, p. 243-246 (2002).
- A.R. Jivani, H.J. Trivedi, P.N. Gajjar and A.R. Jani, Some physical properties of GaX ($X = \text{P}, \text{As}$ and Sb) semiconductor compounds using higher-order perturbation theory // *Physica B* **357**, p. 305-311 (2005).

- A.R. Jivani, H.J. Trivedi, P.N. Gajjar and A.R. Jani, Total energy, equation of state and bulk modulus of AlP, AlAs and AlSb semiconductors // *Pramana - Journal of Physics* **64**, p. 153-158 (2005).
- A.R. Jivani, P.N. Gajjar and A.R. Jani, Application of pseudopotential to III-V semiconductor compounds // *Indian J. Pure and Appl. Phys.* **42**, p. 833-836 (2004).
- A.R. Jivani, S.R. Mishra, Manjul Kumar, P.N. Gajjar and A.R. Jani, Application of model potential to III-V semiconductor compounds // *Solid State Phys. (India)* **45**, p. 469-470 (2002).
- A.R. Jivani, P.N. Gajjar and A.R. Jani, Some static properties of II-VI semiconductor compounds // *Solid State Phys. (India)* **46**, p. 735-736 (2003).
- A.R. Jivani, P.N. Gajjar and A.R. Jani, Elastic and electronic properties of Ga-based semiconductor compounds // *Solid State Phys. (India)* **49**, p. 457-458 (2004).
- T. Soma, The electronic theory of Si-Ge solid solution // *Phys. status solidi (b)*, **95**, p. 427-431 (1979).
- W.A. Harrison, Pseudopotential in the theory of metals, World Scientific, Singapore (1999).
- R. Taylor, A simple useful analytical form of the static electron gas dielectric function // *J. Phys. F* **8**, p. 1699-1702 (1978).
- K. Utsumi and S. Ichimaru, Dielectric formulation of strongly coupled electron liquids at metallic densities IV. Static properties in the low-density domain and the Wigner crystallization // *Phys. Rev. B* **24**, p. 3220-3230 (1981).
- B. Farid, V. Heine, G.E. Engel and I.J. Robertson, Extremal properties of the Harris-Foulkes functional and an improved screening calculation for the electron gas // *Phys. Rev. B*, **48**, p. 11602-11621 (1993).
- A. Sarkar, D. Sen, S. Halder and D. Roy, Static local factor for dielectric screening function of electron gas at metallic and lower densities // *Modern Phys. Lett. B* **12**, p. 639-648 (1998).
- G. Grosso and G.P. Parravicini, *Solid State Physics*. Academic Press, New York (2000).
- J.C. Phillips, *Bonds and Bands in Semiconductors*. Academic Press, New York (1973).
- T. Soma, H. Matsuo, and M. Funaki, The electronic theory of the alloy systems composed of Alkali metal elements II phase diagrams // *Phys. status solidi (b)* **108**, p. 221-227 (1981).
- T. Ito, K.E. Khor and S. Das Sarma, Empirical potential-based Si-Ge interatomic potential and its application to superlattice stability // *Phys. Rev. B* **40**, p. 9715-9722 (1989).
- <http://www.ioffe.rssi.ru/SVA/NSM/semicond/SiGe/mechanic.html>.