

Thermal Expansion of Al_{0.3}Ga_{0.7}As by Molecular Dynamics Simulation

S.Chitra

Head and Associate Professor, Department of Physics, Sri Parasakthi College for Women, Courtallam,
Nellai district, India

ABSTRACT: Thermal expansion of Al_{0.3}Ga_{0.7}As is studied by Molecular Dynamics simulation(MDS) and experimentally also studied here using Fizeau's method to compare the results of simulation method Tersoff's potential is used for the simulation for this alloy. Good agreement between the two is reported here. The results are discussed in comparison to the host GaAs.

KEYWORDS: Thermal expansion, Aluminium Gallium arsenide, Molecular dynamics simulation, Tersoff's potential, Fizeau's experiment.

I. INTRODUCTION

Aluminium Gallium arsenide is a technologically important material with variety of applications. For example Al_{0.3}Ga_{0.7}As/GaAs hetero structure is a promising material for high speed transistors and optoelectronic devices. New devices like modulated doped FET, heterojunction bipolar transistors, hot electron transistors, resonant tunneling transistors, quantum well lasers and other photonic and quantum devices have been developed recently using this heterostructure system. Efficiency and performance of such devices may depend on the defect level present in the material and how likely those defects are to be mobile under device operating conditions. During cooling down in the epitaxial growth, a difference in the thermal expansion can produce a drive force which moves the defects in the heterostructure. Experiments and theory on Ga_xAl_{1-x}As: Si show that at x = 0.22 there exists DX centers and the site symmetry also goes to C_{3v}/1/. So works on this alloy for x > 0.22 are extensively carried out, even though persistent photoconductivity (PPC) exists when x < 0.22.

In many of the device applications, other than the PPC, x > 0.22 is useful. But when such systems Al_xGa_{1-x}As is synthesized, annealing and quenching in the growth, demands a detailed study on the thermal expansion of this alloy. The thermal expansion coefficient (α_{th}) for Al_xGa_(1-x)As has been measured by Leszczynski /2/ (for x=0.30 and x=0.71; T ~750 K). By using least square method, Takahashi /3/ has obtained the linear relationship between α_{th} and x for Al_xGa_{1-x}As to be

$$\alpha_{th}(x) = (5.97 - 1.76x) \times 10^{-6} \text{ K}^{-1}$$

Studies on the expansion coefficient of Al_xGa_{1-x}As/GaAs multilayer structure by Bakmisiuk et al /4/ are also available. As there is no study on Al_{0.3}Ga_{0.7}As by simulation for thermal expansion we have here studied the same by Molecular dynamics simulation. Also we measured the same for the sample by experimental method.

II. MD SIMULATION FOR THERMAL EXPANSION OF Al_{0.3}Ga_{0.7}As

Molecular dynamics simulation (MDS) has been chosen as there is a deliberate time dependence with heat flow. Recently Kurobori et al /5/ have carried out molecular dynamics simulation for the study of thermal expansion coefficient of BaFX (X= Cl, Br) crystals by studying the temperature dependence of lattice parameters (a and c) by constructing a simulation cell of 750 atoms. Similarly they have investigated the other thermal properties by this method / 6/. In all these investigations Born-Mayer potential is used for the simulation. Even though the validity of the

International Journal of Innovative Research in Science, Engineering and Technology

(A High Impact Factor & UGC Approved Journal)

Website: www.ijirset.com

Vol. 6, Issue 9, September 2017

simulation is verified there by working the melting point, there is considerable deviation between the measured and simulated results of thermal expansion for AlGaAs with Tersoff's potential as the basis. Also this is a different approach compared to Kurobori et al /5/. In the present work, simulation cell of dimension 3 x 3 x 3 having four atoms of Ga and As in every cell is constructed. 216 particles are arranged in the zinc blende type lattice and the positions of these atoms are first fixed with the zinc blende basis and the boundary conditions. Then 30% of Ga atoms are replaced by Al atoms in the Al_{0.3}Ga_{0.7}As alloy. The three body potential, Tersoff's potential is considered for the interaction between the atoms. Tersoff's potential has been successfully used to implement the simulation on the semiconducting systems Si and GaAs /7,8/ Similarly Murugan et al /9/ have used this potential to study self and impurity diffusion in GaAs and Jalal /10/ to work out the thermal conductivity in GaAs by MDS. We calculated the Tersoff's potential parameters for Al_{0.3}Ga_{0.7}As alloy using the parameters of GaAs /10/ and are given in Table-2. Here microcanonical ensembles (particles) are considered where all quantities like total energy, volume and number of particles in the ensembles are kept constant. No heat transfer between the cells is allowed. Using the initial positions of the atoms in Al_{0.3}Ga_{0.7}As, possessing zinc blende structure, the cohesive energy at temperature 0K is computed using Tersoff's potential /11/ as,

$$E = \sum_i E_i = \frac{1}{2} \sum_{i \neq j} V_{ij} \quad (1)$$

where V_s represents the Tersoff's potential and is given as

$$V_{ij} = f_c(r_{ij}) [a_{ij} f_R(r_{ij}) + b_{ij} f_A(r_{ij})]$$

$$f_R(r) = A \exp(-\lambda_1 r)$$

$$f_A(r) = -B \exp(-\lambda_2 r)$$

f_R and f_A are the repulsive and attractive potential functions λ_1 and λ_2 are the parameters of attractive and the repulsive potential function, a_{ij} and b_{ij} are the weight factors for the repulsive and attractive parts. f_c is the cutoff function given by

$$f_c(r) = \begin{cases} 1 & r < R - D \\ \left(\frac{1}{2}\right) - \frac{1}{2} \sin\left(\frac{\pi(r-D)}{2D}\right) & \text{for } R - D < r < R + D \\ 0 & r > R + D \end{cases} \quad (2)$$

$$a_{ij} = (1 + \alpha^n \eta_{ij}^n)^{-1/2n}$$

$$\eta_{ij} = \sum_{k(\neq i,j)} f_c(r_{ik}) \exp[\lambda_3^3 (r_{ij} - r_{ik})^3]$$

$$b_{ij} = (1 + \beta^n \zeta_{ij}^n)^{-1/2n}$$

$$\zeta_{ij} = \sum_{k(\neq i,j)} f_c(r_{ik}) g(\theta_{ijk}) \exp[\lambda_3^3 (r_{ij} - r_{ik})^3]$$

$$g(\theta) = 1 + \frac{c^2}{d^2} - \frac{c^2}{[d^2 + (h - \cos \theta)^2]}$$

$\alpha, \beta, \lambda_3, c, n$ and h are the parameters to arrive at the complete potential. Thus the construction of the Tersoff's potential needs the estimation of 13 parameters and they are now computed for the system, Al_{0.3}Ga_{0.7}As as given in Table-1.

International Journal of Innovative Research in Science, Engineering and Technology

(A High Impact Factor & UGC Approved Journal)

Website: www.ijirset.com

Vol. 6, Issue 9, September 2017

Table 1 The parameters of the Tersoff's potential for Al_{0.3}Ga_{0.7}As

Parameter	A(eV)	B (eV)	λ_1 (\AA^{-1})	λ_2 (\AA^{-1})	λ_3 (\AA^{-1})	n	h	β	c	d	R (\AA)	D (\AA)	α (\AA)
	3017.71	373.105	2.383	1.452	0.000	7.495	0.615	0.428	1.455	0.937	4.2	0.118	0.12

Now the force acting on any atom due to other atoms is obtained from the gradient of the potential function. The two body (r) and the three body interaction term (θ) are separately considered for the computation of the force on all the atoms at $t = 0$. Considering the reduced mass of Al_{0.3}Ga_{0.7}As the maximum velocity of the particle v_{\max} is computed using

$$v_{\max}^x = v_{\max}^y = v_{\max}^z = \sqrt{\frac{k_B T}{2m}} \text{ at temperature } T \quad (3)$$

Now, between $-v_{\max}$ and $+v_{\max}$ the velocity of other atoms are assumed to be distributed uniformly. In an one dimensional case, let v_{xi} be the velocity of i_{th} atom in the x direction and the actual temperature is T_A . The temperature of the system is obtained from velocities as

$$T = \frac{2}{3Nk_B} \left\langle \sum m_i v_{xi} v_{xi} \right\rangle \quad (4)$$

That is the velocities are properly averaged in order to take care of the calculation of the velocity of atoms from the previously calculated values during iterative procedure. New velocities are calculated using $v_{xi}^{new} = v_{xi} \sqrt{\frac{T}{T_A}}$. Here Verlet

algorithm is chosen for the computation of the new time dependent displacement, $r(t + \Delta t)$, velocity $v(t + \Delta t)$ and acceleration $a(t + \Delta t)$ from the previous known values of $r(t), v(t), a(t)$. The Verlet algorithm is briefly mentioned here.

$$\begin{aligned} r(t + \Delta t) &= r(t) \Delta t + v(t) \Delta t + (1/2)a(t)(\Delta t)^2 \\ v(t + \Delta t/2) &= v(t) + (1/2) a(t) \Delta t \\ a(t + \Delta t) &= -(1/m)\nabla U(r(t + \Delta t)) \\ v(t + \Delta t) &= v(t + \Delta t/2) + (1/2) a(t + \Delta t) \Delta t \end{aligned} \quad (5)$$

where $r(t)$ and $a(t)$ are position and acceleration of the particle at time t .

The system may not be conserved for energy and linear angular momenta when simulation is tried for some specific trials. Hence it is essential to wait till the system reaches equilibrium. This is called energy equilibration and in our simulation a minimum of 20,000 trials are required to reach that. Fig:1 give the equilibration of kinetic (KE), potential (PE) and total energy (TE) of the system separately when the simulation is done for 30000 trials. Now, 20001st trial will be considered as $t = 0$.

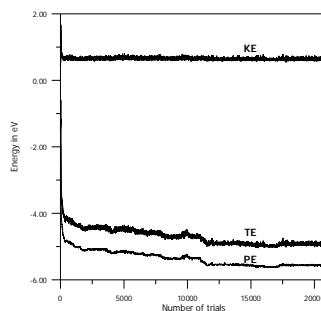


Fig-1: Energy equilibration by MDS

International Journal of Innovative Research in Science, Engineering and Technology

(A High Impact Factor & UGC Approved Journal)

Website: www.ijirset.com

Vol. 6, Issue 9, September 2017

III. FIZEAU'S EXPERIMENT

Fizeau's method is followed here for the measurement of thermal expansion in this $Al_{0.3}Ga_{0.7}As$ to compare the results with that of by MDS. The linear expansivity of the crystal is the increase in length for unit rise of temperature. By Fizeau's experiment technique the linear expansivity of $Al_{0.3}Ga_{0.7}As$ sample is measured, using the formula

$$h = \frac{L\lambda}{2\beta} \quad (6)$$

where 'h' is the height of air wedge or the sample, here a dimension of (10 mm X 6 mm) with about 700 microns thickness of $Al_{0.3}Ga_{0.7}As$ has been used. 'β' is the fringe width, 'λ' be the wavelength of the source of light.

IV. RESULTS AND DISCUSSION

Molecular dynamic simulation is a convenient tool to measure the high temperature activities as anharmonic interactions between atoms are properly considered whereas the conventional lattice dynamical calculations will be complex for the same. MDS is used here to calculate the thermal expansion coefficient, α_{th} by studying the equilibration cohesive energy of the system since thermal properties of $Al_{0.3}Ga_{0.7}As$ like thermal diffusivity and thermal conductivity were already measured by photoacoustic technique and molecular dynamics simulation [12] and showed a very good agreement with the literature values. Tersoff's potential is used to calculate the cohesive energy. When the temperature varies, the lattice constant will vary due to thermal expansion. But for any particular temperature, when the system is in equilibrium, the cohesive energy of the system will be minimum i.e at a particular temperature, the lattice constant is varied slowly and every time the simulation program is run to find the cohesive energy. As a typical example, a graph is given (Figure-2) for two specific temperatures, 300K and 400K. Like this for different temperatures, the program is run. For each temperature, the lattice constant corresponding to the minimum of Cohesive energy is noted. With these data, a graph is drawn (Figure-3) for the variation of the lattice constant with temperature.

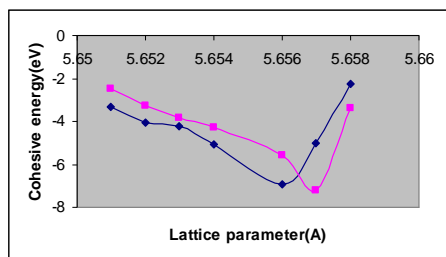


Fig-2 Variation of cohesive energy parameter

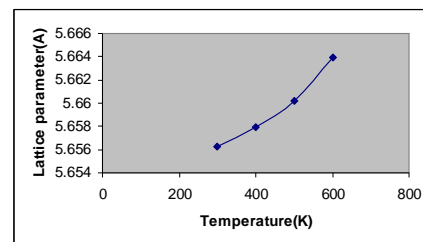


Fig-3 Variation of lattice parameter with with lattice temperature

It is found that there is increase in the lattice parameter with respect to temperature. Figure -(3) shows the expansion of the system. Using the equation

$$\alpha_{th} = \frac{1}{a_o} \left(\frac{\partial a_o}{\partial T} \right)_p \quad (7)$$

the thermal expansion coefficient is then calculated. The results, (Table-2) of MDS agree well with the literature value and also by Fizeau's experiment.

International Journal of Innovative Research in Science, Engineering and Technology

(A High Impact Factor & UGC Approved Journal)

Website: www.ijirset.com

Vol. 6, Issue 9, September 2017

Table-(2) : Thermal expansion coefficient of Al_{0.3}Ga_{0.7}As at room temperature

S.No.	Method	Thermal expansion coefficient $\alpha_{th} \times 10^{-6} \text{ K}^{-1}$
1	Simulation by MDS	5.310
2	Fizeau's experiment	5.432 /4/
3	Literature ^[13]	5.442

ACKNOWLEDGEMENT

Author wish to thank University Grants Commission for providing fellowship under FIP scheme. Also thank Prof. B.M.Arora, Tata Institute of Fundamental Research, Mumbai for providing Al_{0.3}Ga_{0.7}As sample.

REFERENCES

- [1] J.A.Wolk, M.B.Kruger, J.N.Heyman, W.Walukiewicz, R.Jeanloz and E.E.Haller, Phys.Rev.Lett.66, 774(1991)
- [2] M.Leszczynski, Cryst. Res. Technol. **25**, 721(1990)
- [3] N.S. Takahashi, in Properties of aluminium gallium arsenide, EMIS Data reviews Series No.7, edited by S.Adachi (INSPEC (IEE), London, 1993), p.43.
- [4] J.Bak-Misiuk, J.Wolf and U. Pietsch, Phys. Status Solidi A **118**, 209(1990).
- [5] T.Kurobori, Y.Hirose and M.Takeuchi, Phys.Status solidi (b), Rapid Resaerch notes, 220, No.2(2000)R11-R12
- [6] T.Kurobori, S.Kozake, T.Kawamoto and Y.Hirose, Jpn. J. Appl.Phys. 39, No.6A(2000)1537-1540.
- [7] M.Sayed, J.H.Jefferson, A.B.Walker and A.G.Cullis, Nucl.Instr. and Meth.B **102**, 218 (1995)
- [8] W.Sekkal, H.Aourag and M. Certier, J.Phys.Chem. Solids **59**, 1293 (1998)
- [9] P.Murugan and K.Ramachandran, Defects and Diffusion forum (Swiss.), **177-178**, 69 (2000)
- [10] A.Jalal, M.Phil thesis submitted to Madurai Kamaraj University, Oct, 2001
- [11] J.Tersoff, Phys.Rev B, **39**, 5566 (1989)
- [12] S.Chitra and K.Ramachandran, Inter.J. of Mod. Physics C, **14**(2003)
- [13] S.Adachi, GaAs and Related materials (Bulk semiconducting and superlattice propertices) World Scientific, Singapore, 1994