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RESEARCH ARTICLE

THERMAL DIFFUSIVITY OF $Al_{0.3}Ga_{0.7}As$ BY MOLECULAR DYNAMICS SIMULATION AND THERMOGRAPH METHOD

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ABSTRACT

The thermal diffusivity of $Al_{0.3}Ga_{0.7}As$ is studied by Molecular Dynamics simulation (MDS). Tersoff' s potential is used for the simulation for this alloy. Also experimentally studied here using photoacoustic method and thermography. Thermal diffusivity determined experimentally agrees well with the MD simulation and literature values /12/. The results are compared with the host GaAs.

INTRODUCTION

Aluminium Gallium arsenide is a technologically important material and has variety of applications. For example $Al_{0.3}Ga_{0.7}As$/GaAs heterostructure system is a promising material system for high speed transistors and optoelectronic device applications. New devices like modulated doped FETS, heterojunction bipolar transistors, hot electron transistors, resonant tunneling transistors, quantum well lasers and other photonic and quantum devices have been developed recently using this hetero structure 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. The tandem solar cell concept in which high energy photons are converted into high electrical power has been proved with an AlGaAs/GaAs tandem solar cell. The most efficient cell featured an excellent efficiency of 28.85% due to conversion of high energy photons into photovoltage (Ken Takahashi *et al*.) AlGaAs window allows electrons and holes to be created close to the electric field at the junction. It has been reported that low temperature metal insulator semiconductor field effect transistor (MISFET) devices fabricated using $Al_{0.3}Ga_{0.7}$ As have better transconductance frequency dispersion characteristics than low temperature GaAs MISFET devices (Rapeta *et al*., 2001).

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Literature studies shows that there is no earlier study on $Al_3Ga_{0.7}As$ material by simulation hence carried out here and the results are compared with literature values, thermograph and photoacoustic experiment, which are sensitive and accurate method especially for thin sample of material.

Modelling of $Al_{0.3}Ga_{0.7}As$ alloy

GaAs has been modelled and studied previously by Murugan *et al*. (Bak-Misiuk *et al*., 1990) hence the same method is followed here to study AlGaAs. The unit cell of GaAs has zinc blende structure. So it consists of 8 atoms per unit cell. Now to carryout simulation, a simulation cell of dimension 3 x 3 x 3 having four atoms of Ga and As in every cell is constructed i.e. three unit cells along x- axis, three unit cells along y- axis and three unit cells along z- axis. Therefore totally there are 216 particles. All these 216 particles are arranged in the zinc blende type lattice here to start with and the positions fixed with the following basis:

0	0 0; 0 ½ 0	½ ½; ½	0 ½; ½
¼	¼ ¼; ¼ ¾ ¼	¾ ¾; ¾	¼ ¾; ¾

Now, modelling of $Al_{0.3}Ga_{0.7}As$ alloy is done as follows: Al atoms are placed randomly in the place of Ga atoms in the modelled GaAs simulation cell. Thus the Al atoms replace

30% of Ga atoms. Now the modelled crystal is $Al_{0.3}Ga_{0.7}As$. The placement of aluminium atoms in GaAs unit cell is random using random number generator. Here microcanonical ensembles (particles) are considered for the convenience of computation 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. 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.

Simulation to study thermal diffusiivity of $Al_{0.3}Ga_{0.7}As$

Molecular dynamics simulation has been chosen as it is closely tied to kinetic theory and not as closely related to statistical mechanics. In particular, molecular dynamics is less elegant but more direct than statistical mechanics.

(i) Correlation functions

Molecular dynamics (MD) simulation is carried out, by solving all the trajectories of the particles in a given system using velocity auto correlation function, as no such works are reported for this system. Recently Tersoff' s potential has been successfully used to implement the simulation on the semi conducting systems Si and GaAs (Sayed *et al*., 1995; Sekkal *et al*., 1998). Similarly Murugan *et al*. (2000) have used this potential to study self and impurity diffusion in GaAs. Similarly Jalal (2001) has used this potential to work out the thermal conductivity in GaAs, by MDS. Recently Volz and Chen (1999) have extensively investigated the thermal conductivity of silicon using MDS. The diffusivity in a system (of one dimension) is defined from correlations functions as (Frenkel and Smit, 1996).

$$D_x = \int_0^\infty dt \left\langle v_x(t) v_x(0) \right\rangle \tag{2}$$

which is also called Green-Kubo relation. This eqn. (2) in general is valid for all the diffusion processes but here we are interested in the thermal diffusivity and thermal conductivity. The thermal conductivity at any temperature T is given by current (heat flux) correlation function

$$k = \frac{1}{Vk_B T} \int_0^\infty dt < j_z^e(0) j_z^e(t) > \tag{3}$$

where

$$j_z^e = \frac{1}{2} \frac{d}{dt} \sum_{i=1}^{\infty} z_i \left(m_i v_i^2 + \sum_{j \neq i} v(r_{ij}) \right) \tag{4}$$

Eqn. (3) is valid only when the specific heat is independent of temperature. The heat flux is now given by the heat flux operator as,

$$q(t) = \frac{1}{V} \left(\sum_{i=1}^{N} (v_i E_i) + \frac{1}{2} \sum_{j=1, i \neq j}^{N} r_{ij} (f_{ij} v_i) \right) \tag{5}$$

Due to atomic motion, the equilibrium quantities like heat flux, q_0, energy, E_0 and temperature T_0 fluctuate around the equilibrium values and follow the local energy conservation. This can be given as

$$\delta E(t) = -\frac{1}{T_0} \frac{1}{V} \int_V \delta T(r,t) E_0(r,t) dV \tag{6}$$

which produces a resultant heat flux as

$$q(t) = \frac{1}{V} \int_V q_0(r,t) \delta\rho(t) dV + q_0(t) \tag{7}$$

This equation (7) combined with the expression for $\delta\rho(t)$ leads to the thermal conductivity

$$k = \frac{V}{3k_B T^2} \int_0^\infty < q_0(0) q_0(t) > \exp(i\omega t) dt \tag{8}$$

Where

$$< q_0(0) q_0(t) >= \frac{1}{V} \int q_o(0,r) q_0(t,r) \rho_0 dV \tag{9}$$

(ii) MD Simulation

The three body potential, Tersoff's potential is considered for the interaction between the atoms. We then calculated the Tersoff's potential parameters for $Al_{0.3}Ga_{0.7}As$ alloy using the parameters of GaAs (Murugan and Ramachandran, 2000) 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 employing the equilibrium lattice constant at 0 K. The form of energy E, as a function of the atomic coordinates are taken from Tersoff (10) as,

$$E = \sum_i E_i = \frac{1}{2} \sum_{i \neq j} V_{ij} \tag{10}$$

where $V_{ij} = f_C(r_{ij}) \left[a_{ij} f_R(r_{ij}) + b_{ij} f_A(r_{ij}) \right]$

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

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

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

$$f_c(r) = \begin{cases} 1 & r < R - D \\ \left(\frac{1}{2}\right) - \frac{1}{2} \sin\left(\frac{\pi}{2} \frac{(r-D)}{D} \right) & \text{for } R - D < r < R + D \\ 0 & r > R + D \end{cases} \tag{11}$$

and

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

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

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

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

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

$\alpha, \beta, \lambda_3, c, n$ 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, $Al_{0.3}Ga_{0.7}As$ and given in Table-1.

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

A = 3017.71 eV
B = 373.105 eV
λ_1 = 2.383 Å^{-1}
λ_2 = 1.452 Å^{-1}
λ_3 = 0.0 Å^{-1}
n = 7.495
h = -0.615
β = 0.428
c = 1.455
d = 0.937
R = 4.2 Å
D = 0.118 Å
α = 0.12 Å

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

$$v_{\max}^x = v_{\max}^y = v_{\max}^z = \sqrt{\frac{k_B T}{2m}} \text{ at temperature T} \qquad (12)$$

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

$$T = \frac{2}{3Nk_B} \left\langle \sum m_i v_{xi.} v_{xi} \right\rangle \qquad (13)$$

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 $v_{xi}^{new} = v_{xi} \sqrt{\frac{T}{T_A}}$ and these are the velocities that are used for further computations of time dependent positions and velocities. Here Verlet algorithm is chosen for the computation of the time dependent correlation functions. The Verlet algorithm is briefly mentioned here.

$$\begin{aligned} &r(t + \Delta t) = r(t)\,\Delta t + v(t)\,\Delta t + (1/2)a(t)\,(\Delta t)^2 \\ &v(t + \Delta t/2) = v(t) + (1/2)\,a(t)\,\Delta t \\ &a(t + \Delta t) = -(1/m)\nabla U(r(t + \Delta t)) \\ &v(t + \Delta t) = v(t + \Delta t/2) + (1/2)\,a(t + \Delta t)\,\Delta t \end{aligned} \qquad (14)$$

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. 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.2 tells the equilibration of kinetic (KE), potential (PE) and total energy (TE) of the system separately. The value of the velocity from 20001st trial will be considered as t = 0.

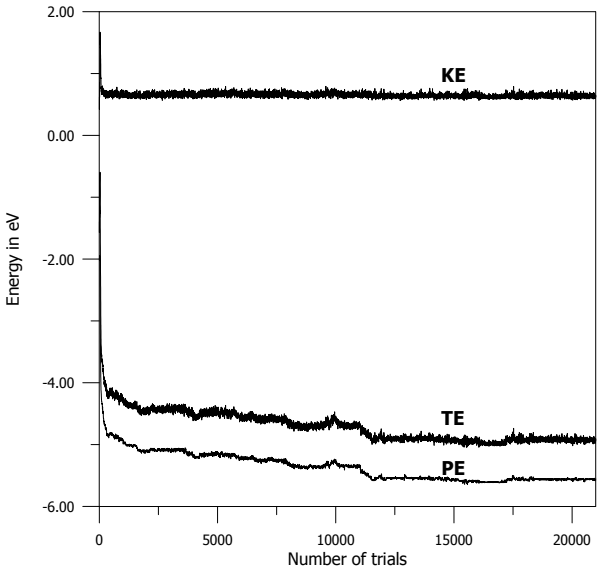

Fig.2. Energy equilibration by MDS

Thermography: Introduction

Infrared thermography, also called as thermal imaging, thermographic imaging, or thermal video, is a type of infrared imaging science. Thermographic cameras detect radiation in the infrared range of the electromagnetic spectrum (roughly 900–14,000 nanometers or 0.9–14 μm) and produce images of that radiation, called thermograms. Since infrared radiation is emitted by all objects based on their temperatures, according to the black body radiation law, thermography makes it possible to "see" one's environment with or without visible illumination. The amount of radiation emitted by an object increases with temperature, therefore thermography allows one to see variations in temperature (hence the name). When viewed by thermographic camera, warm objects stand out well against cooler backgrounds; humans and other warm-blooded animals become easily visible against the environment, day or

night. As a result, thermography's extensive use can historically be ascribed to the military and security services.
The appearance and operation of a modern thermographic camera is often similar to a camcorder. Enabling the user to see in the infrared spectrum is a function so useful that ability to record the output is often optional. A recording module is therefore not always built-in.The CCD and CMOS sensors used for visible light cameras are sensitive only to the nonthermal part of the infrared spectrum called near-infrared (NIR), but not to the part of infrared spectrum useful for thermal imaging (mid- and long-wavelength infrared), so most thermal imaging cameras use specialized focal plane arrays (FPAs) that respond to longer wavelengths. The most common types are InSb, InGaAs, HgCdTe and QWIP FPA. The newest technologies are using low-cost and uncooled microbolometers FPA sensors. Their resolution is considerably lower than of optical cameras, mostly 160x120 or 320x240 pixels, up to 640x512 for the most expensive models.

Thermograph of $Al_{0.3}Ga_{0.7}As$

Thermal diffusivity of AlGaAs sample is also studied by thermograph method. The sample grown by Czheckrolski method in Tata Institute of science is used here for thermographic study. The sample is mounted on a platform and heat wave is generated and passed through the sample for few seconds (here 5 sec) by using a flash light. Fig-(1) shows the thermograph of the sample and Fig-(2) shows the propagation of heatwave through the sample from which $t_{1/2}$ is measured and using the following equation the thermal diffusivity of the sample can be calculated. Table-(2) shows the results.

$D=0.1388L^2/t_{1/2}$

Propagation Vs time of passing

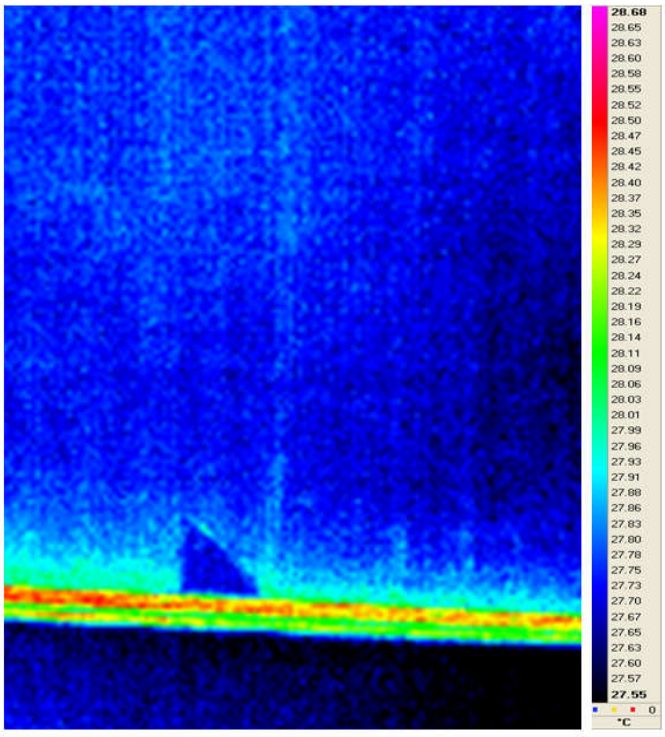

Fig. 1. Thermograph of AlGaAs sample

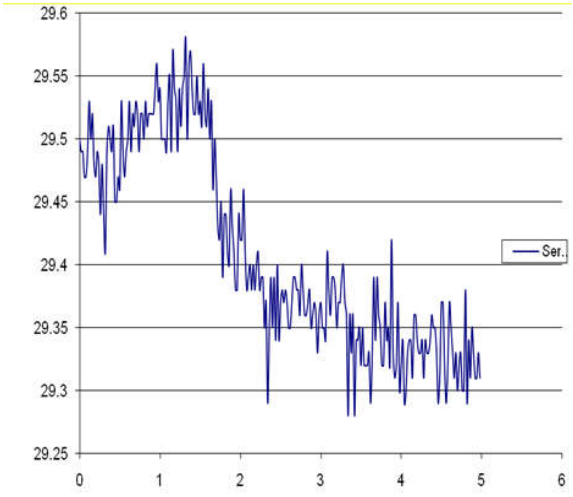

Fig.2. Thermal wave propagation through sample for 5secs

Table 2. Thermal diffusivity of $Al_{0.3}Ga_{0.7}As$ at room temperature

S.No.	Method	Thermal Diffusivity in cm^2/sec
1	Simulation by MDS	0.0745
2	Thermography	0.0803
3	Photoacoustic	0.0708
4	Literature[12]	0.0724

RESULTS AND CONCLUSION

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. The thermal conductivity can be deduced from thermal diffusivity from the relation,

$$\alpha = \frac{k}{\rho C} \qquad (16)$$

where k is the thermal conductivity , ρ is the density of the sample and C, the specific heat capacity at constant pressure. From this equation given above the thermal conductivity can be studied while knowing all the other terms in that equation. Thermal property of $Al_{0.3}Ga_{0.7}As$ particularly thermal diffusivity measured by molecular dynamics simulation showed a very good agreement with the literature values. Thermal diffusivity for GaAs, from other earlier investigations at room temperature are 0.31 cm^2 sec^{-1} whereas for $Al_{0.3}Ga_{0.7}As$, they are 0.0724 cm^2 sec^{-1}. Now our investigations by photoacoustics and thermograph method agree very well with these reported values and such kind of measurements for this system was not reported earlier (Table 2). When these values are compared with host GaAs, we find a reduction in thermal diffusivity because of alloying with aluminium. This is expected as extra aluminium atoms added to the host GaAs system will lead multiple scattering of phonons, thereby reducing the mean free path and the thermal conductivity. It is known that, on doping with n type impurity in GaAs, will increase the above thermal parameters because of the charge carrier (electron) concentration. But here, on alloying, GaAs with Al will not increase the electron concentration and so we find a decrease in the values. But large reduction in the thermal properties may be due to the

large lattice relaxation leading to the existence of DX centers. Large lattice relaxation will affect (a decrease in) the force constant and hence the phonons in the system are affected very much (i.e. decreased very much) affecting the phonon mean free path. This is the reason why there is a large reduction in the thermal values. Similarly the band gap is also measured from photoacoustics and the impact of the alloying by addition of Al atoms is visualized. This is valid because GaAs is a direct band gap material and also upto a concentration of $x = 0.4$, $Al_xGa_{1-x}As$ will be still a direct band gap material. The MD simulations are a useful way of investigating the thermal properties of the materials and also an aid in the design of materials at high temperatures.

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