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Effects of Temperature on the Nanotribology of Gallium Arsenide (GaAs) and Indium Arsenide (InAs)

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Abstract *- Three models were developed in this work through a combination of bond-orbital model, Tomlinson's model and Sang's equation. Using the first model called Jump Energy model for high and low ionic energy gaps,* ΔE *which is the energy barrier that presents the tip jump was calculated for gallium arsenide (GaAs) and Indium arsenide (InAs). The second model called Temperature model was used to study the effects of temperature on nanotribology of the two semiconductors. The results obtained using the first model compares favourably with the values of* ΔE *obtained using Tomlinson model. The results obtained using the temperature model compare favourbly with experimental results for Silicon (Si) found in literature. Hence the model was used for GaAs and InAs. There are no experimental results for GaAs and InAs. Hence these models were used to predict experimental results for these binary compounds for the first time. The models developed in this work will help to reduce problems encountered by nanotribologists in third world countries who find it difficult in carrying out research on nanotribology due to lack of Atomic Force Microscope. The results show that at nanolevel, friction decreases with increase in temperature. The results also indicate that GaAs has better tribological properties than InAs at various temperatures.*

Keywords - nanotribology, temperature, model, friction, wear

1. INTRODUCTION

Nanotribology is the study of the friction lubrication and wear at atomistic length and time scales (Carpick and Salmeron, 1997). The increase in the surface-to-volume ratio that occurs when devices are scaled down in size makes friction increasingly problematic in miniature instruments such as micro and nano-electromechanical systems (Frenken, 2006). Lubrication is not an option because the lubricant would be too viscous on the nanoscale and the adhesion forces introduced by the liquids are strong enough to damage tiny devices. Extracting useful information about nanotribological properties of different materials has been the subject of intense research in various parts of the world. This warless friction is due to instabilities occurring for plastic deformation of the surfaces or from a more atomistic point of view to the process of plucking of atoms proposed by Tomlinson (Gyalog and Thomas, 1997; Chandross et al., 2004; Fraxedas et al., 2002). Robert (2002) worked on viscosity of silica and reported experimental results which show an inverse relationship between temperature and viscosity (Robert 2002). Bennewitz (2004) used Tomlinson's model to study temperature dependence of friction on n-hexadecane and octamethycyclotetrasiloxane at nano level and in each case his results show an inverse relationship between nanotribology and temperature. Bhushan (2004) studied the effect of temperature on friction in silicon using a thermal stage attached to Atomic Force Microscope (AFM) and his results show an inverse relationship between the nanotribology and temperature.

Africans find it very difficult in carrying out research work in nanotribology due to lack of equipment like atomic force microscope (AFM) and Friction force microscope (FFM). In view of this, the aim of the study is to develop workable theoretical models which can be used to predict experimental results. Because experimental results for silicon are available these models were used to study the effects of temperature on the nanotribology of silicon. The results obtained are in good agreement with experimental results for silicon found in literature. Hence the models were also used for gallium arsenide (GaAs) and Indium arsenide (InAs)

2. MATERIALS AND METHODS

Three different models were developed and used for this work. The first two called jump energy models for high and low ionic energy gaps were developed through a combination of bond-orbital model and Tomlinson's model. The third one called temperature model was developed through a combination of Tomlinson model and Sang's equation.

2.1 Development of Jump Energy Models for High and Low Ionic Energy Gaps

From Tomlinson's model the equation describing

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the thermal effects on atomic friction is given by equation 1, (Bennewitz 2004).

$$\frac{dp(t)}{dt} = -f_0 exp\left(-\frac{\Delta E(t)}{K_B T}\right) \text{P (t)} \quad (1)$$

Where f_0 is the characteristic frequency of the system.
ΔE= Energy that prevents the tips jump.
t= Time, k_B=Boltzmann's constant, T= Temperature.

Replacing time with the lateral force f_l gives

$$\frac{dp(f_l)}{df_l} = -f_0 \exp\left(-\frac{\Delta E(f_l)}{K_B T}\right)\left[\frac{df_l}{dt}\right]^{-1} P(f_l) \quad (2)$$

From this model, the force preventing the tip jump is **Δ**E which is the energy barrier.

$$\mathbf{\Delta}E = (X_{max,}\ t) - (X_{min,}\ t) \quad (3)$$

Where X_{max} corresponds to the first maximum observed in the energy profile and X_{min} is the critical point. The energy barrier can be written approximately as shown in equation 4, (Sang et al., 2001).

$$\mathbf{\Delta}E = \mu(\bar{F}\text{-}F_L) \quad (4)$$

Where $\bar{F}$ is close to the critical value $F^* = \frac{\pi E_0}{a}$ (5)

Substituting

$$\frac{dF_l}{dt} = \frac{dF_l}{dx}\frac{dx}{dt} = K_{eff}\, V \quad (6)$$

Into equation (2) and use approximation (4), the maximum probability transition condition $\frac{d^2p(f)}{df^2} = 0$

Then gives

$$F_L(V) = F^* - \frac{K_\beta T}{\mu} \text{Ln}\frac{V_c}{V} \quad (7)$$

Where

$$V_c = \frac{F_0 K_\beta T}{K_{eff}\,\mu} \quad (8)$$

This energy barrier ΔE is given by

$$\mathbf{\Delta}E = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 \quad (9)$$

Simplifying equation (9) gives

$$\Delta E = \frac{h^2}{4\pi^2 2m}\cdot\frac{4\pi^2}{a^2}$$

$$\Delta E = \frac{h^2}{2m}\cdot\frac{1}{a^2} \quad (10)$$

In bond orbital model in binary compounds, if the imaginary (polar) component and real (covalent) component are present, then the energy gap is

$$E_g = -(V_2{}^2 + iV_3^2) \quad (11)$$

But if the imaginary (polar) part varnishes, then the overlap integral contains only the covalent (real) part as shown in equation 12, (Animalu, 1997).

$$\text{Then } E_g = (V_2^2 + V_3^2)^{\frac{1}{2}} \quad (12)$$

Using equation (10), $\mathbf{\Delta}E = E_T$ was calculated for Si, GaAs and InAs. Analysis of the results obtained show that the calculated values of $\mathbf{\Delta}E = E_T$ using Tomlinson's model is related to E_g (from bond-orbital model) by the equation

$$E_{Ts} = \beta\left(E_g - \left(\alpha_c^{\frac{1}{2}} + f_i^2\right)\right) \quad (13)$$

For $\alpha_c \geq 3.85\ eV$

Where α_c is the ionic energy gap, f_i is the iconicity of the material and β is an empirical constant and has the value $\beta = 1.073$. If $\alpha_c < 3.85\ eV$, then another equation holds and is given by

$$E_{Ts} = \beta\left(Eg - f_i^{\frac{1}{2}}\right) \quad (14)$$

Equations (13 and 14) are jump energy models for high and low ionic energy gaps respectively which were developed by the researchers. Equation (14) was used for the three semiconductors under study and the results obtained are presented in table 1.

2.2 Development of Temperature Model

The third model was developed through derivation of an equation for F_l i.e. friction force using Tomlinson's model and Sang's equation. This derived equation was carefully modified so that it can be applied over a wide range of semiconductors including binary compounds.

From Tomlinson's model, the motion of the tip is influenced by:

i. The interaction between the atomic lattices of the surface.
ii. The elastic deformation of the cantilever.

If the cantilever moves with a constant Velocity 'V' in x -direction, the total energy of the system is given by equation 15, (Bennewitz, 2004).

$$E_{tot}(x,t) = -\frac{E_o}{2}\,Cos\frac{2\pi x}{a} + \frac{1}{2}K_{eff}(Vt - x)^2 \quad \ldots(15)$$

At any time't', the position of the tip can be determined by equating to zero the first derivative of the expression $E_{tot}(x,t)$ with respect to x to obtain

$$\frac{dE_{tot}}{dx} = \frac{\pi E_0}{a} Sin\frac{2\pi x}{a} - K_{eff}(Vt - x) = 0 \quad (16)$$

The critical position X^* corresponding $t=t^*$ is determined by equating to zero the second derivative of $E_{tot}(x,t)$ which gives

$$X^* = \frac{a}{4} arcos\left(-\frac{1}{y}\right) \quad (17)$$

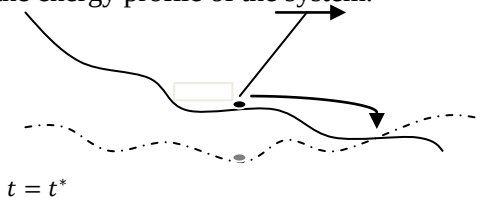
$$y = \frac{2\pi^2 E_0}{K_{eff} a^2} \quad (18)$$

When $t=t^*$ the tip suddenly jumps into the next minimum of the potential profile. The lateral force

$$F^* = K_{eff}(\text{Vt} - \text{x}^*) \quad (19)$$

Which induces the jump can be calculated from (16 and 18) to give $F^* = K_{eff}\frac{a}{2\pi}\sqrt{y^2 - 1}$ (20)

Therefore the stick-slip is observed only when y>1 i.e. only when the system is not too stiff. Figure 1 below shows the energy profile of the system.



ig. 1: Energy profile experienced by FFM tip. (Thick dot) at t=0 (dotted line) and t = t* (continuous line)

In two dimensions, the energy of the system is

$$E_{t0t}(r,t) = U(r) + \frac{K_{eff}}{2}(Vt - r)^2 \quad (21)$$

Using the assumption that $y >> 1$, at a given time $t = t^*$ the tip jump is prevented by the energy barrier ΔE. ΔE decreases with increasing frictional force F_l until it vanishes when $F_l = F^*$

It was observed that the energy barrier ΔE close to the critical point is better approximated by

$$\Delta E = \mu (F^* - F_l)^{\frac{3}{2}} \quad (22)$$

Where μ=0.01 as found by Mate, [Bennewitz, 2004].

Substituting equation (6) into equation (2) and using approximation (22) with the same maximum probability transition condition $\frac{d^2p(f)}{df^2} = 0$

Tomlinson model gives

$$\mu \frac{(F^* - F_l)^{\frac{3}{2}}}{k_\beta T} = ln\frac{V_c}{V} - ln\sqrt{1 - \frac{F^*}{F_l}} \quad (23)$$

Where $V_c = \frac{\pi\sqrt{2}}{2}\frac{f_0 K_\beta T}{K_{eff}}$

If $V << V_c$, then the second logarithm in (23) can be neglected to obtain

$$F_l = F^* - (\frac{K_\beta T}{\mu})^{\frac{2}{3}} (\ln\frac{V_c}{V})^{\frac{2}{3}} \quad (24)$$

Taking the value of V such that $\frac{V_c}{V}$= e, the velocity effect on F_l is suppressed and equation (24) becomes

$$F_l = F^* - (\frac{K_\beta T}{\mu})^{\frac{2}{3}} \quad (25)$$

Rearranging (22) gives $F_l = F^* - \left(\frac{\Delta E}{\mu}\right)^{\frac{2}{3}}$ (26)

Solving (25) and (26) simultaneously gives

$$F_l = F^* - \frac{1}{2}\left[(\frac{\Delta E}{\mu})^{\frac{2}{3}} + (\frac{K_\beta T}{\mu})^{\frac{2}{3}}\right] \quad (27)$$

After series of calculations with equation (27) it was carefully modified based on the fact that temperature effects on nanotribology requires a more sensitive equation which can predict experimental results more accurately. In making these modifications, it was noted that multipliers enhance the sensitivity of a model. The variable T was selected as part of the multipliers to help vary the effects of other multipliers P and $\frac{1}{\mu}$ which are empirical constants. These modifications give the equation

$$F_l = F^* - \frac{P^2T^2}{2}\left[(\frac{\Delta E}{\mu})^{\frac{2}{3}} + \frac{1}{\mu}(\frac{K_\beta T^2}{\mu})^{\frac{2}{3}}\right] \quad (28)$$

Where P which is an empirical constant is given by

$P = (R + x)$

$R = 1.3\,x\,10^{-3} and\ x = (n_i - 1)x\,10^{-3}$. n_i takes values from 1- 4.

The behavior of this model when used justifies the modifications. Hence equation (28) is the temperature model which was developed. This equation was used to study the effects of temperature on nanotribology of Gallium Arsenide (GaA) and Indium Arsenide (InAs). The results obtained are presented in fig. 3. Experimental results for silicon as found in literature together with the results obtained using our model are presented in fig. 2.

F^* for each material was calculated using equation (20). After series of calculations with different values of y, y=100 was adopted to satisfy the assumption that y >> 1.

3. RESULTS AND DISCUSSION

The two models were successfully applied to the semiconductors GaAs and InAs. The results obtained using jump energy model for low ionic energy gap are presented in table 1.

Table 1: The results obtained using jump energy model for low ionic energy gap

Material	Lattice Spacing (A^o)	Bond Energy gap E_g(eV)	Calculated Values of ΔE = E_T using Tomlinson's model (eV)	Calculated Values of Δ E=E_{TS} using equation (14) (eV)
Si	5.42	4.77	5.12	5.12
GaAs	5.65	5.20	4.71	4.98
InAs	6.06	4.58	4.10	4.27

These results show that the values obtained using equation (14) compare favourably with that obtained using Tomlinson's model. Hence with equation (14) bond energy gap of every material which is obtained from bond-orbital model can be used to calculate E for the material which is the energy that prevents the tip jump. The above results show that GaAs has a higher value of E than InAs. Since E decreases with increasing friction force, it follows that GaAs exhibits better tribological properties than InAs at nanolevel. It should be noted that bond-orbital model is an instrument for structural analysis and nanotribology is a structural problem, hence the choice of this model for this study. E = ETS from the table was used in the temperature model (equation 28) for the two materials and silicon. The results obtained using the temperature model for silicon together with experimental results found in literature are presented in figure 2.

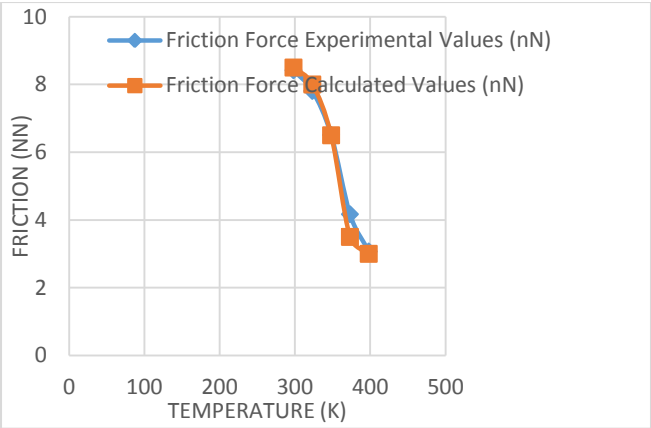


Fig. 2: Graphs of the effects of temperature on nanotribology of Silicon together with experimental results found in literature

The graph above shows that the results obtained using the temperature model for silicon compares favorably with experimental results. The higher deviation observed in the two results at 373K could be attributed to the fact that in the graph of the experimental data, the point plotted for friction at 373K is the only point that falls well off the line of best fit. This is observed in the graph of the results as found in literature. Hence, the model can properly predict experimental results. This model was also use for GaAs and InAs and the results obtained are presented in fig. 3 below

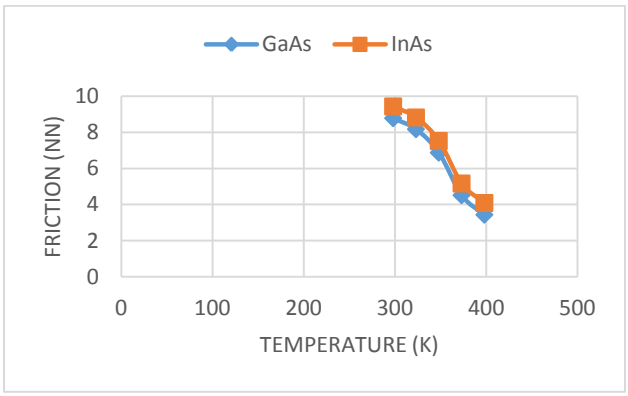


Fig. 3: Graphs of Effects of Temperature on Nanotribology of GaAs and InAs

The results above show that friction at nanolevel decreases with increase in temperature. For instance, at temperatures of 298K and 323K, GaAs has nanotribologies of 8.78nN and 8.17nN respectively. Also, at temperatures of 298K and 323K, InAs has nanotribologies of 9.43nN and 8.82nN respectively. This agrees with the experimental results on viscosity of silica obtained by Robert (2002), which shows an inverse relationship between temperature and viscosity. It also agrees with experimental results obtained by Bhushan (2004), which shows an inverse relation between temperature and nanotribology of silicon. The results obtained by Bennewitz (2004), which show an inverse relationship between temperature and friction of n-hexadecane also agree with this. The results also indicate that GaAs has better tribological properties than InAs at various temperatures. At low temperatures, InAs exhibits high friction. However, as the temperature increase, the friction reduces to low values. From the graph it can be observed that nanotribological properties of elements become better as we move upwards in group III elements in the periodic table. This may be due to less number of electrons present in the elements as we move upwards in the group. This observation suggests that boron and boron compounds may have the best tribological properties in the group with regard to temperature variations.

4. CONCLUSION

The two models developed have been applied successfully in the study of the effects of temperature on the nanotechnology of GaAs and InAs. There are no experimental results for GaAs and InAs. Hence these models were used to predict experimental results for these semiconductors for the first time. Nanotechnology still stands out as an area in which much still remains unknown. Jeong Young Park and co-workers have suggested that “electronic friction” also exists. Further works done with these models have shown that they can be modified and used in studying other parameters that affect Nanotribology of semiconductors such as velocity and normal load.

REFERENCES

Animalu, A.O.E. (1997). Intermediate Quantum Theory of Crystalline Solids, Chap.8, Prentice – Hall Inc, New Jersey, .301p.

Bennewitz, R. (2004). Friction and wear on the atomic scale ed. B.Bhushan, Chap.20, Springer Handbook of Nanotechnology, Springer–Verlag Berlin Heidelberg. 631p.

Bhushan, B. (2004). Nanoscale boundary lubrication studies ed. B.Bhushan, Chap.28, Springer Handbook of Nanotechnology, Springer –Verlag Berlin Heidelberg. 861p.

Carpick, R.W. and Salmeron, M. (1997). Fundamental investigations of tribology with Atomic Force Microscope. Chem. Rev. 97, 1103-1194.

Chandross, M., Webb, E.B., Stevens, M.J. and Grest, G.S. (2004). Systematic study of effects of disorder on nanotribology of self assembled monolayers. Physical review letters 93 (16), 166103- 1661011.

Fraxedas, J., Gracia – Manyes, S., Gorostrizo, P. and Sanz, F. (2002). Nanoindentation: Towards the sensing of atomic interactions. Proceedings of the National Academy of sciences of the united states of America (PNAS). 99, 85228-85232.

Frenken, J. (2006). Nature Nanotechnology: Bringing friction to a halt. News and Views. 1, 20-21.

Gyalog, T. and Thomas, H. (1997). Atomic friction. Z Physics B, 104, 669-674.

Robert, H.D. (2002). Viscosity of Silica. J. Appl. phys 92, 7619-7629.

Sang, Y., Dube, M. and Grant, M. (2001). Thermal effects on atomic Friction. Physical review letters, 87, 174301.