Effect of Velocity on Nanotribiology of Silicon (Si), Germanium (Ge) and Tin (Sn)

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ABSTRACT--- ***Due to constant energetic losses in micro and macro systems, nanotribology remains central in the global scientific research. In this work we developed new models through a combination of bond-orbital model, Tomlinson's model and Sang's equation. Using jump energy models for high and low ionic energy gaps, ΔE which is the energy that prevents the tips jump was calculated for Silicon (Si) Germanium (Ge) and Tin (Sn). Through a combination of Tomlinson model and Sang's equation temperature model was developed. This model was further modified to obtain other models. These final models were used to investigate the effects of velocity on the nanotribology of Silicon. The results obtained compare favorably with experimental results for silicon found in literature. Hence, the models were also used for Germanium and Tin. There are no experimental results for germanium and tin. Hence, we are predicting experimental results for these semiconductors for the first time using our models.***

Keywords-- nanotribology, velocity, model, energy.

1. INTRODUCTION

Nanotribology is the science of friction, lubrication and wear at atomistic length and time scales. [1] Increasing energetic losses in micro-electromechanical and nano-electromechanical systems (MEMS) and (MENS) due to tribology has put this subject at a central point in global scientific research. Extracting information about nanotribological properties of materials has numerous practical applications. Reducing energetic losses due to tribology which will help a car engine to work efficiently, reducing material losses due to wear and optimizing lubricants are important issues for a wide range of industrial and societal applications. With the invention of small devices triggered in part by the tremendous development of silicon micro fabrication techniques, novel problems appear that require knowledge at the nanometer scale. For example the whole technology of information storage as shown by the case of computer hard disks with coatings and lubricants that protect the stored information, with dimensions that are measured in nanometers. [1,2] In investigating the velocity effect on nanotribology, the friction force versus nornmal load relationships of Si (100), Z-15 and Z-Dol (BW) at different velocities were measured. [3,4] The results indicate that for silicon wafer, the friction force decreases logarithmically with increasing velocity up to 10μm\s after which it remains almost constant. The velocity has a much smaller effect on the friction force of Z-dol (BW). It reduced slightly only at very high velocities.

Effective laboratory equipment for nanotribology research like Atomic force microscope (ATM) and friction force microscope (FFM) are extremely difficult to come by in African countries. Hence we decided to develop workable theoretical models which can be used to predict experimental results for velocity dependence of nanotribology over a wide range of semiconductors including binary compounds. These models are;

- Jump energy models for high and low ionic energy gaps.
- Temperature model
- Low and high velocity models

These models were used to study the effects of velocity on nanotribology of silicon. The results obtained compare favourably with experimental results found in literature. Hence the models were also used for Ge and Sn. There are no experimental results for Ge and Sn. Hence, we are predicting experimental results for these semiconductors for the first time using our models. It was found among others that at nano level, friction decreases with increase in velocity.

2. MATERIALS AND METHODS

Five 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 bound-orbital model and Tomlinson model. The third one called temperature model was developed through a combination of Tomlinson model and Sang's equation. The fourth and fifth models called low and high velocity models were developed through modifications of temperature model.

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

From Tomlinson model, the equation describing the thermal effects on atomic friction is given by equation 1. [5]

$\frac{dp(t)}{dt}$= - F_0 exp ($\frac{-\Delta E(t)}{K_B T}$) P (t) ---------- 1

Where F_0 is the characteristics frequency of the system. If we replace time with the lateral force F_L we have

$\frac{dp(F_L)}{dF_L}$= F_0 exp ($\frac{-\Delta E(F_L)}{K_B T}$) ($\frac{dF_L}{dt}$) p ($F_L$) ----------2

From this model, the force preventing the tips jump is ΔE which is the energy barrier.

ΔE = (X_{max}, t) – (X_{min}, t) ---------- (3)

Where Xmax. corresponds to the first maximum observed in the energy profile and X_{min} is the actual position of the tip. The quantity ΔE decreases with the frictional force F_L until it vanishes when F_L = F*. Close to the critical point, the energy barrier can be written approximately as shown in equation 4. [6]

ΔE = μ (F-F_L) ---------- (4)

Where F is close to the critical

Value F* = $\frac{\pi E_0}{a}$ ---------- (5)

If we substitute

$\frac{dF_L}{dt}$= $\frac{dF_L}{dx}\frac{dx}{dt}$ = K_{eff} V---------- (6)

Into equation (2) and use approximation (4), the maximum probability transition condition

$\frac{d^2 p(F)}{dF^2}$= 0 then gives

F_L (v) = F* - $\frac{K_B T}{\mu}$ in $\frac{Vc}{V}$ ---------- (7)

Where V_C = $\frac{F_0 K_B T}{K_{eff}}$ ---------- (8)

This energy barrier ΔE is given by

ΔE = $\frac{\hbar^2}{2m}$ ($\frac{2\pi}{a}$)^2 ----------(9)

Simplifying equation (9) we have

ΔE = $\frac{\hbar^2}{4\pi^2 2m}$ x $\frac{4\pi^2}{a^2}$ ----------(10)

ΔE = $\frac{\hbar^2}{2m}\frac{1}{a^2}$ ---------- (11)

In bond-orbital model in binary compounds, if the imaginary (polar) components are present, then the bond energy gap is

E_g = - (V_2^2 + iV_3^2) ---------- (12)

But if the imaginary (polar) part vanishes, then the overlap integral contains only the covalent (real) part as shown in equation 13. [7]

E_g = (V_2^2 + V_3^2)^{½} ----------(13)

Using equation (11) ΔE = E_T was calculated for Si, Ge and Sn. Analysis of the results obtained shows that the calculated values of ΔE = E_T using Tomlinson model is related to E_g (from bond-orbital model) by the equation

E_{os} = β [E_g – ($\propto_c^{½} + f_i^2$)] ----------(14)

for $\propto_c \geq$ 3.85eV.

Where $\propto_c$ is the ionic energy gap f_i is the ionicity of the material and β is an empirical constant and has the value β = 1.073.

If $\propto_c$ < 3.85eV, then another equation holds and is given by

E_{os} = β (E_g- $f_i^{½}$) ----------(15)

Equations (14) and (15) are jump energy models for high and low ionic energy gaps respectively which we developed. Jump energy model for low ionic energy gap (equation 15) was used to generate results for the materials under study. The results obtained are presented in table 1.

2.2 Development of Temperature Model

The temperature model was developed through derivation of an equation for F_L i.e friction force (lateral force), using Tomlinson model and Sang's equation. This derived equation was carefully modified in two stages so that it can be applied over a wide range of semiconductors including binary compounds. The first stage of modification produced a good model for investigating temperature dependence of nanotribology and the second stage of modification produced the models used in this work.

From Tomlinson model, the motion of the tip is influenced by

1. the interaction with the atomic lattice of the surface
2. 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 $E_{tot}(x,t) = -\frac{E_0}{2}\cos\frac{2\pi x}{a} + \frac{1}{2} K_{eff}(Vt - x)^2$ ----------(16)

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

$\frac{dE_{tot}}{dx} = \frac{\pi E_0}{a}\sin\frac{2\pi x}{a} - K_{eff}(Vt-x) = o$ ----------(17)

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

$x^* = \frac{a}{4}\arccos\left(-\frac{1}{y}\right)$----------(18)

$y = \frac{2\pi^2 E_o}{k_{eff}\, a^2}$ ---------- (19)

when t = t*, the tip suddenly jumps into the next potential profile. The lateral force

$F^* = K_{eff}(Vt - x^*)$ ---------- (20)

Which induces the jump can be calculated from equations (17) and (19) to give

$F^* = K_{eff}\frac{a}{2\pi}\sqrt{y^2 - 1}$ ---------- (21)

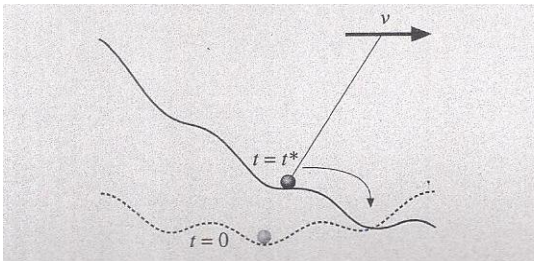
Therefore the stick slip is observed only when y > 1 i.e only when the system is not too stiff.

In two dimension the energy of the system is

$E_{tot}(r,t) = U(r) + \frac{K_{eff}}{2}(Vt - r)^2$ ----------(22)

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 frictions force F_L until is vanishes when $F_L = F^*$.

The figure below shows the energy profile of the system.



Energy profile experienced by FFM tip, (black circle) at t = o (dotted line) and t = t (continuous line)*

Sang observed that the energy barrier ΔE close to the critical point is better approximated by the relation

$\Delta E = \mu(F^* - F_L)^{2/3}$ ----------(23)

Where μ = 0.01 as found by mate. Substituting equation (6) into equation (2) and using approximation (23) with the same maximum probability transition condition

$\frac{d^2 p(F)}{dF^2} = 0$

Tomlinson model gives

$\mu\left(\frac{F^* - FL}{K_B T}\right)^{3/2} = \text{Ln}\frac{Vc}{V} - \text{Ln}\sqrt{1 - \frac{F^*}{F_L}}$ ----------(24)

If $V << V_c$, then the second logarithm in equation (24) can be neglected to obtain

$F_L = F^* - \left(\frac{K_B T}{\mu}\right)^{2/3}\left(\text{Ln}\frac{V_C}{V}\right)^{2/3}$ ----------(25)

If we take value of V such that $\frac{V_c}{V} = e$, then the above equation becomes

$F_L = F^* - \left(\frac{K_B T}{\mu}\right)^{2/3}$ ---------- (26)

Rearranging equation (23) we have

$F_L = F^* - \left(\frac{\Delta E}{\mu}\right)^{2/3}$ ---------- (27)

Solving (26) and (27) simultaneously we obtain

$F_L = F^* - \frac{1}{2}\left[\left(\frac{\Delta E}{\mu}\right)^{2/3} + \left(\frac{K_B T}{\mu}\right)^{2/3}\right]$ ---------- (28)

After series of work with equation (28), we carefully modified it based on the fact that temperature effect on nanotribology requires a more sensitive equation which will predict experimental results more accurately. These modifications led to the equation

$F_L = F^* - \frac{P^2T^2}{2}[(\frac{\Delta E}{\mu})^{2/3} + \frac{1}{\mu}(\frac{K_BT^2}{\mu})^{2/3}]$ ---------- (29)

Where p which is an empirical constant is given by P = (R + X)

$R = 1.3X10^{-3}$ and x = $(n_i - 1) \times 10^{-3}$ n_i takes values from 1- 4.

The above equation is a working model which we have already developed for investigating temperature dependence of nanotribology.

2.3 Development of Low and High Velocity Models

In developing a model for velocity dependence of nanotribology, we note that the above model contains ΔE which has a very essential property of every crystal – lattice spacing, the velocity model can be obtained by modification of the above equation.

Dropping $\frac{P^2T^2}{2}$ in the above model we have

$F_L = F^* - [(\frac{\Delta E}{\mu})^{2/3} + \frac{1}{\mu}(\frac{K_BT^2}{\mu})^{2/3})$ ----------(30)

Substituting V for T in equation (30) and introducing the necessary constants, we have $F_L = \propto_v F^* - [(\frac{\Delta E}{\mu})^{2/3} + (\frac{K_BV^2}{\mu^3})^{2/3}\frac{1}{K}]$ ----------(31)

Where $\propto_v$ and K are constants given by

$\propto_v = 1.043$ and

$K = 1.0 \times 10^{-10}$

Equation (31) holds for

$V \leq 2.0$ μm/s.

If V > 2.0 then another model holds and is given by

$F_L = \propto_v F^* - [[(\frac{\Delta E}{\mu})^{2/3} + (\frac{K_BV^3}{\mu^3})^{2/3}\frac{1}{K}] + C]$ ----------(32)

Where 'C' is another constant given by $C = 2\text{-}22 \times 10^{-9}$

Hence equations (31) and (32) are low and high velocity models respectively which we developed. These models were used to study the effects of velocity on nanotribology of silicon. The results obtained are in good agreement with experimental results for Si found in literature. Hence the models were also used for Ge and Sn. The results obtained for Si together with experimental results found in literature are presented in figure 1. While the results obtained for Ge and Sn are presented in figure 2.

F* was calculated for each element using equation (21). After series of calculations with different values of y, we adopted y = 100 so as to satisfy the assumption that y > >1.

3. RESULTS AND DISCUSSION

The models were successfully applied to the semiconductors: Silicon, germanium and tin. The results obtained using jump energy model for low ionic energy gap are presented in table 1.

Table 1: Results obtained using jump energy model for low ionic energy gap (equation 15).

Material	Lattice spacing (A^o)	Average bond energy gap (eV)	Calculated values of ΔE = E_T using Tomlinson model (eV)	Calculated values of ΔE = E_{os} using equation (15) (eV)
Si	5.42	4.77	5.12	5.12
Ge	5.62	4.31	4.76	4.62
sn	6.46	3.06	3.60	3.28

The results above show that the values obtained using equation (15) compares favourably with that obtained using Tomlinson model. Hence with equation (15), bond energy gap of every material can be used to calculated ΔE for the material which is the energy that prevents tip jump. It should be noted that bon-orbital model is an instrument for structural analysis and nanotribology is a structural problem. Hence ΔE = E_{os} from the table was used in the low and high velocity models for the materials.

The results obtained using low and high velocity models for Si together with the experimental results found in literature are presented in figure 1.below.

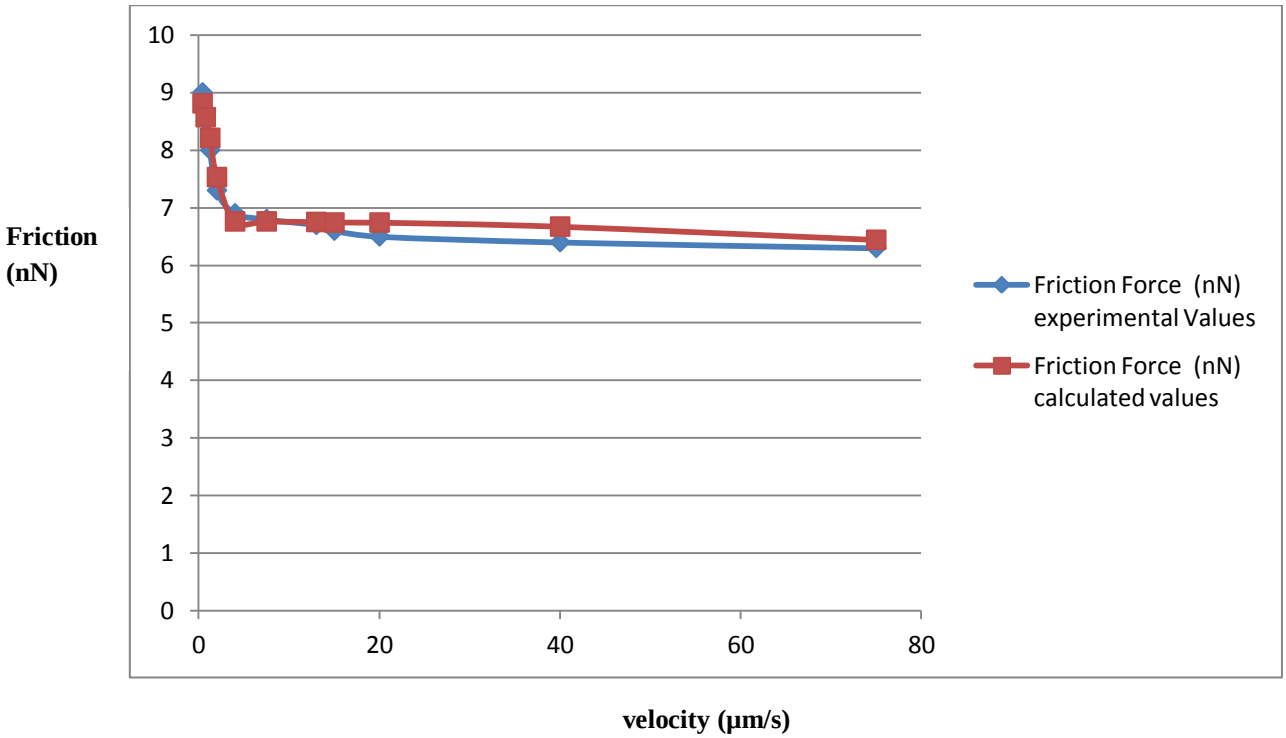


Fig 1: Graphs of the effects of velocity on nanotribology of Si together with experimental results found in literature.

The graph above shows that the results obtained using the low and high velocity models compares favourably with the experimental results for Si found in literature. Hence, the models properly predict experimental results. The models were also used for Ge and Sn and the results obtained are presented in figure 2:

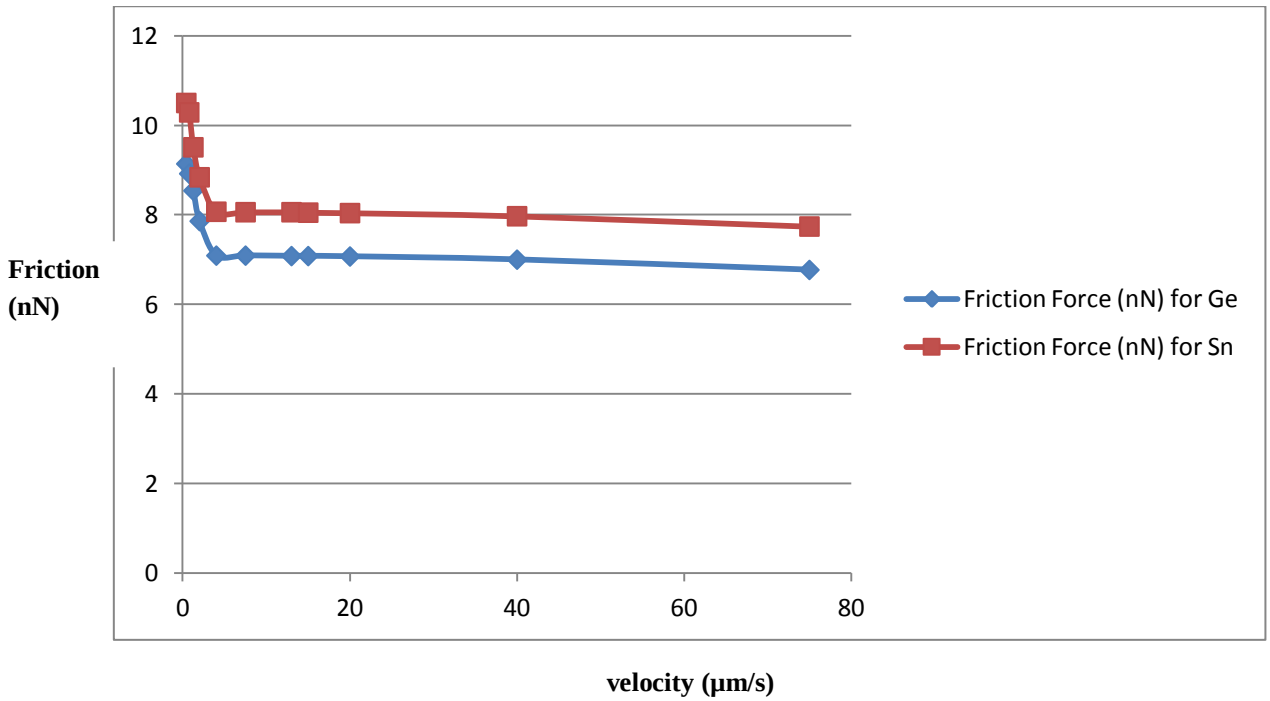


Fig 2: Graphs of the effects of velocity on nanotribology of Ge and Sn.

The above results show that at nano level, friction decreases with increase in velocity. This agrees with the results obtained by Huiwen Liu (2004) [8], Bharat Bhushan (2004), Berman A.D. and Isrealachivili J.N (2004) [9].

The results also show that silicon exhibits better tribological properties at different velocities than the other two elements followed by Germanium. From the results, friction force decreases gradually as velocity increases and tends to be constant as velocity rises above 2.0μm/s. From the graphs, it can also be observed that as we move upwards in group (IV) elements in the periodic table, nanotribological properties becomes better with regards to velocity variations. These observations may be due to fewer numbers of electrons present in these elements as we move upwards in the group.

4. CONCLUSION

The models developed have been applied successfully in the study of the effects of velocity on nanotribiology of Si, Ge and Sn. The results obtained actually compare favorably with experimental results for silicon found in literature. There are no experimental results for Ge and Sn. Hence we are predicting experimental results for these semiconductors for the first time using our models. Extracting information about nanotribological properties of materials remains a big challenge to scientists globally. This challenge is compounded by serious lack of adequate equipment like Atomic force microscope needed to carry out research in this area especially in third world countries. However, the models developed in this work can be used effectively in extracting information about velocity dependence of nanotribology for many semiconductors including binary compounds.

5. REFERENCES

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