Theoretical Studies of Static Friction at Atomic Scale for Unlubricated BCC Solids

by

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"*Though this is madness, yet there is method in 't.*"

– **William Shakespeare**, *Hamlet*

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1 Introduction

1.1 Laws of Friction

The study of friction in its modern form began 500 years ago when Leonardo da Vinci deduced the laws governing the motion of a rectangular block sliding over a flat surface but this work remained unpublished for hundreds of years. In 17^{th} century, Amontons' rediscovered the laws of friction after he studied dry sliding between two flat surfaces. Amontons' conclusions now constitute the laws of friction[1]:.

1. The maximum friction force that resists sliding at an interface is proportional to the normal contact force. If f_l is limiting static frictional force (or limiting friction force, for short) and N is a normal contact force, then f_l/N has a constant value known as the coefficient of friction μ. In general, μ depends on whether one measures the static friction force(f_s) or the kinetic friction force(f_k) needed to maintain sliding.

2. The value of limiting friction force does not depend on the apparent area of contact.

3. Kinetic friction force is independent of the sliding velocity. The third law was given by Coulomb. Researchers have found this rule to be untrue.

1.2 Brief account of ideas to explain friction

Many early investigators thought that friction arose from mechanical interlocking between rigid or elastically deforming asperiries. The friction force in this scenario is obtained by equating the work done by the frictional force to that done against the normal load as the surfaces separate to allow asperiries to slide up and over each other. This model is deeply flawed however, since

[1]Over the years, in the field of Tribology, it has been observed that using special kind of materials and under certain conditions, all the three laws mentioned here are violated, See[12]. To begin with, we will not take into account these pathological cases.

the normal load performs work *on* the system after the asperities have passed over each other and the upper body had settled back into its lowest position: All of the potential energy stored in the "separating" phase of the motion is recovered, so no net energy dissipation, and therefore no friction, can be present.

The view that interlocking between surfaces is a cause of friction is also not right because it can not explain a variety of common macroscopic observations. For example, when two highly polished and smooth metal surfaces are brought into contact, they are far more likely to cold-weld than to exhibit low friction. By mid-1950s, surface roughness had been ruled out as a viable mechanism for most of the everyday friction.

Bowden, Tabor, et al.[2] put forward the adhesive model of friction in which they presumed that friction is proportional to true contact area. They proposed that friction originates from very strong adhesive bonding between true(or microscopic) contact area [2]. This would imply that during sliding, tiny fragments from each surface were being worn away. However, this could not explain the fact that substantial friction exists even in cases where wear is negligible. In fact in 1970s, Israelchvili[3] found clear evidence of wear-free friction. In 1980s, McCelland[4] derived a model based on the vibrations of atomic lattices. Several studies have tried to understand friction by simulations of the interatomic interactions[5,6]. In all these studies the interactions are understood using the potential energy function. However, like Feynman[1] points out, inter-atomic interactions can be understood equally easily using forces. This is one of the motivations for this study.

[2]The frictional force between two solid bodies results from the formation and breakage of bonds at each actual contact point and the total area of actual contact points is called as the true(or microscopic) contact area.

2 Basic assumptions of model

2.1 Objectives

Here, we discuss a simplified model of atomic interactions by *directly* considering the electrostatic forces between atoms. We first put forth our assumptions and try to calculate the value of limiting friction. Lastly, we suggest a reason for the difference between limiting friction and kinetic friction. Our reasoning posits that the *difference* between limiting friction and kinetic friction may actually depend upon the nature of irregularities of the surfaces involved.
The objectives of the project are,

1. Outlining the assumptions of our model.
2. Calculating the effective charge on surface atoms.
3. Finding an expression theoretically for ing friction
4. Calculating the value of limiting friction.
5. Qualitative explanation for why the limiting friction is greater than kinetic friction.

2.2 Assumptions

We put forward the following assumptions for our model:

1. Atoms are spherical in shape having a definite radius (refer Appendix-C).
2. In equilibrium (i.e.when no horizontal force is acting on the system), for every four atoms of the lower surface, there is one atom of the upper surface touching all the four atoms.

This can be easily seen in the solids having body centered cubic(bcc) crystal structure e.g. iron, chromium, niobium, tungsten, etc.

2.3 Justification for second assumption

In the bulk of bcc solids, there is a continuous crystal structure which repeats itself periodically. But, at the surface of the object, the crystal gets terminated. Now there can be two cases, it terminates at upper or lower portion of the crystal where four atoms are present or it can terminate at the central portion where only one atom is present. We will take into account both the cases.

Consider the former case: In this case, the atomic arrangemet at the interface of two bcc solids, when they are kept over each other will be as shown in the Figures-1,2.

Suppose that they come right on the top of each other (see Figure-2), then the second assumption mentioned above can not be true. But this kind of arrangement is in equilibrium because the electrostatic repulsion between the upper and lower atoms cancel each other. Note that the equilibrium is unstable, because even if a horizontal force of small magnitude acts on this system, the atoms will start moving away from each other. This implies that even a small nudge to the upper surface will lead to motion, but this is not what is observed. Thus, this kind of arrangement is ruled out. Same argument can be used to rule out arrangement in which one atom of the upper surface comes right on top of the other atom of the lower surface.

The other arrangement (see Figure-2) is in stable equilibrium and for this arrangement the second assumption holds. Now, consider the latter case: If the crystal gets terminated at the central portion, then the single atom of the upper surface will touch the four atoms of the lower atoms and the system will be in stable equilibrium because of the repulsive forces (Figure-3). If you try to dispalce the atom from the central position, the forces will try to get the atom back to its stable position. Thus, we see that the second assumtion seems reasonable if you consider bcc solids kept over each other. So, it becomes clear that our second assumption actually rules out all the arrangements which are not in stable equilibrium.

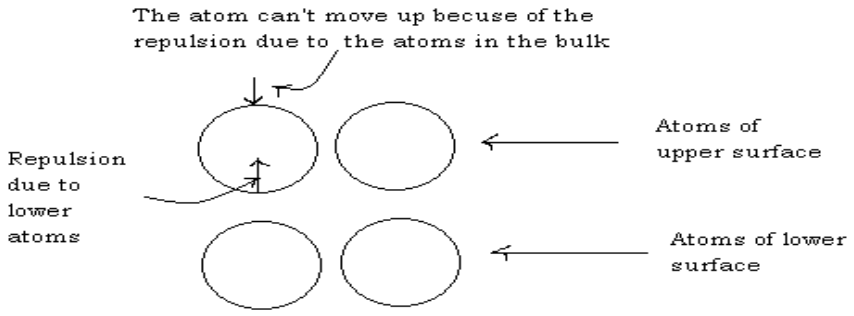

Figure 1: Side-view of the arrangement of atoms at the interface in which four atoms of upper surface come right on top of four atoms of lower surface. This arrangement is in unstable equilibrium.

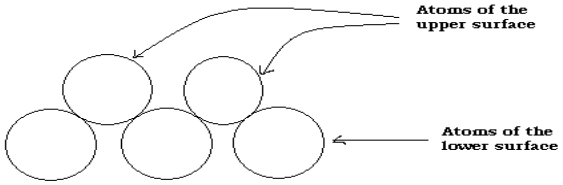

Figure 2: Side-view of the arrangement of atoms at the interface in which four atoms of upper surface settle on the central portion of the lower four atoms. This arrangement is in stable equilibrium.

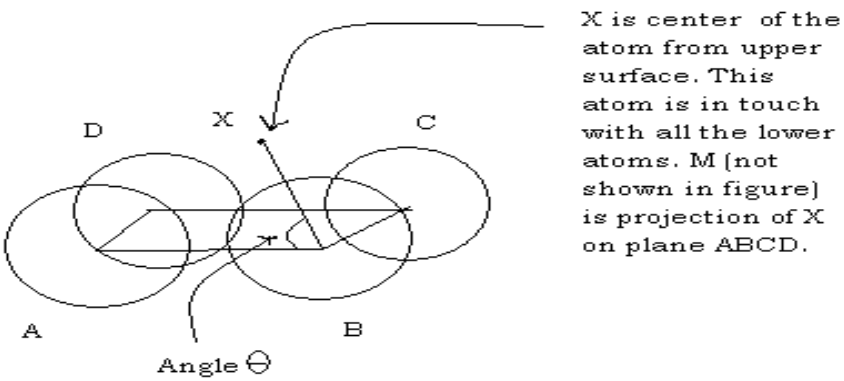

Figure 3: Three-dimensional arrangement of atoms at the interface in which single atom of the upper surface touches the four atoms of lower surface. This arrangement is in stable equilibrium.

3 Calculation of value of limiting friction

3.1 Calculating the net effective charge on the surface atoms

In our calculations, we take into account two iron surfaces. The aforesaid assumptions are quite reasonable in this case because iron has a bcc structure at lower temperature[14]. [3]

Consider an iron cube of side 1 cm kept on another iron surface. We shall make all our arguments with reference to this cube and they are equally valid for surfaces with arbitrary shapes and sizes. As has been noted earlier, friction arises due to electrostatic interactions at actual contact points. We consider one such contact point and calculate the net vertical and horizontal force at this point. Thereafter we calculate the net force on the block by simply multiplying the force into the total (approximate!) number of contact points.

Figure-3 shows the arrangement of atoms at one of the contact points according to our model. We assume that for each atom on the upper surface we can associate four atoms in the lower surface. This assumption seems reasonable for a solid having a bcc crystal structure.

Notice that each atom on the upper surface can be considered as one of the 'central' atoms in the unit cell only at *true* contact points. The interatomic distances can thus be calculated by using the well-known relations between atomic radii(r) and edge length of the unit cell(a) for a bcc crystal lattice. Note that, here we are taking the interatomic distances at the interface of the surfaces to be equal to the interatomic distances in the bulk of the material. At the outset, this assumption may seem incorrect. However, we remind the reader that such a closely-packed structure of atoms of different surfaces *occurs only at the actual contact points*

The surfaces may look smooth at macroscopic level, but at microscopic scales, we always find irregularities. Thus, when we keep two objects on each other,

[3] Upto $910°C$, iron retains its bcc structure, but above that temperature, its structure changes to fcc(face centered cubic).

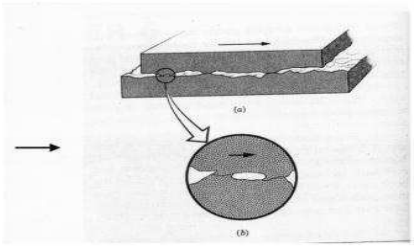

Figure 4: This picture depicts the contact points in a magnified view.

contact points are not formed at all the points. They are formed only at points where two surfaces "touch" each other (see Figure-4).

In this model, the friction arises due to the electrostatic interactions between the four lower atoms and the upper atom. This is possible only if the atoms at the surface have some net effective charge. Note that the net charge in the bulk of the material is zero. However, we would expect the accumulation of some residual charges at the surfaces. We explain the accumulation of the charge on the surface atoms (more specifically at the contact points) as follows. Some residual charges are always induced in a material due to environmental effects as well as minute deformations in the electron cloud. When two surfaces come near each other, due to electron-electron repulsion a net positive charge is induced on the surface. In a metal, these charges always reside on the surface. Moreover, these charges tend to accumulate at the sharp edges or corners of the surface in order to minimize the electrostatic potential energy of the system[7]. Indeed, these 'sharp edges' are nothing but the true contact points. So the atoms at the contact points possess a net

effective charge.

The calculation of the net effective charge on surface atoms however is a daunting task since their causes (i.e. the environmental effects) can be varied and the deformation of the electron cloud is not easy to calculate. We calculate the effective charge on each atom indirectly by equating the net vertical force experienced by all the contact atoms with the weight of the block (since $N = mg$). The net vertical force on the upper atom is given by (refer Appendix-A),

$$N_X = 4F \sin\theta = 327.296 \times 10^{27} \times q_{\text{eff}}^2$$

The net upward force on the block due to all the atoms in actual contact is,

$$N_{\text{total}} = n_{\text{micro}} \times N_X$$

$$N_{\text{total}} = 3.865579 \times 10^{40} \times q_{\text{eff}}^2 \tag{1}$$

This force is equal to the weight of the the block,

$$W = mg = 7.8 \times 10^3 \times 9.8 = 76.44 \times 10^{-3} \text{ newton}$$

taking the density of Iron to be 7.8 gm/cc[9]. Hence, the effective charge on a single atom comes out to be,

$$\boxed{q_{\text{eff}} = 1.4062194 \times 10^{-18} \text{ coulomb}} \tag{2}$$

3.2 Calculation of theoretical value

When no external horizontal force is applied, then the atom in the upper surface is in equilibrium i.e. it is at the central position (Figure-3). As the external force is applied to the upper block, the atom "slides over" the lower atoms. This causes an imbalance between the horizontal components of the forces on the upper atom due to lower atoms (see Figure-8). This gives rise to the frictional force (in a direction opposite to that of the applied force). We calculate the horizontal component of the electrostatic force between the upper and lower atoms (refer Appendix-B). The net horizontal component

of the force on the upper atom is obtained in terms of some geometric parameters of the model,

$$f_s = \frac{c}{8r^3}\sqrt{4x^2 - a^2} - \frac{c\sqrt{4x^2 + 3a^2 - 4a\sqrt{4x^2 - a^2}}}{(4r^2 + a^2 - a\sqrt{4x^2 - a^2})^{3/2}}$$

As a cross check, we see that the value of f_s vanishes when $x = a/\sqrt{2}$ (i.e. when upper atom is at the centre of the cell), which one would expect from symmetry. The maximum value of this frictional force gives us the value of the limiting friction. Figure-5 shows the *Mathematica* plot of the net horizontal force (in newtons) on y-axis as a function of x (in meters), which is a geometric parameter in our model, on x-axis, taking the interval of x from $[a/2, a/\sqrt{2}]$ i.e. $[1.4549 \times 10^{-10}, 2.05754 \times 10^{-10}]$. Clearly, the maximum value of the force is around 1.5×10^{-13} newton for a single atom. This is the "limiting" value of friction for a single atom. The net value of the limiting friction is obtained by summing up the force over the approximate number of atoms in actual contact with the surface (see Appendix-B),

$$\begin{aligned} f_{l(theoretical)} &= n_{\text{micro}} \times f_{l(single\ atom)} \\ &= 11.81 \times 10^{10} \times 1.5 \times 10^{-13} \\ &= 17.715 \times 10^{-3} \text{ newton} \end{aligned} \tag{3}$$

Notice that for a cubical iron block of side 1cm the value of limiting friction is approximately 76.44×10^{-3} newton (taking μ_s for Fe $= 1$ (for dry surface) [11]), i.e.

$$\boxed{f_{l(experimental)} = 76.44 \times 10^{-3} \text{ newton}} \tag{4}$$

$$\boxed{f_{l(theoretical)} = 17.715 \times 10^{-3} \text{ newton}} \tag{5}$$

Thus, the theoretical value matches with the experimental value fairely well!

4 Transfer of applied force to the actual contact points - A Qualitative Explanation

In the derivation of expression for static friction force, we assumed that the applied force on upper body moves the atom of the upper surface without

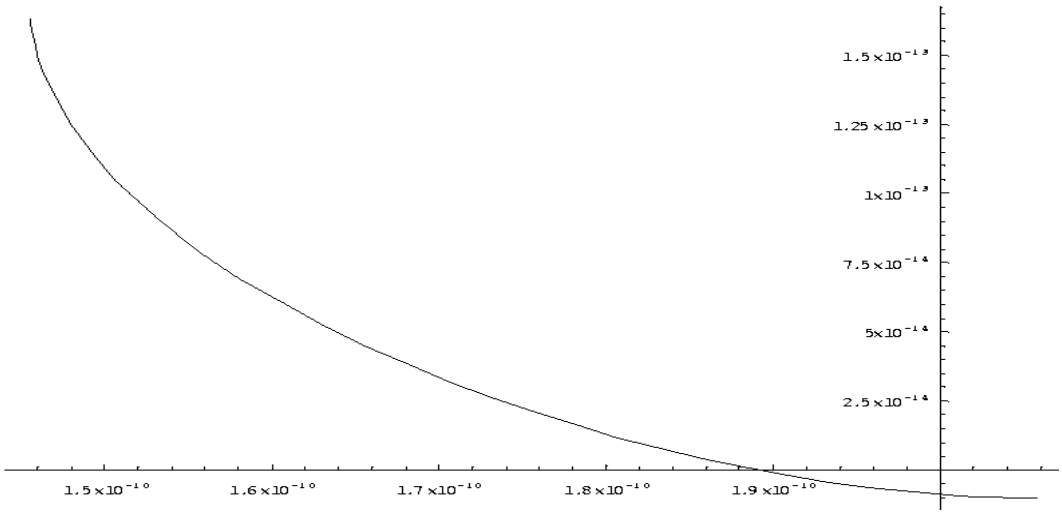

Figure 5: *Mathematica* plot of f_s(in newtons) vs. x (in metres)

the motion of the body itself (since if the body is moving, it is no longer a static friction force). This seems weird at first glance because we don't expect the body to be stationary and lowest layer (where the actual contact points reside) shifting. Thus, we need to explain how the applied force gets transferred to the actual contact point and moves the upper atom without motion of the entire body. This we elucidate as follows:
When a horizontal force is applied on a body, the layers where the force is applied will undergo a small lateral shift, but the layer below it would try to pull it back through forces. This forces can be approximated to be Hooke's law kind of forces (see Figure-6). This approximation is reasonable since, for small deviation from a stable equilibrium system, the forces which try to restore the system to its stable state are Hooke's law type of forces[13]. Let's see what happens at the irregularities which lie in the lowest layer. At irregularities, the situation is shown in (Figure-7).

Thus, the net force has direction of that of applied force. But, note that the transferred force acting at the contact point does not have the magnitude of the applied force because some work is done to stretch the springs between the layers and this energy is stored in the form of elastic potential energy. Quantitatively, we haven't been able to find out what fraction of the applied force will act at contact point. But, whatever that force may be, it will be balanced by the horizontal component of contact force till limiting friction.

5 Why $f_s > f_l$? - A Qualitative Explanation

In the Figure-8, we can see how the upper atom will move as the external force goes on increasing. As the external force on the upper body goes on increasing, the upper layer of atoms tries to shift i.e. the given atom will try to leave the cell. Upto the limiting friction, the atom will remain in the cell because the external force will be nullified by the electrostatic interactions. But if the applied force increases beyond a certain limit, then the electrostatic interactions will fail to balance out the external force and consequently, the atom will leave the cell i.e. the upper layer will "slip" and the body will start

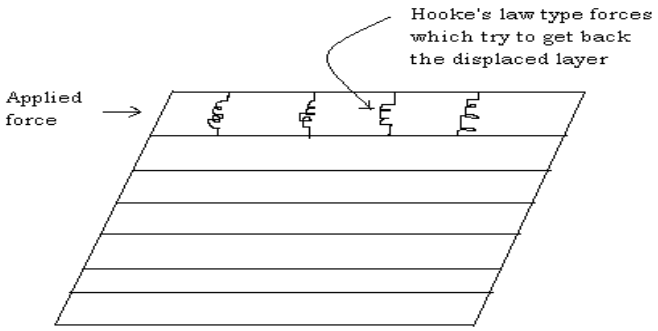

Figure 6: If a horizontal force is applied to solid, the layers near the applied force will undergo a differential displacement.

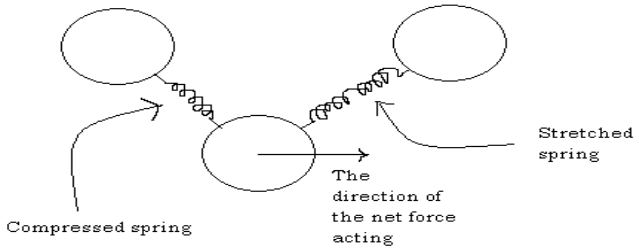

Figure 7: At the actual contact point one atom of upper surface will come close (i.e. spring will get compressed), while the other atom will move away from the central atom of the upper surface (i.e. spring will be stretched). This will result into a net force in the direction of applied force.

moving. In case of the body moving on the surface of the other body, we will have a kinetic force of friction(f_k) which will try to oppose the relative motion between the surfaces.

It is observed that the value of the kinetic friction is generally smaller than the value of limiting friction. The justification often given is that, when a body is in motion, then the surface atoms can not form sufficiently strong bonds as compared to the situation when they are at rest[10]. However this justification is not rigorously confirmed [8].

We think that one way to understand the cause of the difference between kinetic friction and static friction is to see whether the difference depends upon the nature of the irregularities on the two surfaces. Our argument is as follows: when a body with non-uniform irregularities starts to slide over another body, then we would expect that the *probablity of formation of contact points may decrease*. Note that the strength of the bonds at the contact points remains the same. However, *on an average*, the number of contact points may decrease when the body is in motion.

Our argument is somewhat intuitive and we have not been able to give a quantitative explanation. Nevertheless, in such a situation we can easily see that the *difference* in kinetic and limiting friction will increase by making the surfaces in contact more irregular. This fact can be experimentally verified.

6 Conclusion and Future scope

6.1 Conclusion

In this project, we have put forward a model for the static friction between two bodies having bcc crystal structures. We have done so by directly taking into account the electrostatic forces between atoms. We have deduced an equation for calculating the value of static friction in terms of some geometric parameters of the model. The value of limiting friction that we have obtained from this equation matches well with the observed values. This study can be extended to more complicated types of atomic arrangements.

6.2 Future scope

In this study, we have explained the force of static friction by taking into account the electrostatic interactions. We expect that this model can be extended to explain friction in solids having face centered cubic (fcc) crystal structure. We would also like to extend our model for surfaces having different types of atoms. We have also proposed (qualitatively) that the difference between the kinetic friction and the static friction may depend upon the nature of the irregularities of the surfaces involved. We would like to work it out quantitatively. We intend to do this in future. Also, we would like to evade our first assuption and take into the vibrational motion of the atoms in order to explain how heat is produced when two bodies are rubbed aginst each other.

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Appendices

A Calculation of the net upward force on the block

Consider one of the contact points at the interface of the 1 cm iron block kept upon another iron surface. As stated in assumptions, in this unit cell, a single atom of the upper surface (say X) is in touch with the four atoms of the lower surface(say A, B, C, and D). The radius of the atom is r and the edge length of the unit cell is a and the relation between them is-

$$r = \frac{\sqrt{3}a}{4} \tag{6}$$

For Iron atom, $r = 0.126 \times 10^{-9}$ m and $a = 0.29098 \times 10^{-9}$ m [14].
We first calculate the vertical component of the contact force on X due to atoms A, B, C, D. As can be seen, the horizontal component of the contact force gets cancelled because of the symmetrical arrangement of the atoms. The vertical component of the contact force on X due to A is given by,

$$N = F\sin\theta = \frac{1}{4\pi\varepsilon_0}\frac{q_{eff}^2}{4r^2}\sin\theta$$

where F is the total electrostatic force on upper atom due to A. As the distance between upper atom and other three atoms is same as that between X and A, total electrostatic force between any of the lower atom and upper atom is F. Thus, the total electrostatic force between the upper atom and four lower atoms is 4F. Thus, it follows that the total vertical component of the contact force on X is,

$$N_X = 4F\sin\theta = 327.296 \times 10^{27} \times q_{\text{eff}}^2$$

where, from Figure-4,

$$\sin\theta = \frac{a}{4r} = \frac{1}{\sqrt{3}}$$

Now, let n be the number of atoms of the upper surface in a length of 1cm. Hence,

$$a.n = 0.01 \text{ m}$$
$$\therefore n = 3.43667 \times 10^7$$

Then, number of atoms in 1cm^{2}area will be,

$$n_{\text{macro}} = 11.81065 \times 10^{14}\text{atoms}$$

Let σ be the number of atoms per unit area, where this area is apparent (or macroscopic) area. So,

$$\sigma_{\text{macro}} = 11.81065 \times 10^{18}\text{atoms}/m^2$$

But, experiments show that real (or microscopic) area in contact is approximately 10^{-4} times the apparent (or macroscopic) area in contact[8], i.e.

$$A_{\text{micro}} = A_{\text{macro}} \times 10^{-4}$$

Now, let σ_{micro} be the number of atoms per unit microscopic area. Then,

$$\begin{aligned} \sigma_{\text{macro}} &= \sigma_{\text{micro}} \\ \therefore \frac{n_{\text{macro}}}{A_{\text{macro}}} &= \frac{n_{\text{micro}}}{A_{\text{micro}}} \\ \therefore n_{\text{micro}} &= n_{\text{macro}} \times 10^{-4} \\ \therefore n_{\text{micro}} &= 11.81065 \times 10^{10}\text{atoms} \end{aligned} \tag{7}$$

The net normal contact force on the block (N_{total}) is obtained by multiplying N_{total} with the actual number of atoms in touch (i.e. n_{micro}). Thus,

$$N_{\text{total}} = n_{\text{micro}} \times N_X$$

where N_X is the vertical component of the contact force on upper atom X due to A, B, C, and D.

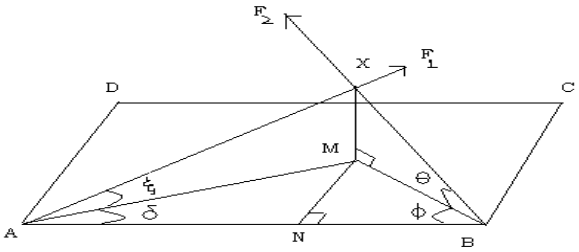

Figure 8: The force imbalance when upper atom is in displaced position.

B Derivation of the formula for Static Friction

Let some external horizontal force be applied on the iron block. Due to this force, there will be an imbalance between the horizontal components of the contact forces on the atom X due to A and D, and due to B and C, because the atom of the upper surface will move in the direction of the force so that its distance from the atoms A and D of the lower surface will change. Let r_1 be the distance of X from A and D, while r_2 be the distance of X from B and C. As r_2 is less than r_1, the net horizontal component of the force will act in a direction opposite to the external force because electrostatic force varies inversely with the square of the distance (see Figure-8). Till limitng friction, the external horizontal force is balanced by the horizontal component of the net contact force.

In Figure-8, ABCD is the plane joining the centres of the atoms A,B,C,D.

Let's draw a perpendicular XM from point X(centre of atom X) on the plane ABCD. Then, in $\triangle$MBX, θ is the angle MBX. Let $MX = y$ and $MB = x$. Then, the relation $x^2 + y^2 = 4r^2$ will always hold (until body slides over)[4]. We then draw MN$\perp$AB, so that in $\triangle$MNB, ϕ is the angle NBM. We here note that due to symmetry, the atom will move in such a way that NM will always be equal to $a/2$. The horizontal component of the force on X due to the atom B will be given by,

$$\varphi_2 = F_2 . \cos\theta . \cos\phi$$

where F_2 is the total electrostatic force on the displaced upper atom due to atom B and is given by,

$$F_2 = \frac{1}{4\pi\varepsilon_0}\frac{q_{\text{eff}}^2}{r_2^2}$$

The same expression will hold for the horizontal component of the force on X due to C. Then, total horizontal component of the force on atom X due to the atoms B and C is given by,

$$\varphi_{BC} = 2F_2 . \cos\theta . \cos\phi$$

where,

$$\cos\theta = \frac{x}{2r} \quad \text{and} \quad \cos\phi = \frac{\text{NB}}{x}$$

From Figure-6, we can see that, in $\triangle$MNB,

$$\text{NB} = \sqrt{x^2 - \frac{a^2}{4}}$$

$$\therefore \cos\phi = \sqrt{1 - \frac{a^2}{4x^2}}$$

Hence, the product is,

$$\cos\theta . \cos\phi = \frac{\sqrt{4x^2 - a^2}}{4r} \tag{8}$$

Similarly, we can compute the horizontal component of the force on the atom X due to the atoms A and D. In $\triangle$XMA, ξ is the angle XAM. Also, in $\triangle$

[4]Note that this makes y, which is the height of center of upper atom from the plane passing through centres of lower atoms, a function of x. Thus, as the atom moves away from the central position, it undergoes vertical displacement too.

AMB, δ is the angle MAB. Let AM=z, so that AX = $\sqrt{z^2+y^2}$. Applying cosine rule in ΔAMB,

$$z^2 = x^2 + a^2 - 2xa\cos\phi$$

$$\therefore z = \sqrt{x^2 + a^2 - 2xa\cos\phi}$$

But,

$$\cos\phi = \sqrt{1 - \frac{a^2}{4x^2}}$$

Thus, expression for z becomes,

$$z = \sqrt{x^2 + a^2 - a\sqrt{4x^2 - a^2}}$$

Then, horizontal component of the force on X due to the distant atom A will be given by,

$$\varphi_1 = F_1.\cos\xi.\cos\delta$$

where F_1 is the total electrostatic force on the displaced upper atom due to atom A and is given by,

$$F_1 = \frac{1}{4\pi\varepsilon_0}\frac{q_{\text{eff}}^2}{r_1^2}$$

The same expression will also hold for the horizontal component of the force on X due to the atom D. Hence, total horizontal component of the force on atom X due to the atoms A and D is given by,

$$\varphi_{AD} = 2F_1.\cos\xi.\cos\delta$$

In ΔAMX, $\cos\xi = \frac{z}{\text{AX}}$. But, AX=$\sqrt{z^2+y^2}$. Thus,

$$\cos\xi = \frac{z}{\sqrt{z^2+y^2}}$$

From ΔBMX, it is clear that $y^2 = 4r^2 - x^2$. Also, we know the expression for z. Thus, above equation becomes,

$$\cos\xi = \frac{\sqrt{x^2 + a^2 - a\sqrt{4x^2 - a^2}}}{\sqrt{x^2 + a^2 - a\sqrt{4x^2 - a^2 + 4r^2 - x^2}}} \tag{9}$$

$$\therefore \cos\xi = \frac{\sqrt{x^2 + a^2 - a\sqrt{4x^2 - a^2}}}{\sqrt{4r^2 + a^2 - a\sqrt{4x^2 - a^2}}} \tag{10}$$

Let's find out an expression for $\cos\delta$. From Figure-8, it is clear that,

$$\cos\delta = \frac{\text{AN}}{z} \tag{11}$$

From ΔANM, we see that

$$\text{AN} = \sqrt{z^2 - \frac{a^2}{4}} \tag{12}$$

$$\therefore \cos\delta = \frac{\sqrt{4z^2 - a^2}}{2z}$$

Using the expression for z, we have-

$$\cos\delta = \frac{\sqrt{4(x^2 + a^2 - a\sqrt{4x^2 - a^2}) - a^2}}{2\sqrt{x^2 + a^2 - a\sqrt{4x^2 - a^2}}}$$

$$\therefore \cos\delta = \frac{\sqrt{4x^2 + 3a^2 - 4a\sqrt{4x^2 - a^2}}}{2\sqrt{x^2 + a^2 - a\sqrt{4x^2 - a^2}}}$$

Hence, the product is,

$$\cos\xi.\cos\delta = \frac{\sqrt{4x^2 + 3a^2 - 4a\sqrt{4x^2 - a^2}}}{2\sqrt{4r^2 + a^2 - a\sqrt{4x^2 - a^2}}} \tag{13}$$

Hence, the net horizontal static frictional force on the atom X until the limiting friction (f_l) reaches, is given by,

$$f_s = \varphi_{BC} - \varphi_{AD} = 2(F_2.\cos\theta.\cos\phi - F_1.\cos\xi.\cos\delta) \tag{14}$$

Substituing the expressions for $\cos\theta$, $\cos\phi$, $\cos\xi$, and $\cos\delta$, we get the final expression for the static frictional force which comes out to be in terms of x, a, r_1, and r_2.

$$f_s = \frac{F_2\sqrt{4x^2 - a^2}}{2r} - \frac{F_1\sqrt{4x^2 + 3a^2 - 4a\sqrt{4x^2 - a^2}}}{\sqrt{4r^2 + a^2 - a\sqrt{4x^2 - a^2}}}$$

Let $c = \frac{q_{\text{eff}}^2}{4\pi\varepsilon_0}$. Then, putting in expressions for F_1 and F_2, above equation becomes,

$$f_s = \frac{c\sqrt{4x^2 - a^2}}{2r_2^2 r} - \frac{c\sqrt{4x^2 + 3a^2 - 4a\sqrt{4x^2 - a^2}}}{r_1^2\sqrt{4r^2 + a^2 - a\sqrt{4x^2 - a^2}}}$$

Here, we note that the way the upper atom is moving implies that r_2 will remain equal to $2r$ till the atom remains within the cell. Thus, putting $r_2 = 2r$, the above expression becomes,

$$f_s = \frac{c\sqrt{4x^2 - a^2}}{8r^3} - \frac{c\sqrt{4x^2 + 3a^2 - 4a\sqrt{4x^2 - a^2}}}{r_1^2\sqrt{4r^2 + a^2 - a\sqrt{4x^2 - a^2}}}$$

Again, from Figure-8, we note that, $r_1^2 = z^2 + y^2$. But, $y^2 = 4r^2 - x^2$. Thus,

$$r_1^2 = z^2 + 4r^2 - x^2$$

Putting in expression for z^2,

$$r_1^2 = 4r^2 + a^2 - a\sqrt{4x^2 - a^2}$$

Then, equation for f_s becomes,

$$\boxed{f_s = \frac{c}{8r^3}\sqrt{4x^2 - a^2} - \frac{c\sqrt{4x^2 + 3a^2 - 4a\sqrt{4x^2 - a^2}}}{(4r^2 + a^2 - a\sqrt{4x^2 - a^2})^{3/2}}} \tag{15}$$

It should be noted that f_s is function of just one geometric parameter, viz. x. To check whether the above expression is consistent or not, we put $x = a/\sqrt{2}$, which corresponds to the state of the system when no external horizontal force is applied and the atom is in the central stable position. *A priori*, we would expect that the static frictional force should be zero and indeed the expression gives zero value when $x = a/\sqrt{2}$!

An important point to be noted here is that we have not considered the electrostatic repulsion that may arise due to the lower atoms in the adjacent cell. It is difficult to calculate the expression for this force. However, the force will be really weak because of the distance at which theses atoms lie. Thus, to first approximation, these effects can be neglected.

C Why to treat atoms classically?

In this section, we would like to justify our first assumption which says that atoms can be dealt in classical manner, i.e. without involving the laws of quantum mechanics.

In general, quantum mechanics is relevant when the de Broglie wavelength of the particle in question (here, atoms) is greater than the characteristic size of the system (d)[13], i.e.

$$\lambda = \frac{h}{p} > a$$

In this case, the characteristic size of the system is edge length(a). In thermal equilibrium at (kelvin) temperature T, the average kinetic energy of the particle is,

$$\frac{P^2}{2m} = \frac{3k_BT}{2}$$

where k_B is Boltzmann's constant. Thus, the typical de Broglie wavelength is

$$\lambda = \frac{h}{\sqrt{3mk_BT}} \tag{16}$$

So, quantum mechanics becomes relevant when $\lambda > a$, i.e. $\lambda > 0.29098 \times 10^{-9}$ m. The mass of the iron atom can be approximately taken as the mass of the nucleons, since mass of electrons is negligible as compared to mass of nucleons. Atomic weight of iron atom is, $m = 55.845$ amu $= 92.7 \times 10^{-27}$ kg. Also, $k_B = 1.38 \times 10^{-23}$ J/K and $h = 6.626 \times 10^{-34}$ Js.

Putting in all the values, we see that iron atoms need to be treated quantum mechanically below temperature of 1.37 K. Thus, it becomes clear that for all practical temperatures, atoms can be treated classicaly.

We have also assumed that atom is like a rigid ball. One shortcoming of this assumption is that this model can't explain heat which is produced when two surfaces are rubbed against each other. We would like to do this in future.


I THINK WE'VE GOT ENOUGH INFORMATION NOW, DON'T YOU?
ALL WE HAVE IS ONE "FACT" YOU MADE UP.
THAT'S PLENTY. BY THE TIME WE ADD AN INTRODUCTION, A FEW ILLUSTRATIONS, AND A CONCLUSION, IT WILL LOOK LIKE A GRADUATE THESIS.