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ADHESIVE CONTACT MODELLING BASED ON LENNARD-JONES FORCE LAW

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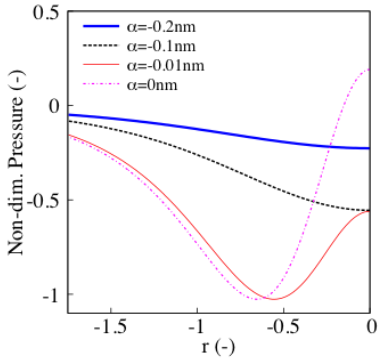
Graphical abstract



Abstract

At diminishing separations, the load carrying capacity of opposing rough surfaces is distributed among asperities across a smaller contact area as compared with the apparent contact area. An improved understanding on asperity interactions is therefore required in order to better predict the tribological behaviour of a rough surface contact. In this paper, based on Weir's method for computing the work of adhesion, a simplistic adhesive contact model is proposed, applying the Lennard-Jones force law, to study an asperity pair interaction. Assuming that the tip represents an asperity, the numerical model is subsequently applied to simulate a Tungsten Carbide (WC) coated AFM tip indenting on a Diamond (111) surface. It was found that the simulated pull-off force agrees with the measured value by Enachescu *et al* for a WC AFM tip on a Diamond (111).

Keywords: Asperity, atomic force microscopy, adhesion, Lennard-Jones and pull-off force

1.0 INTRODUCTION

The size of equipments and measurement devices are decreasing with the advancement in technology and science as forecasted in Moore's law. The miniaturisation of machine elements introduces nano-scale contact in the form of increased surface asperity interactions, which are heavily influenced by intermolecular and surface forces such as boundary adhesion [1]. To understand these contact interactions, one of the earliest theories proposed by Hertz [2] for local elastic deformation of smooth contacting bodies, could be used to describe the normal contact load, deflection of the body and the contact area between two contacting bodies. However, the model excludes any kind of surface forces. By considering surface adhesion, Johnson *et al* [3] proposed a contact model using fracture-mechanics, known as the JKR model. On the other hand, Derjaguin *et al* [4] approximated the effects of adhesion between two contacting spherical bodies by assuming that surface forces occur only outside of the contact region, thus giving the DMT model.

Initially, both models seemed to have produced contradicting ideas, but were later proven to be interrelated by Tabor [5]. However, there are still shortcomings in using the aforementioned models: DMT model is only valid at small values of Tabor's coefficient ($\mu \ll 1$) while the JKR model is only valid at higher values of the Tabor's coefficient ($\mu \ll 1$). This led to further adhesive contact model development by Muller et al [6], using Lennard-Jones potential to describe the behaviour of two contacting spheres and Maugis [7], using the Dugdale model with relation to Tabor's parameter, to illustrate the transition between JKR to DMT. Recently, improved numerical analysis on

the adhesive contact was proposed by Attard and Parker [8], Greenwood [9], Feng [10] and Chong [11].

A common parameter used for the above-mentioned adhesive contact models involves the surface energy for the materials, which is ascertained empirically most of the time. Therefore, by using Weir's [12] method in computing the surface energy, this study proposes a simplistic numerical scheme to solve for an adhesive contact using the Lennard-Jones power law. For validation, the numerical scheme is applied to simulate a Tungsten Carbide (WC) coated AFM tip on a Diamond (111) surface. The predicted pull-off force is then compared with the measured value by Enachescu *et al* [13].

2.0 MATHEMATICAL MODEL

The study attempts to simulate an adhesive contact, considering a spherical cap on the AFM tip indenting a planar surface. The contact problem is illustrated in Figure 1.

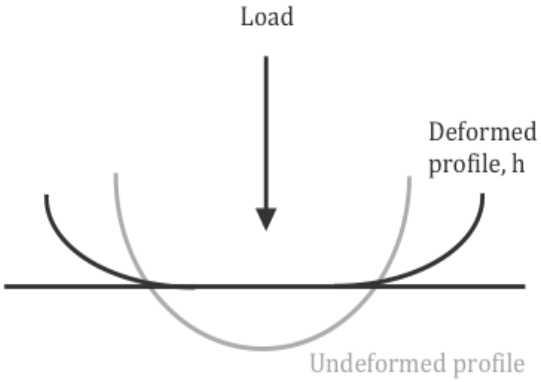


Figure 1 Schematic of spherical cap AFM tip indenting sample

The deformed contact profile, $h(r)$ given in Figure 1 is described as follow:

$$h(r) = -\alpha + z_o + A - \frac{r^2}{2R} - w(r) \qquad \text{(Eq. 1)}$$

where α is the non-deformed indenter or tip approach, Z_o being the equilibrium spacing between two parallel flat surface of 1.65 Å [14,15] with R referring to the curvature radius of the spherical cap on the AFM tip. The deformation of the contact, $w(r)$ is given as:

$$w(r) = \frac{4}{\pi E}\int_0^{r\infty} \frac{\hat{r}p(\hat{r})}{r+\hat{r}} K\left(\frac{2\sqrt{r\hat{r}}}{r+\hat{r}}\right) d\hat{r} \qquad \text{(Eq. 2)}$$

where E represents the reduced modulus of elasticity with K being the complete elliptic integral of the first kind. The term $p(r)$ is the contact pressure within the approaching contact and is expressed as:

$$p(r) = -\frac{8\lambda}{3z_o}\left\{\left[\frac{z_o}{h(r)}\right]^3 - \left[\frac{z_o}{h(r)}\right]^9\right\} \qquad \text{(Eq. 3)}$$

where, $\lambda = 2\left(\gamma_1 + \gamma_2 - 2\sqrt{\gamma_1\gamma_2}\right)$ is the work adhesion.

The surface energy terms, γ are most often obtained experimentally, leading to an empirical solution for the adhesive contact. Therefore, in order to have a more theoretical intensive model, Weir's method [12] is applied in computing the surface energy as follows:

$$\frac{\gamma}{aB} = \frac{1}{(m-2)(n-2)} \qquad \text{(Eq. 4)}$$

where $a = (M/\rho)^{1/3}$, is the material Poisson's ratio, and $B = E/[3(1-2\nu)]$ is the material bulk modulus with M and ρ referring to the molecular weight and density of the material. The terms m and n depend on the power of the Lennard-Jones potential, which are 6 and 12 respectively in this study.

3.0 NUMERICAL APPROACH

Applying the discretisation provided by Feng [10], Equation (1) can then be rearranged to give a residual equation, $\Re$ as follows:

$$\Re(\bar{r}) = H(\bar{r}) + A - \frac{\bar{r}^2}{2} - W(\bar{r}) \qquad \text{(Eq. 5)}$$

The residual is solved iteratively until, $\Re < 1\times10^{-3}$. In this study, the integral term for the discretised surface deflection, W is calculated using Gaussian quadrature. Subsequently, following the numerical scheme as being illustrated in Figure 2, the discretised profile, H is successively relaxed using:

$$H_{new} = H_{old} - 0.001\times\Re_{old} \qquad \text{(Eq. 6)}$$

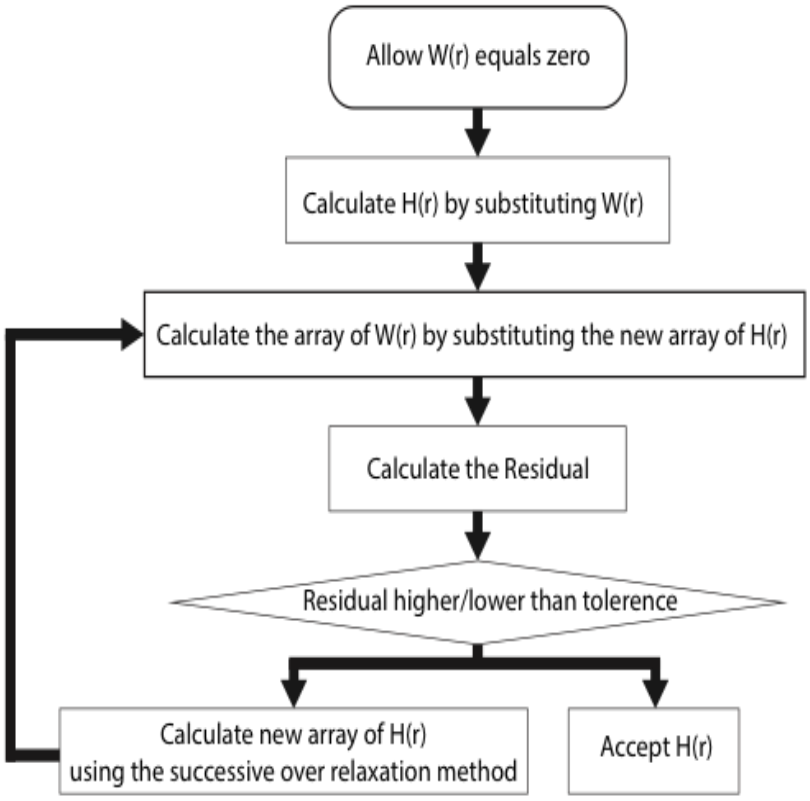


Figure 2 Flowchart for the numerical scheme

4.0 RESULTS AND DISCUSSIONS

In the study, the contact was solved for a domain of 128 elements. The simulation parameters for an AFM tip coated with WC on a Diamond (111) surface are tabulated in Table 1, giving a Tabor's parameter of 0.014, which is well within the DMT domain. This bodes well with the assumption of a spherical cap AFM tip, where deformation of the tip is mainly focused along the tip area.

Figure 3(a) shows the non-dimensional contact and profile at different tip approach locations, illustrating the build-up of compressive stress, which eventually would elastically deform the WC coated AFM tip with a further increase in indentation. Because the investigated contact problem is shown to be within the DMT region, it can be observed that tip deflection is minimal as illustrated in Fig 3(b).

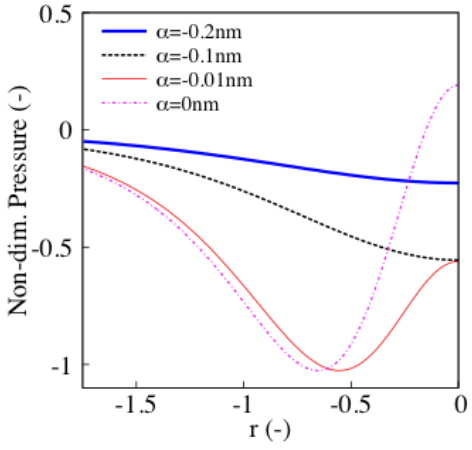


Figure 3 (a) Contact characteristics of the WC coated AFM tip on a Diamond (111) surface: Non-dimensional contact pressure

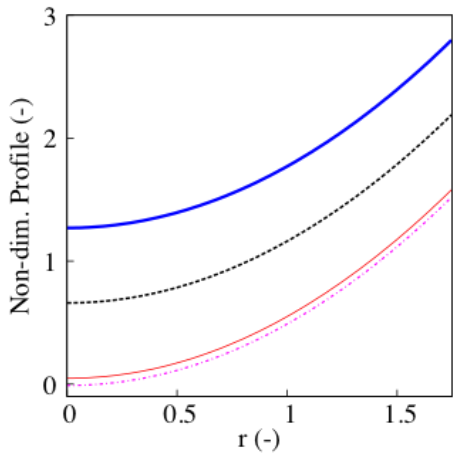


Figure 3 (b) Contact characteristics of the WC coated AFM tip on a Diamond (111) surface: Non-dimensional profile

The force-cantilever displacement curve measured by Enachescu *et al* [13] is given as in Figure 4(a). The definitive parameter from the plot - pull-off force, is given as 7.3nN. Applying the proposed numerical model, using Weir's method [12] in computing the theoretical work of adhesion (see, Figure 4(b)), the predicted pull-off force is obtained as 8.6nN, giving a deviation of 17.8% from the measured value. At such diminishing scale, the difference is deemed to be acceptable because the proposed numerical scheme assumes an ideal contact between the AFM tip and the surface. Whereas, in reality other factors may also reduce the "stickiness" of the contact (e.g. foreign particles between contacts, nano-scale surface asperity interactions along the coated tip or surface).

Table 1 Simulated parameters for a WC coated AFM on a Diamond (111) surface

	Diamond (111) [16]	Tugnsten Carbide [17]
Molar Mass (kg)	1.99×10^{-26}	3.25×10^{-25}
Density (kg m^{-3})	3500	15250
Young's Modulus (GPa)	1164	600
Poisson's Ratio	0.079	0.2

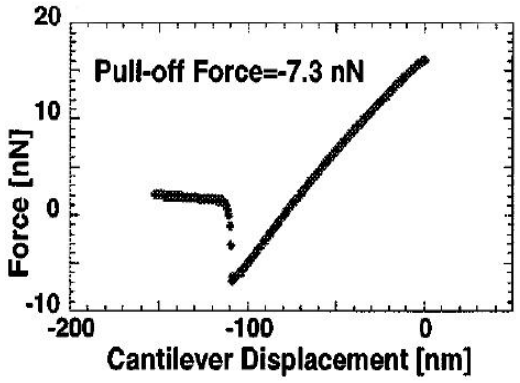


Figure 4 (a) Measured and simulated force curves for a WC coated AFM on a Diamond (111) surface: Force-Cantilever displacement [13]

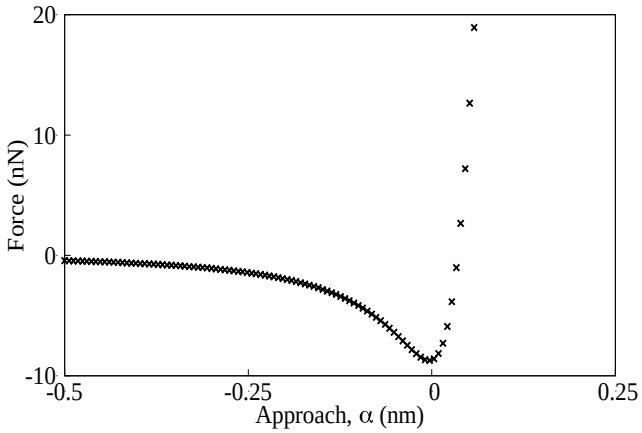


Figure 4 (b) Measured and simulated force curves for a WC coated AFM on a Diamond (111) surface: Force-Tip approach

4.0 CONCLUSION

A numerical scheme is proposed, solving for the adhesive contact using the Lennard-Jones force law together with Weir's method in computing the theoretical value for the work of adhesion, λ. For a WC coated AFM tip on a Diamond (111) surface, the pull-off force predicted is shown to deviate by 17.8% from the measured value. This is in agreement with the experimental measurement, looking at the fact that the proposed numerical model assumes a theoretical work of adhesion, based on Weir's method. The study prepares a platform to further investigate the relevance of Weir's approach in predicting the work of adhesion for an adhesive contact with higher value of Tabor's parameter.

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References

[1] Chong, W. W. F., Teodorescu, M., and Rahnejat, H. 2013. Nanoscale Elastoplastic Adhesion Of Wet Asperities. *Proc. IMechE Part J: J. Eng. Trib.* 227(9):996–1010.

[2] Heinrich, H. 1881. On The Contact Of Elastic Solids. *J. Reine Angew. Math.* 92(110):156–171.

[3] Johnson, K. L., Kendal, K. I., and Roberts, A. D. 1971. Surface Energy And The Contact Of Elastic Solids. *Proc. Roy Soc Lon. A. Math. & Phy Sci*. 324(1558):301– 313.

[4] Derjaguin, B. V., Muller, V. M., and Toporov, Y. P. 1975. Effect Of Contact Deformations On The Adhesion Of Particles. *J. Coll. & Int. Sci*. 53(2): 314–326.

[5] Tabor, D. 1977. Surface Forces And Surface Interactions. *J. Coll. & Int. Sci.* 58(1): 2–13.
[6] Muller, V. M., Derjaguin, B. V., and Toporov, Y. P. 1983. On Two Methods Of Calculation Of The Force Of Sticking Of An Elastic Sphere To A Rigid Plane. *Coll. & Surf.* 7(3): 251–259.
[7] Maugis, D. 1992. Adhesion Of Spheres: the JKR-DMT Transition Using A Dugdale Model. *J. Coll. & Int. Sci*. 150(1): 243–269.
[8] Attard, P. and Parker, J. L. 1992. Deformation And Adhesion Of Elastic Bodies In Contact. *Phys Rev A*. 46(12): 7959–7971.
[9] Greenwood, J. A. 1997. Adhesion Of Elastic Spheres. *Proc. Roy. Soc. A: Math, Phy. & Eng. Sci*. 453(1961): 1277–1297.
[10] Feng, J. Q. 2001. Adhesive Contact Of Elastically Deformable Spheres: A Computational Study Of Pull-Off Force And Contact Radius. *J Colloid Interface Sci*. 238(2): 318–323.
[11] Chong, W. W. F. 2013. A Numerical Model For Wet-Adhesive Line Contact. *Procedia Eng*. 68: 579– 585.
[12] Weir, G. 2008. Implications From The Ratio Of Surface Tension To Bulk Modulus And Nearest Neighbour Distance, For Planar Surfaces. *Proc. Roy. Soc. A: Math, Phy. & Eng. Sci*. 464(2097): 2281–2292.
[13] Enachescu, M., Van Den Oetelaar, R. J. A., Carpick, R. W., Ogletree, D. F., Flipse, C. F. J., Salmeron, and M. 1998. Atomic Force Microscopy Study Of An Ideally Hard Contact: The Diamond (111)/Tungsten Carbide Interface. *Phy. Rev. Lett*. 81(9): 1877.
[14] Israelachvili, J. N. 2011. Intermolecular And Surface Forces: Revised Third Edition. *Acad. Press*.
[15] Butt, H., Cappella, B., and Kappl, M. 2005. Force Measurements With The Atomic Force Microscope: Technique, Interpretation And Applications. *Surf. Sci. Rep.* 59(1): 1– 152.
[16] Klein, C. A. 1992. Anisotropy Of Young's Modulus And Poisson's Ratio In Diamond. *Mat. Res. Bull.* 27(12): 1407–1414.
[17] AZoNetwork. Tungsten carbide - An overview, October 2014.