Intermolecular Force and Surface Roughness Models for Air Bearing Simulations for Sub-5nm Flying Height Sliders

Du Chen and David B. Bogy

Computer Mechanics Laboratory

Dept. of Mechanical Engineering

University of California

Berkeley, CA 94720

Abstract

When the spacing between the slider and the disk is less than 5 nm, the intermolecular forces between the two solid surfaces can no longer be assumed to be zero. The model proposed by Wu and Bogy can be viewed as a flat slider–disk intermolecular force model. The local distance between the slider and disk needs to be considered in this model when the slider-disk spacing is in the contact regime. To get more accurate intermolecular force effects on the head disk interface, we need to consider the slider and disk surface roughnesses when the flying height is comparable to the surface RMS roughness value or when contact occurs. With the intermolecular force model and asperity roughness model implemented in the CML air bearing program, we analyze the effect of intermolecular adhesion stress on the slider at low flying height in a static flying simulation. It is found that the intermolecular adhesion stress between the slider and the disk has slight effect on the slider-disk interface for a flying slider.

1. Introduction

The effect of intermolecular force on air bearing sliders in hard disk drives has been extensively investigated recently, starting with the paper by Wu and Bogy [1]. The intermolecular force between the slider and the disk is usually modeled based on the Leonard-Jones potential, which describes the potential energy between two atoms as a function of the distance between them. In the implementation of this potential in closely spaced air bearings the force is expressed as a function of the distance between the slider and the disk, i.e. the local flying height (FH). However, when the FH is less than 3nm, a contact distance ε (0.3nm-0.5nm) needs to be considered and the intermolecular force then turns out to be a function of $FH + \varepsilon$. Thus for very close spacing the intermolecular force is overestimated in Wu and Bogy [1], and others. After this correction is made there does not occur an unbounded repulsive intermolecular force when the FH is less than 0.5nm, or down to contact.

The model resulting from this modification can be viewed as a flat slider-disk intermolecular force model. To get more accurate intermolecular force effects on the head disk interface the slider and disk surface roughnesses need to be considered when the flying height is comparable to the surface RMS roughness value or when contact occurs. The improved DMT (IDMT) models [2, 3 and 4], which are suitable for small, stiff spherical asperities, can be used to approximate the rough slider-disk intermolecular adhesion force. The intermolecular adhesion between measured rough slider and disk surfaces is calculated using the IDMT models, and the results are compared with the intermolecular force between the corresponding flat slider and disk surfaces. With this improvement implemented in the CML air bearing program, the effect of adhesion stress on the slider at low flying heights is analyzed in the static flying simulation.

2. Intermolecular force model

As a special case of the Mie Potential, the Lennard-Jones potential is widely used to describe the interaction between two atoms or molecules. It is expressed as,

$$w(r) = -C / r^6 + D / r^{12}, \tag{1}$$

where r is the center-to-center distance between the atoms and C and D are constants. For two atoms in vacuum the values C=10^{-77}Jm^6 and D=10^{-134}Jm^{12} are usually used [1]. Differentiating the Lennard-Jones potential with respect to the distance r, we obtain the Lennard-Jones force as,

$$f = \frac{dw}{dr} = \frac{6C}{r^7} - \frac{12D}{r^{13}}, \tag{2}$$

where the direction of adhesion is the positive direction of the force.

If we ignore the anisotropy, non-additivity, and retardation effects of the Lennard-Jones potential, and make the continuum assumption, we get through appropriate integration the potential between an infinite-half space and a unit area of a parallel infinite half space, as shown in Fig.1,

$$U = \rho_2 \int_h^\infty (-\frac{\pi C \rho_1}{6z^3} + \frac{\pi D \rho_1}{45 z^9}) dz, \tag{3}$$

where ρ_1 and ρ_2, respectively, are the number densities of atoms or molecules in these two infinite half spaces and h is the distance between the two center planes of the surface atoms or molecules. If we differentiate this potential with respect to the distance h, we get the intermolecular adhesion stress between two half spaces,

$$P(h) = \frac{dU}{dh} = \frac{A}{6\pi}\frac{1}{h^3} - \frac{B}{45\pi}\frac{1}{h^9}, \tag{4}$$

where the Hamaker constant A=$\pi^2 C \rho_1 \rho_2$ and another constant $B = \pi^2 D \rho_1 \rho_2$. This result is similar to the intermolecular force expression in Wu and Bogy [1] except that here h is

the center-plane-to-center-plane distance instead of the flying height. We assume that the surfaces of the two half spaces are in contact when the total potential energy is a minimum [5]. If the minimum potential is at the distance $h=\varepsilon$, then the flying height is equal to $h-\varepsilon$. We see that $P(h=\varepsilon)=0$ when the potential takes the minimum. Then, using Equation (4) we find

$$\varepsilon = (\frac{2B}{15A})^{1/6}. \tag{5}$$

So Equation (4) can be written as,

$$P(h) = \frac{A}{6\pi\varepsilon^3}[(\frac{\varepsilon}{h})^3 - (\frac{\varepsilon}{h})^9]. \tag{6}$$

If we take the difference in surface energy before and after contact as the required energy to separate the two contacting surfaces against the intermolecular adhesion, then we have

$$\Delta\gamma = \gamma_1 + \gamma_2 - \gamma_{12} = \int_{\varepsilon}^{\infty} P(h)dh = \frac{A}{16\pi\varepsilon^2}, \tag{7}$$

where γ_1 and γ_2 are the surface energies of the two surfaces before contact, and γ_{12} is the surface energy of their interface.

The contact distance ε between two half-spaces was suggested to be 0.3-0.5 nm [2, 3, and 4]. Recently Yu and Polycarpou [6] calculated ε based on the relationship between the ground-state property of a crystal and its interatomic potential, which is dominated by the nearest neighbors. This approach is valid for molecular crystals, in which the total energy is primarily the sum of all interaction potentials between the molecules, and this weak intermolecular interaction can be approximated by the Lennard-Jones potential. However, for covalent crystals, such as diamond, or metals, the interatomic bonds are covalent bonds or metallic bonds, which cannot be described by the Lennard-Jones potential [7]. Another issue is the incompatibility between the continuum approach and

the molecular approach with the nearest neighbor assumption. The continuum approach considers the interaction between one atom or molecule and those non-nearest neighbors. So if we assume that the nearest neighbors contribute most of the interaction energy in the molecular approach, the obtained results can not be applied to the continuum approach.

Notice that $\Delta\gamma = \gamma_1 + \gamma_2 - \gamma_{12} \approx 2\gamma$ for two surfaces composed of the same material, where γ is their surface energy. Thus for two diamond-like carbon (DLC) surfaces, we know the surface energy $\gamma \approx 0.04 J/m^2$ [8] and the Hamaker constant $A = 1.80 \times 10^{-19} J$ [9], then we can estimate the contact distance ε for DLC surfaces through Equation (7). This estimation gives $\varepsilon = 0.22nm$. So it is a good approximation if we take $\varepsilon = 0.3nm$.

If we take $\varepsilon = 0.3nm$, then the flying height can not be approximated by *h* when the flying height is comparable to ε. Fig.2 shows the adhesion stresses with *FH=h* and *FH=h-ε.* When *FH=0,* i.e. *h=ε*, the two surfaces are in contact, and the contact force can be obtained through contact mechanics. So if the contact distance ε is considered, we will not have the result that an infinite repulsion will occur between the slider and disk when the flying height approaches zero. This is reasonable since the slider may contact the disk and even crash on the disk.

3. Improved DMT model

If we also consider the surface roughness we cannot use the above simple integration method to calculate the total potential and adhesion pressure of two half spaces. We need to turn to other asperity-based adhesion models. For a single asperity contact, Derjaguin et al. [5] proposed the DMT model, which assumes that the adhesion is the sum of all the intermolecular interactions outside the contact zone, and there is no contribution from the

contact area. Another, somewhat opposite model, called the JKR model [10], assumes that the adhesion is confined to the contact region. As pointed out by Tabor [11], these two models work under different conditions, which are determined by the adhesion parameter λ,

$$\lambda = (\frac{R\Delta\gamma^2}{E^2\varepsilon^3})^{1/3}, \tag{8}$$

where E is the equivalent Young's modulus and R is the radius of curvature of the asperity. It was shown that low values of λ ($\lambda<1$) correspond to a regime where the DMT model applies and high values of λ correspond to the JKR regime. The Maugis model [12], which used the Dugdale approximation [13] to the Lennard-Jones force, can be viewed as a bridge between the DMT and JKR models, and it applies to a wide range of adhesion parameters.

For a slider-disk interface, R is on the order of 10^1μm, E is on the order of 10^1 GPa and $\Delta\gamma$ is around 10^{-2}J/m^2, then though Equation (8) we determine that λ is around 0.15, which is much less than 1. So we can use the DMT model for the adhesion problem in the slider-disk interface. Of course here we have made the assumption that the adhesion between the slider and disk is quasi-static.

The contact between two rough surfaces can be modeled by an equivalent single rough surface contacting a flat rigid plane. Some of the asperities on the equivalent rough surface are in contact with the flat surface, while others are not in contact. So we need to use the improved DMT model [4] to consider the adhesion between those non-contacting asperities and the flat surface as well as the adhesion due to contacting asperities. Since the DMT model only uses the Hertz profile of an elastically deformed asperity for all contacting asperities, Chang, et al [2] proposed a CEB-IDMT model with the profile obtained through the volume conservation theory for plastic contact; Kogut and Etsion [3]

developed the KE-IDMT model with the asperity profile from their FEM solution. The difference between the CEB-IDMT model and KE-IDMT model, numerically shown in [3], partially comes from the inaccuracy of Equation (19a) in [3], which occurs when the dimensionless interference is less than 0.1. Here we directly use Equation (15) in [3] for the KE-IDMT model.

We use the equivalent slider and disk surface parameters as given in [14], shown in Table I, and calculate the adhesion stresses based on these three adhesion models, i.e. IDMT, CEB-IDMT and KE-IDMT. The results are shown in Fig.3. Here the FH is a function of position and is defined as the distance between the mean asperity surfaces of the slider and the disk, while the FH between an ideally flat slider and disk is just the distance between the slider and the disk. It is found that the difference predicted by these various adhesion models is very small for low values of the plasticity index, which characterizes the elastic-plastic deformation of asperities. Asperities are mostly elastically deformed in the contact interfaces with the smaller plasticity index. If we compare the adhesion stress obtained using the IDMT model with that obtained using the intermolecular force model, i.e. the results shown in Fig.2 with those in Fig.3, we find that the IDMT models give much smaller adhesion stress than the intermolecular force model.

4. Net adhesion stress

Asperity contacts occur when the distance between the slider and the disk is below the glide height. In the simulations we can take three times the standard deviation of the surface height as the glide height. The asperity contact pressure increases as the distance between the slider and disk surfaces decreases towards zero. Then the net adhesion stress on the slider is the asperity adhesion stress minus the asperity contact pressure.

To model the slider disk asperity contact we assume that all of the contacts are quasi-static. For the multi-asperity static contact between two parallel surfaces, the GW model [15], CEB model [16] and KE model [17] give different relationships between the contact pressure and the distance between two parallel surfaces. The GW model assumes that all of the contacting asperities are elastically deformed. The CEB model assumes that the contacting asperities are either elastically deformed when the interference is less than a critical value, or directly become fully plastically deformed when the interference is greater than the critical interference. In the KE model the elastic-plastic deformation of a single contacting asperity is analyzed using the finite element method. Although the results of these three models are different, the difference is negligible when the plasticity index of the contact interface is small and only a few of the contacting asperities are fully plastically deformed. Fig.4 shows the contact pressures versus flying height between the slider and the disk, using the surface parameters in Table I. The results of these three models are close to each other for these three contact interfaces, except that the CEB model gives slightly larger contact pressure than the others when the plasticity index is 0.836. The reason is that the total contact force of a fully plastically deformed asperity is much larger than for an elastically or elastic-plastically deformed asperity. So the assumption of the CEB model is expected to give a larger contact pressure.

Fig.5 shows the net adhesion stress for these three slider-disk interfaces for the three models versus the flying height. The net adhesion stress in Fig.5 is much smaller than the intermolecular adhesion stress shown in Fig.2. Also, for the rougher slider-disk interface the net adhesion stress can become negative at low flying height, which means a repulsion effect instead of adhesion effect on the slider.

5. Static simulation of an air bearing slider

Next the adhesion stress calculation needs to be implemented in the air bearing simulation for the flying slider in order to analyze the effect of the intermolecular adhesion. We can not make a simple assumption that the effect of adhesion is negligible when the FH is above 3nm simply because in Fig.2 or Fig.5 the adhesion stress is close to zero when the flying height is above 3nm. The reason is that the adhesion stress may still be comparable to the air bearing pressure although it looks very small in Fig.2 or Fig.3 for a FH greater than 3nm. In addition, different places on the slider have different flying heights, due to the pitch, roll and the air bearing surface (ABS) design features of the slider, and hence they have different adhesion pressures. The correct way to analyze the effect of adhesion stress is to consider the adhesion stress in slider flying simulations. As shown above, the choices among these asperity contact and adhesion models do not make much difference for the flying slider/disk interface. So we picked the KE-IDMT adhesion and KE contact models in the following slider static simulation.

The CML air bearing static simulation program is used to analyze the effect of intermolecular adhesion. In this program the generalized Reynolds equation is modified by the Fukui-Kaneko slip correction to account for the rarefaction of the air at the slider/disk spacing down to asperity contact. The modified Reynolds equation is then discretized using Patankar's control volume method, and the final discretization equations are solved using the alternating direction line sweep method combined with the full multi-grid algorithm. The ABS is discretized to small grids, which are approximately parallel to the disk surface with various flying heights. Then the intermolecular force model or asperity adhesion/contact models are applied to each grid. Air bearing shear stress on the ABS is also considered in the simulation program and its effects on the pitch

and roll of the slider have been analyzed previously [19]. The effect of the slider-disk asperity contact on the air bearing pressure is not considered due to the negligible real contact area as compared with the air bearing surface. In addition, the surface roughness effects are not included in the air bearing model. For a given ABS design the static simulation program uses the quasi-Newton method to calculate the slider's static flying altitude, i.e., the equilibrium state.

In the simulation we use a CML designed femto slider with the ABS shown in Fig.6 and two types of slider-disk surface roughness parameters, case 2 and case 3 in Table I, and also a flat slider/disk interface. The asperity adhesion/contact models are applied to the first two cases and the last one uses the intermolecular force model. Fig.7 shows the relationship between the disk RPM and the slider's minimum flying height for the various cases. As the disk RPM decreases, the slider's minimum flying height also decreases. Both the original and modified intermolecular force models show significant flying height decreases due to the intermolecular adhesion stress. At the same disk RPM the minimum flying height obtained with the modified intermolecular force model is higher than that obtained with the original intermolecular force model. This can be explained by the smaller adhesion stress that occurs with the consideration of the contact distance in the modified intermolecular force model. However, the rougher and smoother slider disk interfaces using the asperity adhesion/contact model show less effect of adhesion stress, and the minimum flying height is close to that obtained without considering the slider disk adhesion, when the minimum flying heights are above the glide height, i.e., 3 times the standard deviation of the surface height. When the minimum flying height is below the glide height, the rougher slider/disk interface, i.e. case 2 in Table I, has a higher minimum flying height than in the case without considering

slider/disk adhesion or contact, while the smoother slider/disk interface, i.e., case 3 in Table I, shows the opposite trend. This indicates that the net adhesion stress takes effect only when the minimum flying height is less than the glide height. For the rougher slider/disk interfaces, the net adhesion stress becomes negative at a flying height below the glide height. Hence the slider has a higher minimum flying height. On the other hand, for the smoother slider/disk interface the net adhesion stress is positive, and it increases as the flying height deceases, so the slider has a lower flying height.

In Fig.7 we also see that the modified intermolecular force model produces two minimum flying heights for one low value of disk RPM as does the original intermolecular force model. The smaller of the two flying heights corresponds to an unstable equilibrium [18]. However, this unstable equilibrium has not been found in experiments. The asperity contact/adhesion models do not produce such an unstable flying height, and therefore they agree better with experimental results, which is understandable, since practical slider and disk surfaces always have certain roughnesses.

6. Conclusion

This paper investigates the intermolecular force model and asperity adhesion/contact models for ultra-low flying height sliders. A contact distance is introduced and included in the original intermolecular force model, after which it is found that no infinite repulsive force occurs as the flying height approaches zero. The IDMT model and GW models are recommended for multi-asperity adhesion and contact simulations, respectively. Other improved models have negligible difference for the slider/disk interface, which has a low plasticity index and high hardness and Young's modulus. Asperity adhesion/contact models are implemented in the CML static air bearing simulation program and the following conclusions may be drawn from the simulations,

1. The intermolecular force model overestimates the slider disk adhesion due to the neglect of the roughness of the slider and disk surfaces.

2. For practical slider and disk surfaces with certain roughnesses, the effect of asperity adhesion/contact is negligible when the minimal flying height is above the glide height.

3. The modified intermolecular force model that incorporates the contact distance predicts a smaller reduction in FH than the original intermolecular force model. The effect is further reduced when surface roughness is included.

4. When the slider/disk roughness is considered, the slider static simulation does not obtain an unstable equilibrium at low disk RPM.

5. When the slider's minimum flying height is less than the glide height, the minimum flying height is higher on rougher slider/disk interfaces since the net adhesion stress is smaller and may even become negative for rougher interfaces.

Acknowledgement

This research was supported by the Information Storage Industry Consortium (INSIC), the Computer Mechanics Laboratory (CML) at the University of California at Berkeley, and the National Science Foundation under Grant CMS-0408484.

References

[1] Wu, L. and Bogy, D. B., 2002, "Effect of the Intermolecular Forces on the Flying Attitude of Sub-5 NM Flying Height Air Bearing Sliders in Hard Disk Drives ," ASME Jour. of Trib., 124:562-7.

[2] Chang, W. R., Etsion, I and Bogy, D. B., 1988, "Adhesion model for Metallic Rough Surface," ASME Jour. of Trib., 110:50-6.

[3] Kogut, L. and Etsion, I, 2003, "Adhesion in elastic–plastic spherical microcontact," J. Colloid and Interface Sci., 261:372-8.

[4] Muller, V. M., Derjaguin, B. V., and Toporov, V. P., 1983, "On Two Methods of Calculation of the Force of Sticking of an Elastic Sphere to a Rigid Plane," Colloid and Surfaces, 7:251-259.

[5] Derjaguin, B. V., Muller, V. M. and Toporov, Y. P., 1975, "Effect of Contact Deformations on the Adhesion of Particles," J. of Colloid and Interface Sci., 53:314-26.

[6] Yu, N. and Polycarpou, A. A., 2004, "Adhesive contact based on the Lennard-Jones potential: a correction to the value of the equilibrium distance as used in the potential", J. Colloid and Interface Sci., 278:428-35.

[7] Israelachvili, J. N., Intermolecular and Surface Forces, second edition, Academic Press, San Diego, 1992.

[8] Ostrovskaya, L. Y., 2003, "Studies of diamond and diamond-like film surfaces using XAES, AFM and wetting," Vacuum, 68:219-38.

[9] Zhang, B., and Nakajima, A., 2003, "Possibility of surface force effect in slider air bearings of 100 Gbit/in2 hard disks," Tribol. Int., 36:291-296.

[10] Johnson, K. L., Kendall, K. and Roberts, A.D., 1971, "Surface Energy and the

Contact of Elastic Solids," Proc. R. Soc. London, A324:301-13.

[11] Tabor, D., 1977, "Surface Forces and Surface Interactions," J. Colloid and Interface Sci., 58:1-13.

[12] Maugis, D., 1992, "The JKR-DMT Transition Using a Dugdale Model," J. Colloid Interface Sci., 150:243-69.

[13] Dugdale, D. S., 1960, "Yielding in Steel Sheets Containing Slits," J. Mech. Phys. Solids, 8:100–104.

[14] Suh, A. Y. and Polycarpou, A. A, 2005, "Adhesive contact modeling for sub-5-nm ultralow flying magnetic storage head-disk interfaces including roughness effects," J. Applied Physics, 97:104328-38.

[15] Greenwood, J.A., and Williamson, J.B.P., 1966, "Contact of Nominally Flat Surfaces," Proc. Roy. Soc. (London), A295:300-319.

[16] Chang, W.R., Etsion, I. and Bogy, D.B., 1987, "An Elastic-plastic Model for the Contact of Rough Surfaces," ASME Jour. of Trib., 109:257-263.

[17] Kogut, L. and Etsion, I., 2003, "A Finite Element Based Elastic-Plastic Model for the Contact of Rough Surfaces," Trib. Trans., 46:383-390.

[18] Gupta, V. and Bogy, D. B., 2006, "Effect of Intermolecular Forces on the Static and Dynamic Performance of Air Bearing Sliders: Part I—Effect of Initial Excitations and Slider Form Factor on the Stability", ASME Jour. of Trib., 128: 197-202.

[19] Chen, D and Bogy, D. B., 2005, "A Comparison of Two Rarefaction Models in the Compressible Reynolds Equation used in air bearing design for hard disk drives", Technical Report No. 2005-010, Computer Mechanics Lab, Department of Mechanical Engineering, University of California, Berkeley.

Table I Slider/disk equivalent roughness parameters

Equivalent roughness parameter	**Case 1 (slider/disk 1)**	**Case 2 (slider/disk 2)**	**Case 3 (slider/disk 3)**
Standard deviation of surface height (nm)	1.619	1.245	0.654
Asperity radius (μm)	3.331	5.452	6.384
Asperity density (μm-2)	7.393	7.177	9.871
Standard deviation of asperity height (nm)	1.417	1.143	0.578
Plasticity index Ψ	0.836	0.587	0.386
Glide height (nm)	4.857	3.735	1.962

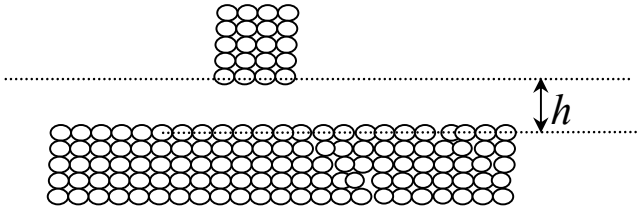

Fig. 1. An infinite half space and a unit surface area of a parallel infinite half space.

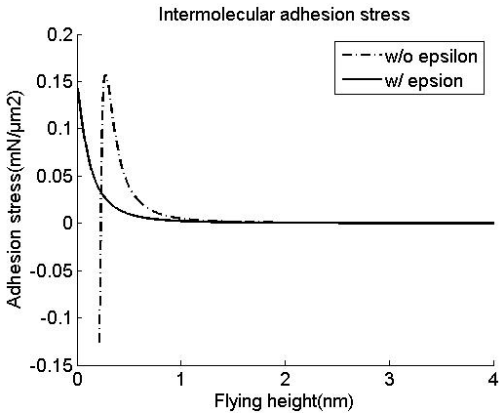

Fig. 2. Adhesion stress obtained through intermolecular force model with and without considering the contact distance ε.

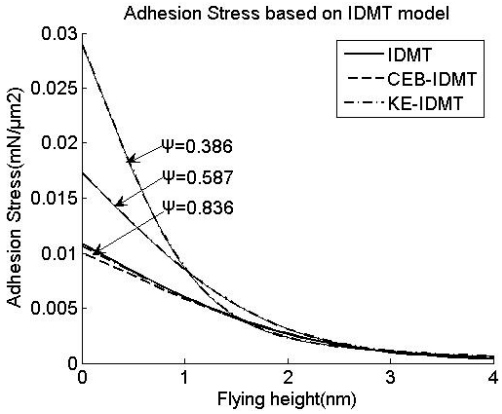

Fig. 3. Adhesion stresses obtained thorough the IDMT, CEB-IDMT and KE-IDMT model.

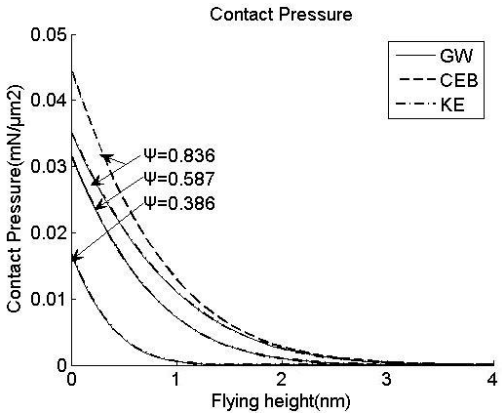

Fig. 4. Contact pressure obtained thorough the GW, CEB and KE model.

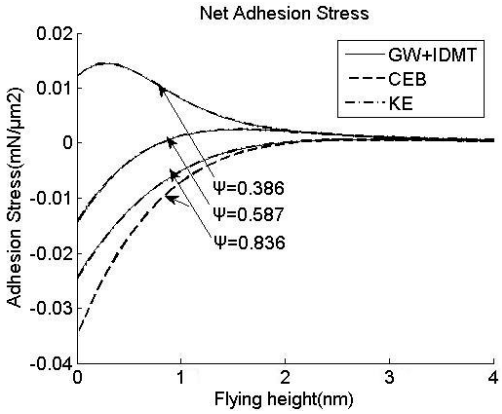

Fig. 5. Net adhesion pressure obtained thorough the GW, CEB and KE contact and adhesion models.

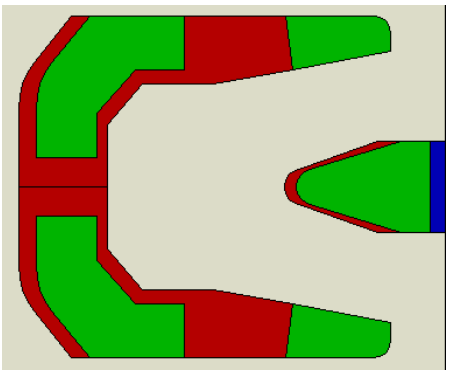

Fig. 6. Air bearing surface of CML femto slider.

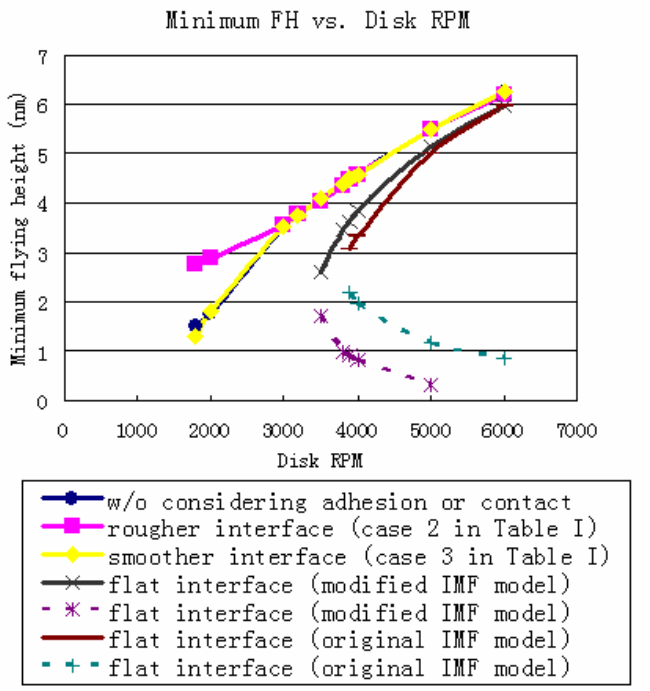

Fig. 7. Minimum flying height versus disk RPM for the rougher slider/disk surfaces (case 2 in Table 1), smoother slider/disk surfaces (case 3 in Table 2), flat slider/disk interfaces and the case without considering the slider/disk adhesion or contact (the solid lines represent stable equilibria and the dotted lines represent unstable equilibria).