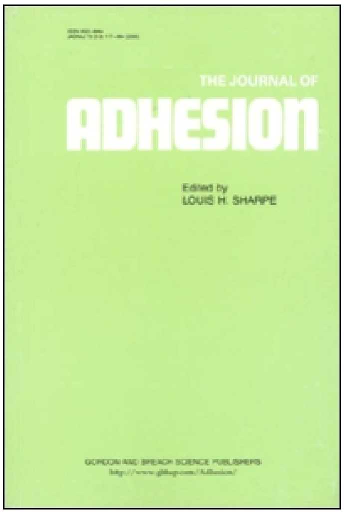

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Particle Removal Mechanisms Under Substrate Acceleration

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Particle detachment due to substrate acceleration is studied. The magnitude of the critical acceleration required to remove a particle from a surface based on the theory of critical moment and sliding detachment is determined. The special cases of spherical and cylindrical particles are examined, and the role of particle geometry on adhesion and detachment is studied. For different adhesion models, the critical substrate acceleration for particle removal is evaluated. The theoretical predictions are compared with the available experimental data and discussed.

KEY WORDS adhesion; particle removal; substrate acceleration; particle detachment; critical moment; sliding detachment.

INTRODUCTION

Developing models capable of describing the mobility of particles on a surface subjected to external forces have attracted considerable attention due to their applications in the semiconductor industry. Numerous studies concerning the particle detachment mechanism from the surface were reported in the literature. Extensive reviews of particle adhesion mechanisms were provided by Corn,[1] Krupp,[2] Visser,[3] Tabor,[4] Bowling,[5] and Ranade.[6] Accordingly, the van der Waals force makes the major contribution to the particle adhesion force on a surface under dry conditions.

Derjaguin[7] studied the effect of contact deformation on the adhesion force. Johnson *et al.*[8] used the surface energy and surface deformation effects to develop an improved contact model which is referred to as the JKR model. Derjaguin *et al.*[9] developed a new theory based on the Hertzian profile assumption. In this model (the so-called DMT theory) the force required to detach the particle from the surface is 4/3 as large as the JKR theory. Further progress was reported by Muller *et al.*[10,11]

Recently, Tsai *et al.*[12] proposed a new model (here it will be referred to as the TPL model) which considered the effect of material properties in the deformation and

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adhesion force of particle-surface systems. Rimai *et al.*[13] reported the significant effects of Young's modulus and material properties on the surface-force-induced contact radius of spherical particles.

To measure particle adhesion force, several techniques have been developed. Extensive reviews of the experimental methods were provided by Corn[1] and Zimon.[14] Ranade[6] noted that vibration, centrifuge, and hydrodynamic or aerodynamic methods are the most efficient techniques for removing submicron particles from surfaces.

Derjaguin and Zimon[15] used an ultrasonic vibrational method to generate acceleration of the order of 10^4 g. Recently, Mullins and Ranade[16] used an ultrasonic horn to study adhesion of micrometer-size metal flakes. The shortcoming of this method is that it can not be applied to fragile substrates, and at high frequencies, violent cavitation in liquid media may cause problems due to material erosion. Brodov *et al.*,[17] Agabalyants *et al.*,[18] and Lowe and Parasher[19] suggested that the action of collapsing cavitation bubbles at a surface contributes significantly to particle detachment. Shwartzman *et al.*[20] noted the formation of the pressure waves due to collapsing bubbles as the mechanism for particle removal. They proposed a megasonic cleaning system operating at frequencies from 850 to 900 kHz.

Kordeki and Orr[21] studied the centrifuge method to measure the adhesion force. They used a maximum acceleration of about 2000 g in their experiment, and observed that a significant fraction of small particles can be removed. Bohme *et al.*[22,23,24] used an ultracentrifuge to generate an acceleration of more than 10^6 g.

The hydrodynamic methods for measuring the adhesion force have advanced significantly in the last two decades. Visser[25] used a hydrodynamic method to measure the force of adhesion between submicrometer carbon black (0.2 μm diameter) and cellophane substrates in a rotating concentric cylinder. Zimon[26] studied the role of a drag force on particle removal by air as well as by water flow.

Much work has been reported in the literature concerning particle detachment mechanisms. Wang[27] studied the effect of inceptive motion on particle detachment from surfaces and concluded that the removal of spherical particles is more easily achieved by the rolling motion, rather than sliding or lifting. This result is consistent with the experimental observation of Masironi and Fish.[28]

Cleaver and Yates[29] developed a particle resuspension model based on the lift force arising from turbulent bursts. A dynamical model for the long term resuspension of small particles from smooth and rough surfaces in turbulent flow was developed by Reeks *et al.*[30] and Reeks and Hall.[31] Recently, Tsai *et al.*[32] proposed the critical moment model for particle detachment. Soltani and Ahmadi[33] studied turbulent resuspension models based on sublayer and turbulent burst/inrush flows using the theory of rolling detachment and sliding removal.

In this work, particle removal due to substrate acceleration is studied. The theory of rolling and sliding detachment are used and the critical acceleration needed for removing particles from a surface under different conditions are evaluated. Different adhesion models and various detachment mechanisms are used in this study. Effects of shape (spherical or cylindrical) on particle removal are studied and discussed. A comparison of model predictions with the available experimental data is also presented.

ADHESION MODELS

In this section, the adhesion models for spherical and cylindrical particles used in this study are described.

Spherical Particles

According to the JKR model (Johnson *et al.*[8]), the pull-off force, F_{po}, and the contact radius, a, of a spherical particle at the onset of detachment are given by

$$F_{po}^{JKR} = \tfrac{3}{4}\pi W_A d, \tag{1}$$

$$a = \left(\frac{3\pi W_A d^2}{8K}\right)^{1/3}, \tag{2}$$

where K is the composite Young's modulus given as

$$K = \frac{4}{3}\left[\frac{(1-\nu_1^2)}{E_1} + \frac{(1-\nu_2^2)}{E_2}\right]^{-1}. \tag{3}$$

Here, d is the diameter of the spherical particle, W_A is the thermodynamic work of adhesion, and ν_i and E_i are, respectively, the Poisson's ratio, and the Young's modulus of material $i(i = 1$ or $2)$.

For the DMT adhesion model which was described by Derjaguin *et al.*,[7] the detachment force is given by

$$F_{po}^{DMT} = \pi W_A d, \tag{4}$$

which is 4/3 times the JKR force given by equation (1). The contact radius in the absence of external force is, $a_o = (\pi W_A d^2/2K)^{1/3}$, which is identical to that of a Hertzian contact. The DMT theory predicts that, at the moment of separation, the contact area is reduced to zero.

For the TPL adhesion model as developed by Tsai *et al.*,[32] the corresponding force and contact radius are given by

$$F_{po}^{TPL} = F_o\{0.5\exp[0.124(\text{Ц} - 0.01)^{0.439}] + 0.2\text{Ц}\}, \tag{5}$$

where the adhesion parameter, Ц , is defined as

$$\text{Ц} = \left[\frac{25A^2 d}{288 z_o^7 K^2}\right]^{1/3}, \tag{6}$$

and

$$F_0 = \pi W_A d. \tag{7}$$

Here z_o is the minimum separation distance and A is the Hamaker constant. The corresponding contact radius is given as

$$\frac{a}{d} = \sqrt{\frac{K_{20} z_o}{2d}}, \tag{8}$$

with

$$K_{20} = 0.885[\exp(0.8\text{П}^{0.5}) - 1.0] \quad \text{П} \leq 1.6, \tag{9}$$

$$K_{20} = 0.735\text{П}^{0.178} + 0.52\text{П} \qquad \text{П} > 1.6. \tag{10}$$

The adhesion parameter, II, for particle diameter between 0.01 to 100 μm varies from 0.01 to 5 for metals and oxides, and from 5 to 200 for polymers.

Cylindrical Particles

Mullins *et al.*[34] applied the classical Hamaker approach to evaluate the adhesion force for a cylinder oriented parallel to an infinite planar body. Accordingly, the adhesion force is given as

$$F_{po}^{M} = \frac{LA\sqrt{d}}{24\sqrt{z_0^5}}, \tag{11}$$

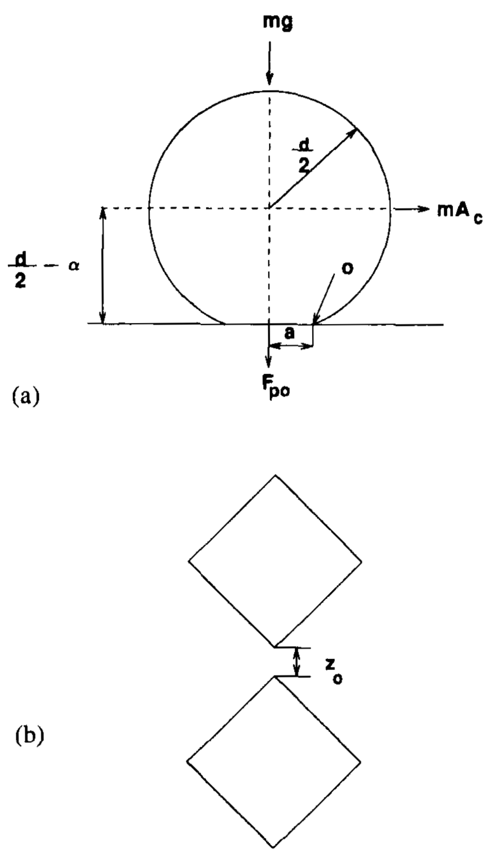

FIGURE 1 (a) Geometric features of a spherical or a cylindrical particle attached to a smooth surface. (b) Geometric features of two rectangular particles.

where A is the Hamaker constant, z_0 is the minimum separation distance, and d and L are, respectively, the diameter and length of the cylinder.

Vold[35] studied the adhesion force between two rectangular rods such that the edges are parallel. Figure 1b shows the geometric features of such rectangular particles. Accordingly, the adhesion force is given as

$$F^V_{po} = \frac{AL}{6\pi z_0^2}, \tag{12}$$

where L is the length of the prism. In the limit, for small particles, the prisms may be considered as cylinders. According to Mullins *et al.*,[34] the experimental results for cylindrical particles fit the prediction of Vold's model closely. It is observed that the adhesion force based on the Vold model is independent of the width of the prism (or diameter of the cylinder).

Note there is no exact expression for the contact radius between the cylindrical particle and a plane surface. Therefore, as a first approximation the contact radius from the JKR adhesion model for spherical particles is used in this study.

PARTICLE DETACHMENT

Figure 1a shows the geometric features of a spherical or a cylindrical particle (cross sectional) which is attached to an accelerating plane surface. The substrate acceleration causes an effective inertial force to act on the particle parallel to the surface. Particles are removed when this force overcomes the adhesion force and the weight of the particle. The acceleration of the substrate may be generated by vibration (ultrasonic and megasonic), centrifuge or impact.

Spherical—Rolling

Consider a particle which is attached to a accelerating surface as shown in Figure 1a. Applying the angular momentum balance about point "O", the critical acceleration, A_c, for particle removal becomes

$$A_c = \frac{(\frac{F_{po}}{m} + g)a}{\frac{d}{2} - \alpha}, \tag{13}$$

where m is the mass of the particle, g is the acceleration of gravity, a is the contact radius, d is the particle diameter, α is the relative approach between the particle and surface (at the equilibrium condition). In most practical cases, α in comparison with $d/2$ is very small, and it is neglected.

Using the JKR adhesion theory (equations (1) and (2)) in equation (13), the acceleration needed for removing the particle from the surface is given as

$$A_c^{JKR} = (4.5W_A + \rho_p d^2 g)\left(\frac{3\pi W_A}{\rho_p^3 K d^7}\right)^{1/3}. \tag{14}$$

Since the contact radius at the moment of separation is zero in the DMT model, it follows that there is no adhesion resistance to rolling motion. That is, the particles will roll on the surface under any slight force, which is unrealistic. Lack of static equilibrium for the DMT model was also noted by Tsai *et al.*[12] To improve this rolling detachment model, the DMT theory (and Hertzian contact) must be re-evaluated for particles under combined normal and tangential forces on frictional surfaces. However, this matter is not pursued in this study.

Similarly, using the TPL adhesion model, (*i.e.*, equation (5)), the acceleration required to detach the particle from the surface becomes

$$A_c^{TPL} = \left[W_A\{0.5\exp[0.124(\text{Л} - 0.01)^{0.439}] + 0.2\text{Л}\} + \frac{1}{6}\rho_p d^2 g \right] \frac{8.48\sqrt{\frac{K_{20}z_o}{d^5}}}{\rho_p}. \tag{15}$$

Here ρ_p is the density of the particle and g is the acceleration of gravity. It should be noted that the equation (15) is valid for $\text{Л} > 0.01$.

Spherical—Sliding

According to the sliding detachment model the particle starts to slide when the external force equates the friction force, *i.e.*,

$$A_c = k\left(g + \frac{F_{po}}{m}\right), \tag{16}$$

where A_c is the critical surface acceleration along the interface, and k is the static friction coefficient. Using the JKR adhesion model, the critical acceleration required for sliding detachment becomes

$$A_c^{JKR} = (4.5W_A + \rho_p d^2 g)\frac{k}{\rho_p d^2}. \tag{17}$$

Similarly, using the TPL adhesion theory, it follows that

$$A_c^{TPL} = \left[W_A\{0.5\exp[0.124(\text{Л} - 0.01)^{0.439}] + 0.2\text{Л}\} + \frac{1}{6}\rho_p d^2 g \right] \frac{6k}{\rho_p d^2}. \tag{18}$$

Figures 2 and 3, respectively, compare the acceleration required to remove the particle from the surface for graphite and copper according to rolling and sliding detachment mechanisms. The coefficient of friction for graphite-graphite and copper-copper interfaces are 0.1 and 1.6, respectively. The corresponding material properties are listed in Table I. A value of 4×10^{-10} m is used for z_0. It is observed that the particle rolling detachment is much easier than particle sliding detachment. For example, an acceleration of about 5000 g is needed to detach a 10 μm graphite particle by the rolling mode. However, an acceleration of about 10000 g is required to detach the same particle by sliding motion. The exception is for small particles, where the rolling mode leads to a slightly higher value of critical acceleration for the graphite-graphite case.

Figures 2 and 3 also show that the model predictions for the JKR and TPL adhesion theories are in close agreement. When the contribution of gravity is neglected or its

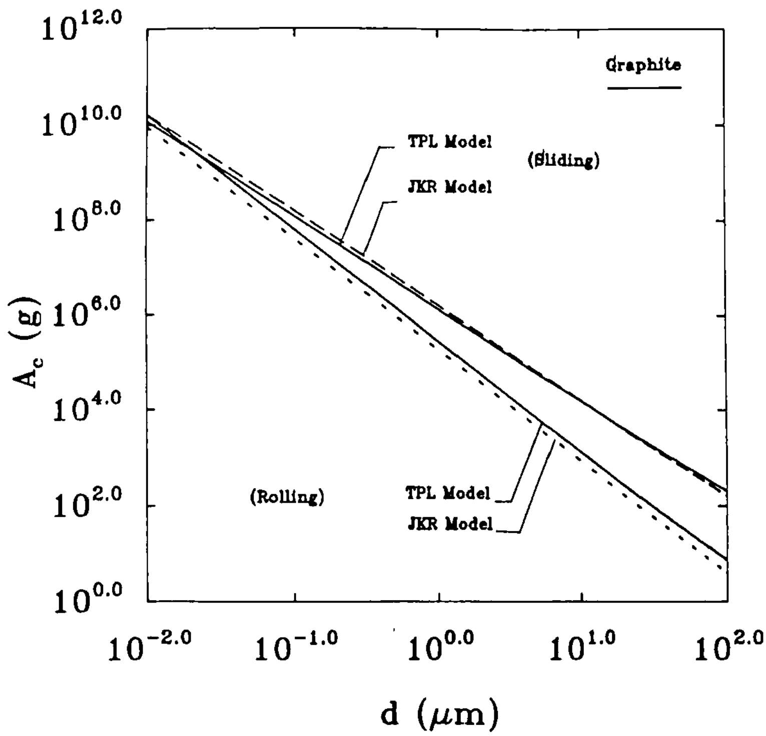

FIGURE 2 Comparison of the acceleration needed to detach spherical graphite particles from a graphite substrate according to various detachment mechanisms and different adhesion models.

direction is varied, there is no noticeable difference in the results. Therefore, the effect of acceleration of gravity is essentially negligible.

Spherical—Lifting

According to this model the particle will be removed when the external lifting forces overcome the adhesion force and the particle weight, *i.e.*,

$$A_c = g + \frac{F_{po}}{m}. \tag{19}$$

TABLE I
Material Properties

Material	E (10^{10} N/m^2)	A (10^{-20} J)	W_A 10^{-3} J/m^2)	ν_i	ρ (10^3 Kg/m^3)	k	*Ref.*
Graphite	67.50	46.90	77.75	0.16	2.2	0.1	38
Copper	13.00	28.30	46.91	0.34	8.89	1.6	39
Aluminum	6.9	33	54	0.33	2.7	1.9	39
Glass (Dry air)	6.9	8.5	14	0.2	2.18	0.9	40
Glass (moist air)	6.9	320	530	0.2	2.18	0.9	36

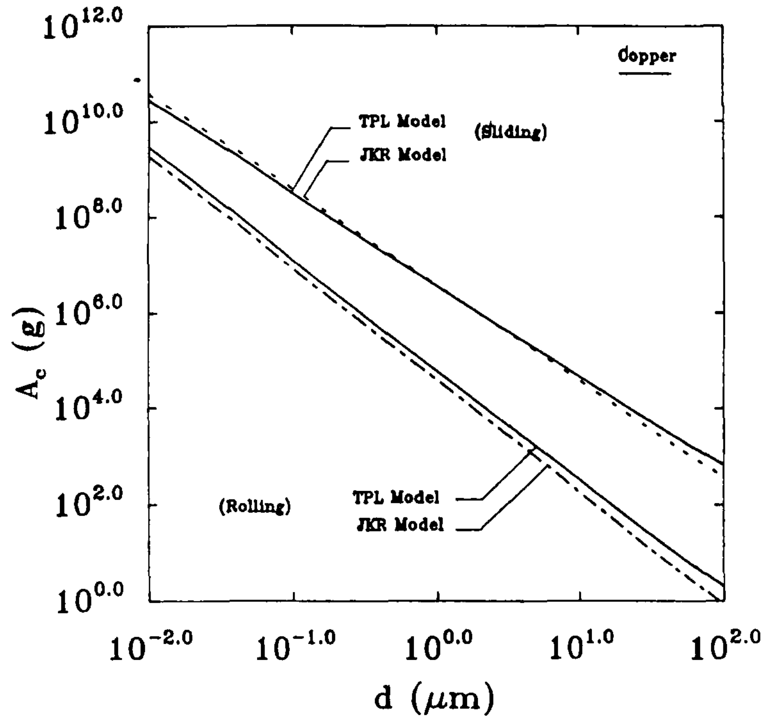

FIGURE 3 Comparison of the acceleration needed to detach spherical copper particles from a copper substrate according to various detachment mechanisms and different adhesion models.

For $k = 1$, equation (16) shows that the critical accelerations for sliding detachment and lifting removal are equal. Similarly, for the TPL and JKR adhesion models, the corresponding critical accelerations, respectively, become

$$A_c^{TPL} = \left[W_A\{0.5\exp[0.124(\Pi - 0.01)^{0.439}] + 0.2\Pi\} + \frac{1}{6}\rho_p d^2 g \right] \frac{6}{\rho_p d^2}, \tag{20}$$

$$A_c^{JKR} = (4.5W_A + \rho_p d^2 g)\frac{1}{\rho_p d^2}. \tag{21}$$

Cylindrical—Rolling

The critical accelerations for radial rolling detachment of cylindrical particles are studied in this section. Using the adhesion force of Mullins *et al.*,[34] as given by equation (11) and the JKR estimate for the contact radius, the acceleration needed to detach the particle becomes

$$A_c^M = \left[\frac{A\sqrt{d}}{3\sqrt{z_0^5}} + 2\pi\rho_p d^2 g \right] \left(\frac{3W_A}{8\rho_p^3 \pi^2 K d^7} \right)^{1/3}. \tag{22}$$

For the adhesion force of Vold,[35] using equation (11), the corresponding critical acceleration becomes

$$A_c^V=\left[\frac{4A}{3\pi z_0^2}+2\pi\rho_p d^2 g\right]\left(\frac{3W_A}{8\rho_p^3\pi^2 K d^7}\right)^{1/3}. \tag{23}$$

It should be emphasized that equations (22) and (23) are rough approximations, since the contact areas for the Mullins *et al.* and the Vold models are not known. Here the JKR estimate for the contact radius was used as a crude approximation. Note also that the critical acceleration as given by equations (22) and (23) are independent of the length of the cylindrical particle.

The possibility of axial rolling detachment (by rotation about the end of a cylindrical particle) is also considered. Figure 4 shows a sketch of the geometric features of a cylindrical particle on a surface. Applying the angular momentum balance with respect to point C, the critical acceleration for (axial) rolling becomes

$$A_c=\frac{F_{po}L}{md}+\frac{gL}{d}. \tag{24}$$

Using the Mullins *et al.*, and the Vold adhesion models the corresponding critical accelerations, respectively, become

$$A_c^M=\frac{LA}{6\rho_p\pi\sqrt{(z_0 d)^5}}+\frac{gL}{d}, \tag{25}$$

and

$$A_c^V=\frac{2LA}{3\rho_p\pi^2 z_0^2 d^3}+\frac{gL}{d}. \tag{26}$$

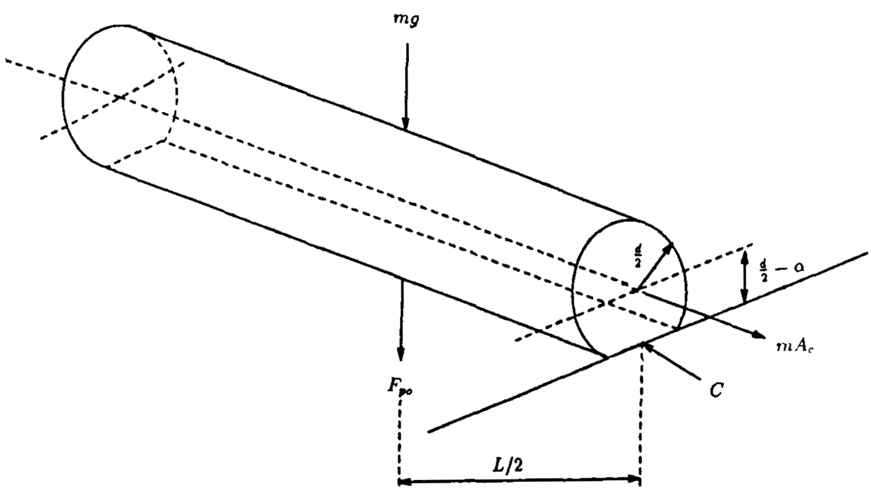

FIGURE 4 Geometric features of a cylindrical particle attached to a smooth surface.

Cylindrical—Sliding

The sliding motion of cylindrical particles is examined in this section. Using the balance of forces acting on the particle, and the Mullins *et al.* adhesion model, the critical acceleration for sliding detachment becomes

$$A_c^M = \frac{Ak}{6\rho_p \pi \sqrt{z_0^5 d^3}} + gk. \tag{27}$$

Using the Vold adhesion model, it follows that

$$A_c^V = \frac{2Ak}{3\rho_p \pi^2 z_0^2 d^2} + gk. \tag{28}$$

Figure 5 provides a comparison of the critical accelerations needed to detach the cylindrical graphite particles according to various detachment mechanisms as predicted by Mullins *et al.*,[34] and Vold[35] adhesion models. The corresponding critical acceleration for rolling detachment of spherical particles as predicted by the JKR adhesion model is shown in this figure for comparison. It is observed that the (radial) rolling detachment of cylindrical particles is more easily achieved when compared with the sliding removal mode.

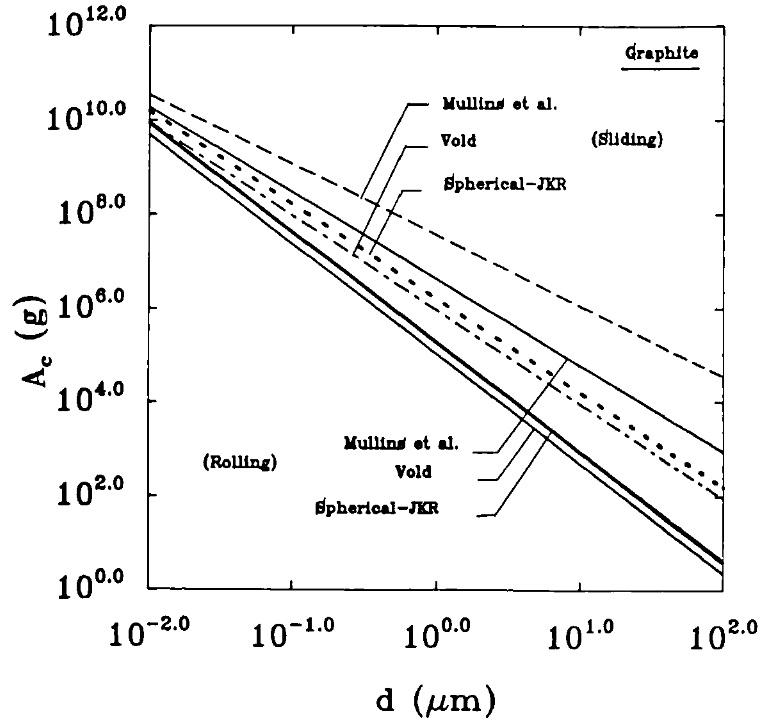

FIGURE 5 The acceleration needed to detach cylindrical graphite particles according to various detachment mechanisms and different adhesion models.

For sliding and (radial direction) rolling detachments, the critical accelerations predicted by the Vold model are lower than those of the Mullins *et al.* model and the JKR prediction for a spherical particle of the same diameter.

Figure 6 compares the critical substrate accelerations for cylindrical and spherical graphite particles according to various detachment mechanisms. The Mullins *et al.*, and the JKR adhesion models, respectively, for cylindrical and spherical particles are used. It is observed that the spherical particles will be removed at lower acceleration in comparison with the cylindrical particles. In this figure, the bold solid line corresponds to the axial rolling motion of the cylindrical particle as predicted by the Mullins *et al.* model (eq. (21)). Here, it is assumed that the length of the cylindrical particle is equal to its diameter (*i.e.*, $L = d$). As expected, the corresponding critical accelerations for rolling in the axial direction are much higher than those for the radial direction. Figure 6 also shows that the (radial) rolling detachment for both geometries is easier than the sliding detachment.

COMPARISON WITH EXPERIMENTAL DATA

A comparison of the theoretical model prediction and the experimental data of Mullins *et al.*,[34] is presented in this section. Mullins *et al.*, used an ultrasonic horn for measuring

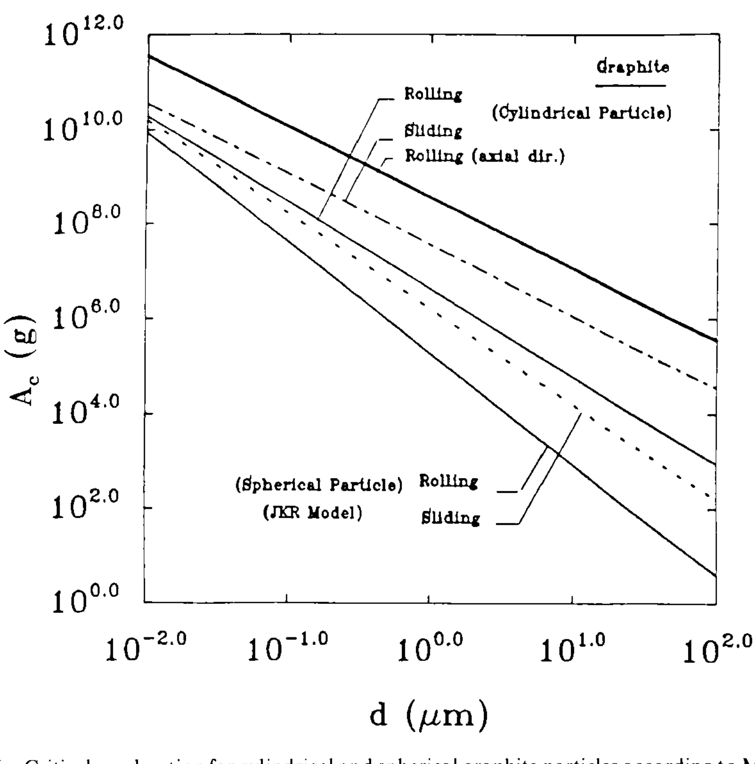

FIGURE 6 Critical acceleration for cylindrical and spherical graphite particles according to Mullins *et al.* adhesion model and various detachment mechanisms.

particle adhesion in their experiment. The particles were deposited on a horizontal flat surface which was vibrating at a frequency of about 20,000 Hz in a direction perpendicular to the surface. Therefore, the particles were detached mainly by the lifting mechanism.

Variations of critical accelerations with diameter for spherical aluminium particles as predicted by the JKR adhesion model according to lifting detachment mechanism are shown in Figure 7. Material properties for aluminum are listed in Table I. Experimental data of Mullins *et al.*,[34] for removal of 5 μm aluminum particles are reproduced in this figure for comparison. Figure 7 shows that the experimental data for 96% removal are in good agreement with the model predictions. The experimental results also indicate that a certain percentage of particle removal could be achieved at lower substrate accelerations. It is conjectured that the particle detachments at lower A_c are due to the presence of small surface roughnesses.

Critical accelerations as predicted by the JKR adhesion model for lifting detachment are compared with the experimental data of Mullins *et al.*,[35] for spherical glass particles in Figure 8. The corresponding material properties used for glass are listed in Table I. Note that the value of the Hamaker constant for glass in moist atmosphere is different from that in dry air (or vacuum). Tomlinson[36] reported a value of about 320×10^{-20} J for moist air, whereas Visser[37] found a value of 8.5×10^{-20} J for the dry air condition. The results for both dry and moist air conditions are presented in Figure 8. This figure

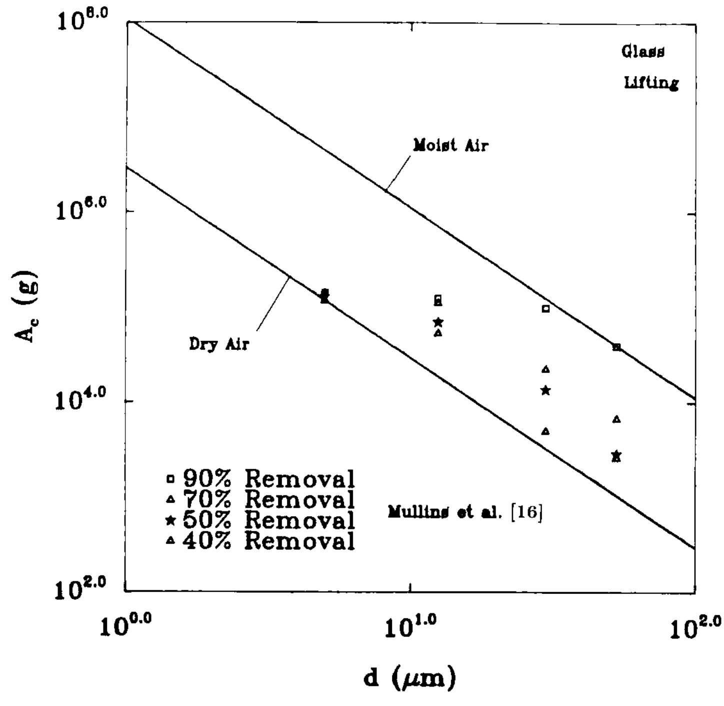

FIGURE 7 Comparison of the predicted critical accelerations with the experimental data of Mullins *et al.* [16] for aluminum particles.

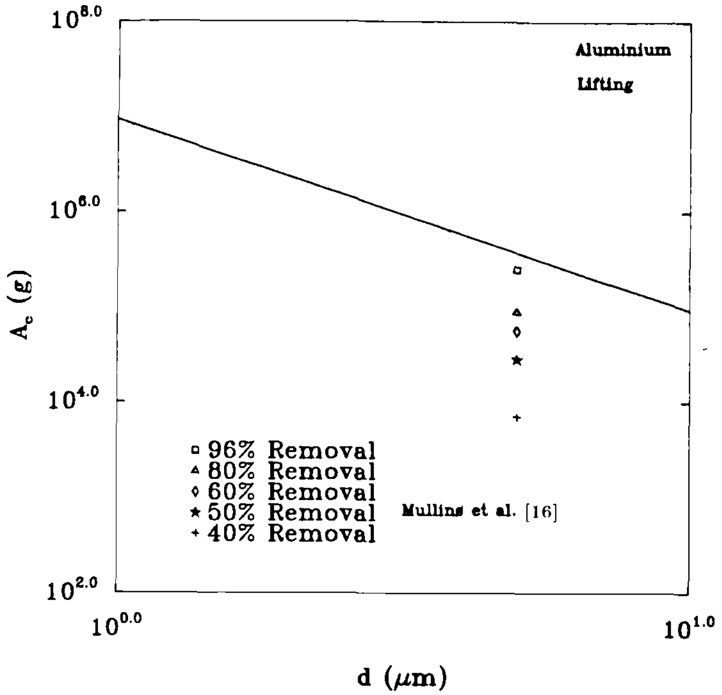

FIGURE 8 Comparison of the predicted critical accelerations with the experimental data of Mullins *et al.* [16] for glass particles.

shows that the experimental data points are between the critical accelerations predicted for the moist and dry air conditions. This implies that the dry air assumption is inconsistent with the experimental results. The particle removal at accelerations lower than those predicted by the moist air and smooth surface conditions could be due to variations in the surface roughness and/or particle size distribution. It should be noted here that the presented comparisons with experimental data were only for the lifting removal condition. Unfortunately, no explicit data for the substrate critical accelerations for rolling or sliding detachments were found for further comparsion.

CONCLUSIONS

Particle removal mechanisms based on the theory of rolling and sliding detachments for the case of an accelerating substrate have been studied. The general expressions for the critical acceleration required to detach a particle from a surface according to various adhesion models have been evaluated. The effect of particle geometry on particle removal has been studied. Based on the presented results, the following conclusion may be drawn:

1. Rolling detachment is the dominant detachment mechanism for spherical and cylindrical particles.

2. The critical acceleration for radial rolling detachment of a cylindrical particle is independent of its length.
3. The critical accelerations for axial rolling of cylinders are much higher when compared with those for their radial rolling or sliding.
4. The effect of the gravity on particle detachment is essentially negligible.
5. The model predictions are in reasonable agreement with the experimental data.
6. Particle removal at accelerations lower than those predicted by the model could be due to the presence of small surface roughnesses.

The presented results are for smooth surfaces. The effect of surface roughness is not included in this study. However, this important issue is left for future study.

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