MICROMECHANICS OF ULTRAFINE PARTICLE ADHESION – ENERGY ABSORPTION AT CONTACT

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Abstract - The mechanical product behaviour of dry, ultrafine cohesive powders (d < 10 µm) is characterized by insufficient flowability and large compressibility. Consequently, a comparatively large energy input is necessary to promote the non-rapid frictional shear flow in powder handling practice. When two adhesive particles are coming in contact, the constitutive models of four stressing modes, namely by compression and detachment (tension), sliding, rolling and spinning (torsion) have to be modelled, see the previous papers of Tomas [1, 2]. Next, the consequences of elastic-dissipative, elastic-plastic, frictional unloading and reloading paths of normal and tangential forces, rolling and torsional moments are discussed with respect to energy absorption. The total energy absorption comprises contributions by elastic-dissipative hysteresis due to microslip within the contact plane and by fully developed friction work when the friction limits of displacements are exceeded during contact sliding, particle rolling or rotation. With increasing contact flattening by normal load, these friction limits, hysteresis and friction work increase. Thus, the understanding of the micromechanics of particle adhesion is essential to assess the powder product quality and to improve the process performance in particle technology.

1. INTRODUCTION

The consolidation and non-rapid shear flow of dry, ultrafine, cohesive and compressible powders were referred to the dominant microscopic effect of variable adhesion forces at particle contacts. That was the physical basis of universal models for particle adhesion that includes the elastic-plastic and viscoplastic particle contact behaviour with hysteresis and consequently, energy dissipation. Various contact elastic-plastic deformation paths for non-rapid (quasi-static) loading, unloading and contact detachment were discussed. As a result, the varying adhesion forces between particles directly depend on this frozen irreversible deformation. Thus, the adhesion force was found to be load dependent [3-5].

Considering these load dependent van der Waals adhesion forces, the four stressing modes by compression and detachment, sliding, rolling and torsion were modelled when two adhesive particles are in contact [1, 2]. To continue these new constitutive models, the consequences of elastic-dissipative as well as elastic-plastic, frictional unloading and reloading paths of normal and tangential forces, rolling and torsional moments are discussed with respect to the energy absorption. This energy absorption comprises contributions by elastic-dissipative hysteresis due to microslip within the contact plane and by fully developed friction work when the friction limits of displacements are exceeded during contact sliding, particle rolling or rotation. Therefore one may expect that with increasing contact flattening by normal load the friction limits, hysteresis and friction work increase.
2. CONTACT MODELS OF ELASTIC-PLASTIC AND FRICTIONAL BEHAVIOUR

A comprehensive literature review may be read in previous papers [2, 4, 5]. The essential force-displacement and moment-angle models for the adhesive contact of smooth ultrafine spheres from the last papers [1, 2] are briefly demonstrated in Fig. 1. During sole normal loading, the spheres approach, form an elastic contact, start with yielding, form an elastic-plastic contact, can be unloaded at point U, achieve the adhesion limit at point A, and finally, detach with increasing separation, Fig. 1a). Within the contact plane both particles can be sheared. But the elastic range is very small and limited by the tangential displacement $\delta_{C,H}$, Fig. 1b). At this Coulomb friction limit (black point, index C) the elastic behaviour is transmitted into the frictional behaviour of contact sliding shown by a constant tangential force. In terms of particle rolling, the elastic range is restricted by the limit of rolling angle $\gamma_{C,H}$, Fig. 1c). At this limit the elastic behaviour is transmitted into the contact rolling shown by constant rolling moment. Additionally, when both particles rotate (twist or spin) around their principal axis (normal of the contact area), the elastic range is restricted by a constant friction limit of rotation angle $\phi_{C,H}$, Fig. 1d). At this Coulomb friction limit the elastic behaviour is transmitted into the contact sliding shown by constant torque.

All necessary force-displacement and moment-angle relations are derived in form of algebraic functions so that they can be analytically integrated to obtain the mechanical work [6].

3. COMPARISON OF LOAD DEPENDENT ADHESION AND FRICTION LIMITS

It is worth to note here that the load dependent adhesion and the friction limits determine the energy absorption within the contact plane. Thus, diagram Fig. 2 is shown to compare the sensitivity of load dependent adhesion $F_{H}(F_N)$ on the friction limits of sliding, rolling and torsion of these four stressing modes. The following material data of ideally assumed, smooth mono-disperse particles with the mechanical properties of limestone are used to calculate the curves of Fig. 2 to Fig. 4:

1. Median particle diameter $d_{50,3} = 1.2 \, \mu m$ and solid density $\rho_s = 2740 \, kg/m^3$,
Hamaker constant $C_{H,sls} = 3.8 \times 10^{-20}$ J. The characteristic adhesion force of rigid sphere-sphere contact $F_{H0} = -2.64$ nN was back calculated from powder shear tests.

The plastic micro-yield strength $\sigma_f = 300$ N/mm$^2$, equilibrium centre separation for dipole interaction $a_0 = 0.336$ nm, elastic-plastic contact area coefficient $\kappa_A = 5/6$, plastic repulsion coefficient $\kappa_p = 0.153$, elastic-plastic contact consolidation coefficient $\kappa = 0.224$,

Modulus of elasticity $E = 150$ kN/mm$^2$,

Poisson ratio $\nu = 0.28$, shear modulus $G^* = 34$ kN/mm$^2$ and

Contact friction coefficient $\mu_i = 0.76$.

The tangential force or maximum resistance $F_{T,C,H}(F_N)$ to let the contact begin to slide is larger than to pull-off and separate the particles by maximum adhesion force $F_H(F_N)$. The microscopic rolling moment or maximum resistance $M_{R,C,H}(F_N)$ to let roll the contact is larger than to let rotate or twist the particles by maximum torsional moment $M_{to,C,H}(F_N)$.

![Force and moment - normal force diagram of limestone particles to compare the load dependent elastic-plastic adhesion limit $F_H$ as positive force and the load dependent elastic-plastic friction limits of tangential force $F_{T,C,H}$, rolling moment $M_{R,C,H}$ and torsional moment $M_{to,C,H}$. The microscopic normal load $F_N$ is equivalent to macroscopically moderate average pressures $\sigma_{M,st} = 1$ to 25 kPa (or major principal stresses $\sigma_1 = 2$ to 40 kPa), frequently applied in powder handling.](image)

4. COMPARISON OF THE AVERAGED AND LOCAL ENERGY DENSITIES

The load dependent specific hysteresis and friction work of the four stressing modes of one particle contact are compared and briefly discussed for normal forces from 3 to 130 nN.

4.1 Comparison of the specific hysteresis work of the four stressing modes

First, the sensitivity of load dependent adhesion $F_H(F_N)$ on the maximum specific work of elastic-dissipative hysteresis (during unloading and reloading) of normal loading, sliding, rolling and spinning (torsion) is demonstrated for the four stressing modes in Fig. 3. The specific energy input that is required to compensate the energy absorption within one loop of the elastic hysteresis for unload/reload in the normal and tangential direction is nearly in the same order $W_{m,N,diss} \approx W_{m,T,max}$.
But in contrast to this, the maximum specific hysteresis work necessary for one loop torsion \( W_{m,\text{to,} \text{max}} \) is much larger than for rolling \( W_{m,\text{R,} \text{max}} \).

Fig. 3: Particle mass related hysteresis work - normal force diagram. The single contact behaviour is shown to compare the load dependent maximum work of elastic hysteresis of normal deformation \( W_{m,N,diss} \), tangential microslip \( W_{m,T,\text{max}} \), rolling friction \( W_{m,R,\text{max}} \) and torsional microslip \( W_{m,\text{to,} \text{max}} \).

### 4.2 Comparison of the specific detachment and friction work of the four stressing modes

The influence of normal load and load dependent adhesion on the work of contact detachment and friction work during sliding, rolling and spinning is shown for the four stressing modes in Fig. 4:

Fig. 4: Particle mass related friction work - normal force diagram. The single contact behaviour is shown to compare the load dependent maximum work of contact detachment in the normal direction \( W_{m,N,A} \), tangential sliding \( W_{m,T,C} \), rolling friction \( W_{m,R,C} \) and spinning \( W_{m,\text{to,} C} \) [2, 6].
The smallest values of energy absorption are calculated for the direct contact approach and separation in the normal direction, i.e. the specific detachment work $W_{m,N,A} = 2 - 50 \, \mu J/g$. If one compares maximum (or selected) specific friction work of sliding $W_{T,C}$, rolling $W_{R,C}$, and torsion $W_{T,C}$, only the factors are different, namely $2 \mu_i$, 1 and $2/3 \mu_i$ [2, 6]. These comparatively small differences in the mass related energy absorption of different loading/unloading procedures are compared in Fig. 4 with respect to tangential sliding, rolling and spinning (torsion).

### 4.3 Comparison of the local energy densities of surface activation

The logical consequence of the model stiff particles with soft contacts is that only the mass fraction of the deformed contact matter is considered to describe the local intensity of energy absorption during mechanical stressing of two particles. For the sake of simplicity, the averaged mass of the locally deformed contact zone is geometrically approximated by the caps of spheres 1 and 2 with their heights or displacements $h_{K,1} = h_{K,2} = h_{K,U}/2$ [6]. The same factors $2 \mu_i$, 1 and $2/3 \mu_i$ are found as well when one compares the characteristic (maximum) local energy densities of surface activation by contact sliding, particle rolling and torsion, Eqs. (2), (3) and (4) in Table 1:

#### Table 1: Activation energy of deformed contact zone. The symbols are explained in section 3 (median particle radius $r_{1,2} = d_{50}/4$ of surface curvature, $\tilde{M} = 100 \, g/mol$ molecular mass of limestone).

<table>
<thead>
<tr>
<th>Microprocess</th>
<th>Work</th>
<th>$W_{M} = \tilde{M} \cdot W_{m}$ in kJ/mol</th>
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<tbody>
<tr>
<td>Compression &amp; detachment</td>
<td>$W_{m,N,act} = 2 \cdot \frac{p_f}{\rho_s} \left[ \kappa_A + \kappa_p \cdot \frac{a_0}{h_{K,U}} + \frac{2 \cdot F_{H_0} \cdot a_0}{\pi \cdot r_{1,2} \cdot p_f \cdot h_{K,U}} \right]$</td>
<td>(1) $W_{M,N,act} = 20 - 40$</td>
</tr>
<tr>
<td>Sliding</td>
<td>$W_{m,T,C,act} = 8 \cdot \mu_i \cdot \kappa_A \cdot \frac{p_f}{\rho_s} \cdot \frac{r_{1,2}}{h_{K,U}}$</td>
<td>(2) $W_{M,T,C,act} = 1000 - 3000$</td>
</tr>
<tr>
<td>Rolling</td>
<td>$W_{m,R,C,act} = 4 \cdot \kappa_A \cdot \frac{p_f}{\rho_s} \cdot \frac{r_{1,2}}{h_{K,U}}$</td>
<td>(3) $W_{M,R,C,act} = 660 - 2000$</td>
</tr>
<tr>
<td>Spinning (torsion)</td>
<td>$W_{m,to,C,act} = \frac{8 \cdot \mu_i \cdot \kappa_A}{3} \cdot \frac{p_f}{\rho_s} \cdot \frac{r_{1,2}}{h_{K,U}}$</td>
<td>(4) $W_{M,to,C,act} = 330 - 1000$</td>
</tr>
</tbody>
</table>

The enormous local energy densities of these various stressing modes are found to be in the orders of magnitude of 0.02 to 3 MJ/mol. These theoretically estimated molar energies are directly compared with the lattice enthalpies of various ionic crystals of 0.7-15 MJ/mol. The values are also located within the range of the energy accumulated in lattice dislocations of about 100-1000 kJ/mol and are more than the sublimation (evaporation) enthalpies of solids of about 200-500 kJ/mol. It is worth to note here that the local activation energy of tribochemical reactions within the contact zone nearly amounts to the same orders of magnitude and varies from 62 to 744 kJ/mol [8, 9].

This local energy consumption is meaningful for surface activation, particle conversion, product formulation, macroscopic non-rapid frictional shear flow of cohesive ultrafine powders and the agglomerate disintegration in powder processing and handling. Thus, the micromechanical approach is qualitatively and quantitatively consistent and conclusive concerning the constitutive force-displacement and moment-angle laws and the estimated maximum specific energy absorption.

### 5. CONCLUSIONS AND OUTLOOK

The consolidation and non-rapid flow of ultrafine and cohesive powders was referred to the dominant effect of adhesion forces at particle contacts. That was the physical basis of universal models
for particle adhesion, which includes the elastic-plastic particle contact behaviour with hysteresis and consequently, energy absorption. The four stressing modes by compression and detachment (tension), sliding, rolling and torsion were considered when two adhesive particles are in contact. By the model stiff particles with soft contacts and the contact force equilibrium, universal models were shown that include the elastic-plastic particle contact behaviour with adhesion, load-unload hysteresis and a load dependent adhesion force function. With increasing adhesion force the tangential, rolling and torsional friction limits increase.

The consequences of elastic-dissipative as well as elastic-plastic, frictional unloading and reloading paths of normal and tangential forces and rolling and torsional moments for the load dependent energy absorption and the friction work are discussed and compared. The different quantities between the averaged and local intensity of the energy absorption are explained for single stressing events of contact compression, sliding, rolling and torsion. The averaged energy densities of these various stressing modes are found to be in the orders of magnitude of about 0.4 - 6 mJ/g. But the enormous local energy densities amount to 0.2 - 30 kJ/g or in molar units 0.02 - 3 MJ/mol.

In this context, the light emission due to mechano-luminescence effects by elastic, elastic-plastic contact deformations and, consequently lattice dislocations, crystal phase conversions and particle breakages can be explained qualitatively at intensive and multiple stressing of particles in grinding processes with large local energy densities, see Aman and Tomas [10].

This microscopic energy absorption macroscopically leads to the significant influence of pre-consolidation stress on the non-rapid frictional flow of ultrafine cohesive powders and to the remarkable macroscopic energy consumption that is well-known in powder storage and handling practice [7]. This is also meaningful for the agglomerate disintegration in powder processing and generates inelastic contact and particle deformations, surface defects, surface asperity abrasion, particle-wall abrasion and micro-cracking up to particle breakage. Those agglomerate disintegration effects are undesired and cause product damage and quality reduction, see Antonyuk et al. [11].

6. REFERENCES