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Simulation of normal impact of micron-sized particle with elastic-plastic contact

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1. Introduction

The handling of powder materials is attached of great importance in pharmaceutical, food, cement, chemical and other industries. Most of powders are treated as cohesive granular materials. Thus, understanding the fundamentals of particle adhesion with respect to product quality assessment and process performance is very essential in powder technology.

Cohesive granular materials are currently being studied by applying experimental, theoretical and numerical methods. Recently, the discrete (distinct) element method (DEM) introduced by Cundall and Strack [1] has become a powerful tool for solving many scientific and engineering powder technology problems. It started with its first application to simulate the dynamic behaviour of noncohesive granular material, which is presented as an assembly of grains. Interaction of particles described by the Hertz contact theory is usually used to describe repulsive contact forces independently on specific particle size.

Fundamentals of the particular DEM models of noncohesive granular material may be found in [2-4], aplication examples in [5-7] while important details of DEM simulation technique and software implementation in [8-10]. Behaviour of adhesive particle is generally investigated basing on three different concepts model DMT (Derjaguin, Muller and Toporov) [11-13], JKR (Johnson, Kendall and Roberts) [14-16], MD (Maugis and Dugdale) [17]. Normal impact of cohesive particles can be expressed on the basis of cohesive elastic-plastic-dissipative contact model. Adhesive elastic-plastic micromechanical model has been developed by Tomas [18-20]. Particle adhesion force between adhesive deformable bodies was shown by Zhou [21] and between rigid boundary by Feng [22].

Strength of adhesive joints of packages made from printing materials was first implemented by Kibirkstis and Mizyuk [23].

The focus of investigation is an attempt to illustrate the behaviour of micron-sized particle during normal impact and the role of various energy dissipation mechanisms combined with possible variation of data parameters. Total amount of dissipation may be characterised by single parameter, i.e. by coefficient of restitution (COR), which may be defined in terms of velocities, energy or other state variables. It is complex parameter and comprises several effects. Explanation of its nature in terms of both interpretation experimental results and theoretical models is, however, not unique.

The coefficient of restitution characterises the inelastic deformation work of particle contact. Dissipation for elastic-plastic behaviour is regarded by Thornton and coworkers [24-26]. A dissipation model based on continuum damage mechanics for the description of nonlinear response during loading of a single particle until fracture has been investigated by Tavares and King [27] and for rock materials by Imre et al. [28]. This model is being also capable of explaining irreversible nature elastic hysteretic dissipation of brittle contact.

A viscous damping dominant dissipation related to force $\boldsymbol{F}_{diss}^{n}$ is typical for coarse cohesionless particles moving with comparatively large velocities ($\upsilon > 1$ m/s). Various models of the nonlinear elastic contact with viscous spring-dashpot behaviour were developed. Because of difficulties in obtaining data values, particular case heuristic critical damping based approach developed by Tsuji et al. [29] was frequently employed. Combinations of various dissipation mechanisms to simulate sticking and rebounding behaviour of contacting micron-sized particle were also shown [30, 31]. Also impact of viscoplastic bodies: dissipation and restitution was presented by Ismail [32].

In spite of huge progress in the theoretical developments, precise weighting of particular dissipation mechanisms and their contribution to integral COR is still problematic. This is not only because of incompletion of models but also of statistical distribution of material data and surface properties.

The problem is challenging because the available experimental evidence of particle restitution issue is also non unique. Collision experiments with micron-sized silica spheres impacting silica and silicon targets were presented by Poppe et al. [33], where measured values of coefficient of restitution are provided. Significant scattering of experimental date indicates uncertainty of the interaction parameters. In contrary, measurements of adhesion forces between silica particles (effective radius R_{eff} varies in the range of 0.1-1.2 μm**)** and a silicon wafer performed with AFM by Kappl in Tykhoniuk et al [34] and showed that the plastic deformation of the particle occurs and mainly takes place in the first load-unload cycle. The same statement concerning the first cycle was confirmed Imre et al. [28] while the CORs of the present rock samples never reached 1.00.

Summating the above diverse facts it could be stated that further research to evaluate of the coefficient of restitution at a particle collisions is required.

Normal impact of the stiff micron-sized particle with soft contact at deformable substrate was investigated numerically.

2. Mathematical model and simulation methodology

The DEM methodology based on the Langrangian approach is applied to simulate dynamic behaviour of the cohesive particles under normal impact. The motion of arbitrary particle i is characterized by a small number of global parameters: positions $\mathbf{x}_i$, velocities $\dot{\mathbf{x}}_i = d\mathbf{x}_i / dt$ and accelerations $\ddot{\mathbf{x}}_i = d^2\mathbf{x}_i / dt^2$ of the mass center and force applied to it. Translational motion is described by the Newton's second law applied to each particle i

$$m_i \ddot{\mathbf{x}}_i(t) = \mathbf{F}_i(t) \qquad (1)$$

where m_i is the mass, while vector $\mathbf{F}_i$ presents the resultant force act on the particle i due to contacts with j neighbour particles. It may comprise prescribed and field forces.

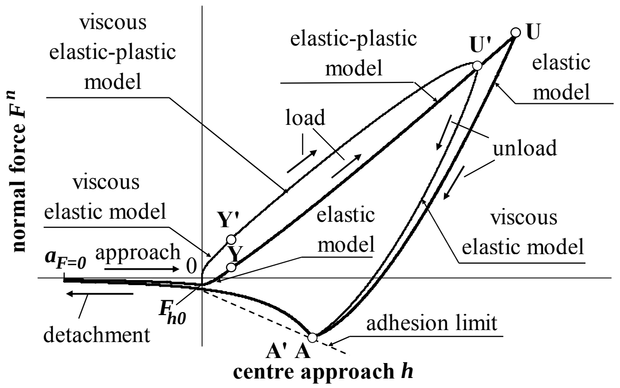

Fig. 1 Force displacement relations for soft contact of particles

The methodology of calculating of the forces $\mathbf{F}_{ij}(t)$ in Eq. (1) depends on the particle size, shape and mechanical properties as well as on the constitutive model of the particle interaction.

The constitutive model for the normal impact under consideration combines displacement-dependent elastic–plastic contact deformation behaviour and includes adhesion as well as velocity-dependent dissipative term (Fig. 1). Negative range of approach displacement h means contactless interaction while positive range illustrates contact behaviour. Here Y' and Y denotes yield point, U' and U unload point, A and A' separation point with and without viscous respectively.

Constitutive model shown in Fig. 1 is presented in a form of algebraic force-displacement functions and is used later to describe particles. Consequently, a normal interaction force required in Eq. (1) during collision comprises three components of slightly different nature in Eq. (1)

$$\mathbf{F}_{ij}^n = \mathbf{F}_{ij}^n\left(\mathbf{F}_{deform}^n + \mathbf{F}_{adh}^n + \mathbf{F}_{diss}^n\right) \qquad (2)$$

where $\mathbf{F}_{deform}^n$ is displacement dependent deformation force, adhesion force $\mathbf{F}_{adh}^n$, elastic-plastic and velocity-dependent dissipative force $\mathbf{F}_{diss}^n$. This approach recovers reversible and irreversible effects and various linear and nonlinear expressions may be applied to evaluate particular force components.

The displacement-dependent terms are formulated basing on the resent developments of Tomas [18-20]. The corresponding deformation history is indicated by O-Y-U-A path. The elasticity limit illustrated by yield point Y is actually characterised by the microyield strength p_f within contact plane.

The velocity-dependent dissipative term is defined according Tsuji [29] and is defined by damping constant η. The hysteric viscoelastic behaviour is illustrated by O - Y'- U'-A' path.

Motion of a particle during impact is shown in Fig. 2. The particle movement starts by approach with initially velocity υ_0 at the minimal initial distance $a_{F=0}$ (Fig. 2, a). It could be state that adhesion forces F_{adh} acting on particle in at distance $a_{F=0}$ is sufficient to attract particle without any initial velocity. This process is so called "jump in". When the particle reaches the surface contact deformation occurs and lasts until complete rebound (Fig. 2, b-d). Here particle reach max overlap value h_U (Fig. 2, c). Dependently on accumulations of kinetic energy it may detach or remain stick to the substrate (Fig. 2, e) with residual overlap.

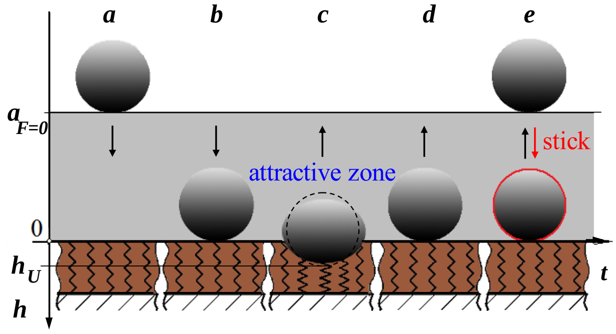

Fig. 2 Movement of micro-sized particle

The discussed contact model along with integration of differential Eq. (1) was implemented into the original program code written on Fortran basis.

3. Problem description and basic data

Simulation addresses normal impact of the smooth spherical silica particle of $R = 0.6$ µm on plane surface of the substrate. The particle is assumed to be smooth on a subnanometer scale. Mass of silica sphere was $1.8\cdot10^{-15}$ kg. Other values of the property parameters are selected from available sources (Zhou and Peukert [21], internet data source [35]) and experimental results. Elastic constants, modulus is $E = 75$ GPa, Poisson's ratio $\nu = 0.17$. Adhesion parameters are separation distance at zero load $a_{F=0} = 0.336$ nm, adhesion force $F_{H0} = 5.0$ nN back calculated from shear experimental test results of industrial silica powder for particles with median (effective) radius 0.6 µm. Taking Hamaker constant $C_H \approx 3.216\cdot10^{-20}$ J the remainder parameters such as interface energy $\gamma = 3.78$ mJ/m^2 [34].

Plasticity properties [18-20] are characterized by microyield strength in compression p_f. This parameter, especially, for ultrafine inorganic/organic powders is normally unknown. One of the possibilities to evaluate p_f is based on macroscopic considerations. By comparing yield inception according to von Mises yield criterion with maximal limit contact pressure it is easy to show that the microyield strength p_f is related to the yield limit σ_y of the sphere material by dimensionless function depending on the Poisson's ratio v (Brizmer et. al. [36]). The failure inception of brittle materials may occur when the maximum tensile stress reaches the failure strength σ_f of the material. The available internet data source [35] gave us additional parameters: the apparent elastic limit $\sigma_{ya} = 55$ MPa and extreme large compressive strength $\sigma_{yc} = 1.1$ GPa. It is already known [36] that $p_f \approx 3\sigma_{ya}$ responds generally the soft plastic behaviour, the dimensionless parameters $E/p_f = 454 > 200$ would indicate very stiff material in compression. Another parameter $E/\sigma_{ya} = 1364 > 1000$ and Poisson's ratio $v = 0.17 < 0.25$ indicate preferably brittle properties in tension.

For fine particles p_f is related to microscopic parameter attractive van der Waals pressure, see Tomas [18-20], and may be significantly influenced by surface microproperties of the particles, because of surface defects a soft plastic behaviour is generally expected, nano-asperities and immobile/mobile adsorption layers.

Omitting discussions about details we choose three acceptable different values of yield strength $p_{f1} = 150$ MPa, $p_{f2} = 300$ MPa, $p_{f3} = 500$ MPa which will be used in future simulations.

Elastic substrate is considered by assigning elasticity properties identical to the particle.

4. Numerical investigation of normal contact

Series of numerical calculations with initial velocity υ_0 varying up to 50 m/s was conducted to investigate normal contact of micron-sized silica particle with plane surface of the deformable substrate in order to investigate sticking and detachment of a particle and various available dissipation mechanisms. Adhesion parameters are assumed independent on the substrate. Coefficient of restitution e is obtained on the results of rebound velocities.

The first series of calculations deals with particle impact on deformable substrate by applying purely elastic but dissipative model solutions in Fig. 3, a, as elastic limit curves which corresponds to involve theoretically expected restitution values.

Three restitution curves *1*, *2*, *3* represent variations of COR against impact velocity υ_0 respond to three different damping factors α_d equal to: 0, 0.15 and 0.35 yielding 0, 20 and 40% reduction of maximal COR. Zero point of undamped model of restitution curve *1* is defined at in elastic zone. Here critical sticking velocity is $\upsilon_{0,st} = 0.041$ m/s corresponds to absorbed contact energy. However, damping plays decisive role, especially near the critical velocity, where viscous dissipation is even faster.

Comparing elastic branches shown in Fig. 3, it is easy to recognise similar character of our elastic curves to those of elastic wave [24] dissipation mechanisms.

The second series reflect the behaviour of viscous-elastic-plastic model with fixed microyield stress $p_f = 500$ MPa. Numerical results represented by three restitution curves *1*', *2*' and *3*' having the same damping factors as curves *1*, *2* and *3* are exhibited in Fig. 3, b. In the points Y_1, Y_2, Y_3 restitution curves switches from purely elastic to elastic-plastic contact.

An influence of microstrength along with properties of the substrate is considered in next series of numerical calculations. Numerical results in terms of variation of COR against impact velocities are presented in Fig. 4. Three curves *1*, *2* and *3* correspond to three values of the microstrength (microhardness) $p_f = 500$, 300, 150, respectively without damping - α_d equal to 0.

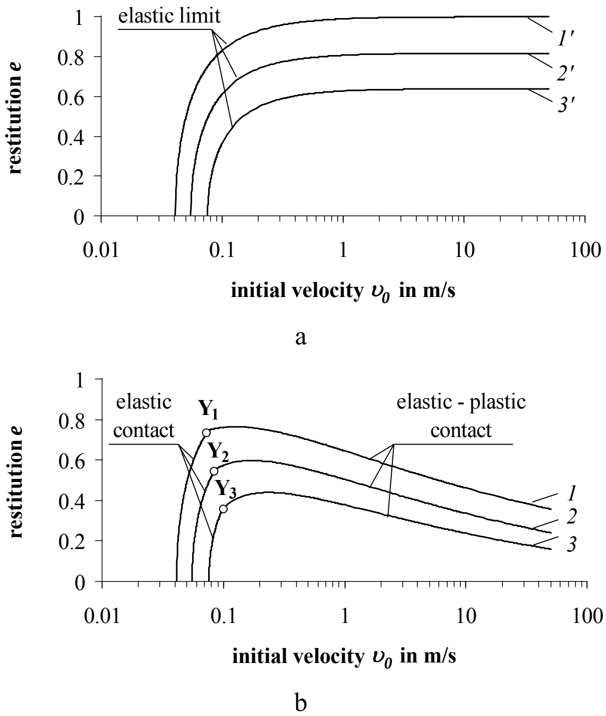

Fig. 3 Variation of COR due to viscous damping against impact velocity for various damping factors

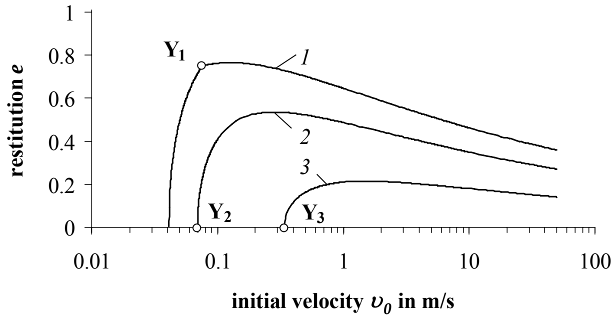

Fig. 4 Variation of COR against impact velocity for various microstrength values

Here points Y_1, Y_2, Y_3 denote origin of elastic-plastic contact. Curve *1* contains restitution values branch of purely elastic and the branch of elastic-plastic contact, while curves *2* and *3* contain values only of elastic-plastic contact.

Simulation results are checked against impact experiment with identical silica particles by Poppe et al. [33], Fig. 5. Two curves *1*, *2* correspond to two values of $p_f =$ = 500, 300 MPa respectively without damping. Additional dashed line indicates purely elastic case. The collisions between the dust particles and the fixed target are observed by optical imaging of the particle trajectories. The measured values of coefficient of restitution for impact velocities υ_0 ranging between 1 and 10 m/s are characterized graphically by thin lines. Generally, our results envelop experiment with compare of both results. It is easy to show the character of COR numerically obtained on the plasticity relation properly respond to the tendency of experimental results. It could be stated that plasticity mechanism indicates lower bound while elastic dissipation responds to the upper bound. However, further research is still required for recovering of the experimentally observed dissipation mechanisms.

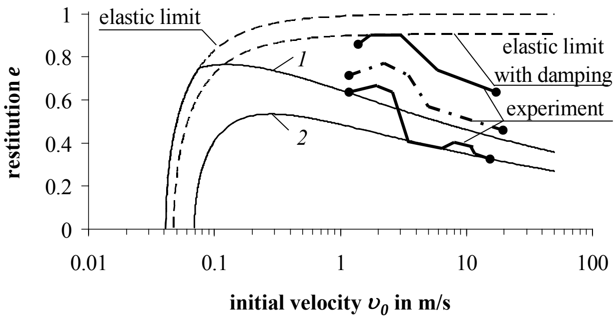

Fig. 5 Variation of COR against impact velocity for various microstrength values and substrates- interpreting of Poppe et al. [33] results

It should be noted that the results illustrates dynamic experiment. In many cases dynamic load yields the increase of statically obtained values as the rate dependent material property effects.

5. Concluding remarks

On the basis of numerical simulation of silica particle impacting plane substrate it could be stated that elastic or elastic-plastic hysteric deformation combined with viscous damping can yield similar dissipation-restitution evaluations. Numerical results also confirmed that plastic deformation is the dominant source of the dissipation mechanism at higher initial impact velocities while adhesive elastic dissipation is the dominant at lower initial impact velocities. Simulation results could be used for reasonable explanation of experimental evidence. Considering comparison with experiment it could be stated that experimental results may be enveloped by various combinations of dissipation mechanisms.

6. Acknowledgements

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NORMALINIO TAMPRIAI PLASTINIO MIKROSKOPINIO DYDŽIO DALELĖS SMŪGIO MODELIAVIMAS

R e z i u m ė

Straipsnyje aprašytas skaitiškai tirtas normalinis dalelės smūgis į deformuojamą pagrindą. Mikroskopinio dydžio dalelė yra $R = 0.6$ µm spindulio sfera. Netiesinis disipacinis kontaktas formuojamas centrinio smūgio jėgų modelyje. Deformacija aprašyta tampriai plastiniu kontakto modeliu, apkraunant ir nukraunant. Slopinimas aprašytas netiesiniu Tsuji modeliu. Nuo apkrovimo priklausantis atsiskyrimas – netiesinis. Uždavinys sprendžiamas diskrečiųjų elementų metodu. Buvo tirti skirtingi disipaciniai mechanizmai. Skaitiniai rezultatai lyginami su eksperimento duomenimis. Parodyta, jog atsistatymo koeficiento sklaida gali būti įvertinta įvairiais disipaciniais mechanizmais.

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SIMULATION OF NORMAL IMPACT OF MICRON-SIZED PARTICLE WITH ELASTIC-PLASTIC CONTACT

S u m m a r y

Central impact of a particle at deformable substrate was investigated numerically. The micron-sized particle presents a sphere with the radius $R = 0.6$ µm. The nonlinear-dissipative contact model with adhesion was developed to model central impact forces. Deformation behaviour is described by elastic-plastic contact model with loading and unloading. Damping was described by the nonlinear Tsuji model. The load-dependent detachment is of nonlinear character. The problem was solved by the Discrete Element Method. Different dissipation mechanisms were examined. Numerical results are compared with published experiment results.

Р. Ясевичюс, Ю. Томас, Р. Качянаускас

МОДЕЛИРОВАНИЕ НОРМАЛЬНОГО УПРУГОПЛАСТИЧЕСКОГО УДАРА ЧАСТИЦЫ МИКРОСКОПИЧЕСКОЙ ВЕЛИЧИНЫ

Р е з ю м е

Нормальный удар частицы с деформируемым субстратом был исследован численно. Частица микроскопической величины представляет собой сферу радиусом $R = 0.6$ мкм. Нелинейная – диссипативная модель контакта с адгезией была разработана для нормальных сил удара. Деформации описаны упругопластической моделью контакта с загрузкой и разгрузкой. Демпфирование описано нелинейной моделью Тсуи. Зависимо от нагрузки отсоединение имеет нелинейный характер. Программа была решена методом дискретных элементов. Изучены разные диссипативные механизмы. Численные результаты сравнены с экспериментом. Экспериментально доказано, что наблюдаемое рассеивание коэффициента восстановления может быть огибающим с помощью различных механизмов диссипации.

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