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Raimondas JASEVIČIUS

THE NUMERICAL MODELLING OF NORMAL INTERACTION OF ULTRAFINE PARTICLES

SUMMARY OF DOCTORAL DISSERTATION

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Scientific Supervisor

Prof Dr Habil Rimantas KAČIANAUSKAS (Vilnius Gediminas Technical University, Technological Sciences, Mechanical Engineering – 09T).

Consultant

Dr Darius MARKAUSKAS (Vilnius Gediminas Technical University, Technological Sciences, Mechanical Engineering – 09T).

The dissertation is being defended at the Council of Scientific Field of Mechanical Engineering at Vilnius Gediminas Technical University:

Chairman

Prof Dr Habil Mindaugas Kazimieras LEONAVIČIUS (Vilnius Gediminas Technical University, Technological Sciences, Mechanical Engineering – 09T).

Members:

Dr Robertas BALEVIČIUS (Vilnius Gediminas Technical University, Technological Sciences, Mechanical Engineering – 09T),

Prof Dr Habil Saulius BALEVIČIUS (State Research Institute Center for Physical Sciences and Technology, Physical Sciences, Physics – 02P),

Prof Dr Habil Rimantas BARAUSKAS (Kaunas University of Technology, Physical Sciences, Informatics – 09P),

Prof Dr Habil Marijonas BOGDEVIČIUS (Vilnius Gediminas Technical University, Technological Sciences, Mechanical Engineering – 09T).

Opponents:

Dr Algis DŽIUGYS (Lithuanian Energy Institute, Technological Sciences, Mechanical Engineering – 09T),

Prof Dr Vytautas TURLA (Vilnius Gediminas Technical University, Technological Sciences, Mechanical Engineering – 09T).

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Address: Saulėtekio al. 11, LT-10223 Vilnius, Lithuania.
Tel.: +370 5 274 4952, +370 5 274 4956, fax +370 5 270 0112;
e-mail: doktor@vgtu.lt

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Raimondas JASEVIČIUS

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Mokslinis vadovas
prof. habil. dr. Rimantas KAČIANAUSKAS (Vilniaus Gedimino technikos universitetas, technologijos mokslai, mechanikos inžinerija – 09T).
Konsultantas
dr. Darius MARKAUSKAS (Vilniaus Gedimino technikos universitetas, technologijos mokslai, mechanikos inžinerija – 09T).
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Pirmininkas
prof. habil. dr. Mindaugas Kazimieras LEONAVIČIUS (Vilniaus Gedimino technikos universitetas, technologijos mokslai, mechanikos inžinerija – 09T).
Nariai:
dr. Robertas BALEVIČIUS (Vilniaus Gedimino technikos universitetas, technologijos mokslai, mechanikos inžinerija – 09T),
prof. habil. dr. Saulius BALEVIČIUS (Valstybinis mokslinių tyrimų institutas Fizinių ir technologijos mokslų centras, fiziniai mokslai, fizika – 02P),
prof. habil. dr. Rimantas BARAUSKAS (Kauno technologijos universitetas, fiziniai mokslai, informatika – 09P),
prof. habil. dr. Marijonas BOGDEVIČIUS (Vilniaus Gedimino technikos universitetas, technologijos mokslai, mechanikos inžinerija – 09T).
Oponentai:
dr. Algis DŽIUGYS (Lietuvos energetikos institutas, technologijos mokslai, mechanikos inžinerija – 09T),
prof. dr. Vytautas TURLA (Vilniaus Gedimino technikos universitetas, technologijos mokslai, mechanikos inžinerija – 09T).
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Tel.: (8 5) 274 4952, (8 5) 274 4956, faksas (8 5) 270 0112;
el. paštas doktor@vgtu.lt
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Introduction

Problem Formulation. Simulation of the dynamic behaviour of solids and structures has been traditionally considered in the field of mechanical engineering and the related areas worldwide for many years. Recently, a major effort has been increasingly focussed on the investigation of various materials including particulate solids and processes herein. The Discrete Element Method (DEM) is a numerical technique that can provide information on the time-history behaviour of individual particles, which is difficult to obtain by the conventional experimental techniques. In spite of huge progress, modelling of cohesive particulates, including ultrafine particles, still requires more profound knowledge.

This work deals with mechanical modelling of ultrafine spherical particles and presents the investigation of their normal interaction. It involves the development and validation of a theoretical model and its implementation in the DEM. Its performance was proved by various numerical experiments and a comparison with the available results. The influence of the characteristic energy dissipation mechanisms as well as sticking and rebound, are considered in detail.

Topicality of the Problem. Recently, powders of the size d ($0.1\ \mu m < d < 10\ \mu m$) have been referred to ultrafine particles. The particle shape considered is assumed to be a sphere of the diameter d. The handling of powders is of great importance for processing of pharmaceuticals, cement, chemicals and other products. Most of these technological processes involve powder compaction, storage, transportation, mixing, etc, therefore, understanding of the fundamentals of particles interaction behaviour is very essential in the design of machines and equipment as well as in powder technology, cleaning of environment and other areas.

The dynamic behaviour of particulate systems is very complicated due to the complex interactions between individual particles and their interaction with the surroundings. Understanding the underlying mechanisms can be effectively achieved via particle scale research. The problem of a normal contact may be resolved in a number of ways. In spite of huge progress in experimental techniques, direct lab tests with individual particles are still rather time-consuming and expensive.

The interaction of particles as solid bodies is actually a classical problem of contact mechanics. In the case of ultrafine particles, the reduction of the particle size shifts the contact zones into the nanoscale or subnanoscale. Thus, steadily increasing contribution of adhesion has to be considered in the development of the physically correct constitutive models and numerical tools.

Consequently, it may be stated that particle-particle or particle-substrate interaction models are based on the knowledge of continuum mechanics, micromechanics, as well as intermolecular and interatomic interaction. The investigation of normal interaction between particles and a substrate is a new contribution to the microscopic theory of ultrafine particles and numerical modelling. Further applications to solving practical problems may be expected.

The Object of Research. A theoretical model of normal interaction behaviour of ultrafine particles and its application to discrete element simulations are considered.

The Aim and Tasks of the Work. The aim of the present work is to formulate and numerically investigate the model of normal interaction between the ultrafine spherical particles.

To achieve this aim, the following tasks should be performed:

1. To formulate and describe the constitutive models of the normal adhesive elastic and elastic-plastic interaction of particles, based on the concept of rigid particle with soft contacts.
2. To evaluate the characteristic mechanisms of energy dissipation for adhesive normal interaction.
3. To investigate the conditions of the particle rebound and sticking and the character of the postcollision processes.

To develop software tools for investigating the normal interaction of ultrafine particles.

Methodology of Research. Research was performed by using analytical methods and numerical simulations. The numerical experiment was performed using the discrete element method.

Scientific Novelty. The contribution to the field of mechanics involves:

1. The development of the constitutive models of normal interaction for ultrafine spherical particles comprising adhesive elastic and elastic-plastic behaviour with the characteristic mechanisms of energy dissipation.
2. The development and DEM implementation of the history-dependent mechanism of energy dissipation associated with adhesion. The development and DEM implementation of the history-dependent mechanism of energy dissipation associated with viscous damping to be used for assessing the particle's sticking process.
3. Evaluation, estimation and description of sticking and rebound conditions.
4. The provision of a reasonable explanation of the results of physical impact experiment conducted with silica particles.

Practical Value. The proposed theoretical model demonstrates the ability to capture various effects in normal interaction behaviour of ultrafine spherical particles. The developed software is an appropriate tool applicable to DEM simulations. It serves as the basis for large-scale simulations and design of technological equipment.

Defended Propositions

1. The proposed constitutive model of normal interaction for ultrafine spherical particles comprising adhesive elastic and elastic-plastic behaviour with the characteristic mechanisms of energy dissipation.
2. The explanation of the role of separate energy dissipation mechanisms during the particle impact on the substrate for various initial interaction velocities.
3. The proof of the development of plastic deformation during the impact of silica particles on the plane substrate.

Approval of the Work. Seven presentations on the topic of dissertation were delivered at scientific conferences in Lithuania and abroad, and seven articles were published.

The Structure of the Research Paper. The scientific work consists of the introduction, 5 chapters, general conclusions, list of literature, list of author publications. The dissertation consists of 124 pages, 48 pictures, 2 tables and 102 formulas.

1. Mechanics of Interaction and Numerical Method

Review and fundamentals of the normal interaction with Van der Waals adhesion along with backgrounds of the Discrete Element Method are presented in this chapter.

Mechanics of Adhesion. Adhesive interaction presents coupled behaviour of the repulsive contact and attractive adhesive forces. A contact model is based on the Hertz contact theory, but the physical basis of universal models with hysteresis has to include the elastic-plastic and viscous properties and characteristic energy dissipation mechanisms.

Consideration of adhesion is basically governed by two original models. The JKR model suggested by Johnson, Kendall and Roberts (1971) assumes that the surface attraction force is associated with the surface energy within the contact area. The DMT model suggested by Derjaguin, Muller and Toporov (1975) assumes that the surface attraction forces are within a finite range and,

therefore, also act beyond the contact zone where surface separation is small. Both cases present limiting solutions of adhesive interactions. Series of modifications of the adhesive models were elaborated later. The constitutive interaction model of the *stiff particles* with *soft contacts* suggested and developed by Tomas (2001, 2007) on the basis of micromechanical approach could be emphasised. Particle is called as micron sized powder component.

Methodology of Discrete Element. The time-driven Discrete Element Method (DEM) introduced by Cundall and Strack (1979) has become recently a dominant numerical tool to solve scientific and practical problems of particle mechanics.

The DEM is a particle oriented method dealing with each individual particle by tracking its movement and interactions with the neighbour particles and surroundings over time t. An arbitrary particle i having mass m_i is characterized by global vector parameters: positions $\boldsymbol{x}_i(t)$, velocities $v_i = \mathrm{d}\boldsymbol{x}_i/\mathrm{d}t$ and accelerations $\boldsymbol{a}_i = \mathrm{d}^2\boldsymbol{x}_i/\mathrm{d}t^2$ of the mass centre and forces $\boldsymbol{F}_i(t)$ applied to it. The particles motion obeys the Newton's second law and is described by a set of fully deterministic ordinary differential equations. Restricting to translational motion:

$$m_i \cdot \boldsymbol{a}_i(t) = \boldsymbol{F}_i(t). \tag{1}$$

Dynamic equilibrium of inertia, external and inter-particle contact forces has to be satisfied during entire time period under consideration, therefore, suitable constitutive models of particle's interactions need to be specified.

2. Theoretical Models of Interaction

A new theoretical model assessing the specific small-size body effects is proposed and developed for the description of the normal interaction of ultrafine spherical particles. The model employing the above mentioned concept of the stiff particle with a soft contact involves adhesive interaction coupled with elastic and elastic-plastic contact deformation as well as characteristic energy dissipation mechanisms. This model recovers reversible and irreversible effects and will be able to describe various loading-unloading-reloading interactions.

Particles Adhesive Interaction with Deformable Contact. Evaluation of the interaction forces in Eq. (1) depends on the particle size, shape and mechanical properties as well as on the constitutive model of the interaction. Consequently, a normal interaction force during collision comprises three components of slightly different nature:

$$\boldsymbol{F}_{ij}^{N} = \boldsymbol{F}_{ij}^{N}(\boldsymbol{F}_{deform} + \boldsymbol{F}_{adh} + \boldsymbol{F}_{diss}), \tag{2}$$

where $\boldsymbol{F}_{deform}$ is the displacement dependent contact deformation force, $\boldsymbol{F}_{adh}$ is the adhesion force and $\boldsymbol{F}_{diss}$ is the dissipative force. Various linear and non-linear expressions may be applied to evaluate particular force components.

The constitutive model under consideration combining elastic-plastic contact deformation behaviour and load dependent adhesion is shown in Fig. 1. It naturally captures energy dissipated by plastic deformation but the model will be extended to incorporate other dissipation mechanisms.

The model is expressed in terms of the relationship between the force $\boldsymbol{F}^N$ and displacement h plotted in nanoscale. Here, the compression force is defined as positive, while the tension force is described as negative. The positive displacement characterises the contact behaviour (loading and unloading) and means the particle overlap in compression, while the negative displacement characterises the short-range interaction (approach and detachment) and denotes the distance between the interacting surfaces. First contact loading and unloading in the opposite direction are shown by the arrows.

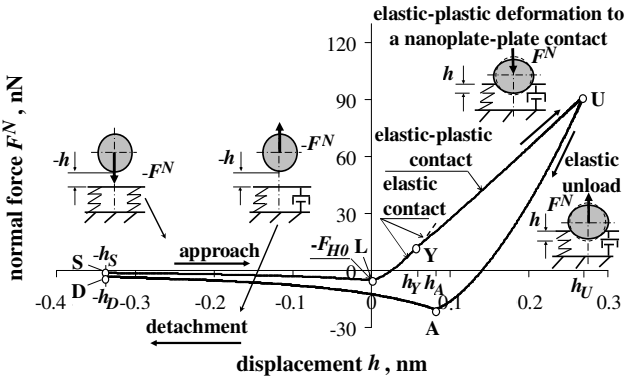

Fig. 1. Adhesive elastic-plastic interaction. Normal force F^N versus displacement h

The respective particle motion path is indicated by S-L-Y-U-A-D path (Fig. 1). The particle approach is denoted in the graph by S-L. The particle movement during approaching between h_S and 0 is assumed to be formed without any contact deformation by a short-range attractive Van der Waals force. The decay of this force is dictated by the inverse square dependence of the surface distance h as:

$$\boldsymbol{F}^{N}(t) = F_H(h) = -\frac{F_{H0} \cdot a_{F=0}^2}{(a_{F=0} - h(t))^2} \cdot \tag{3}$$

Thus, analytical description of the adhesive approach path is relevant to two parameters – minimum distance $a_{F=0}$ and adhesion force F_{H0}. Actually, fixed position $a_{F=0}$ means here a remaining intermolecular separation limit $a_{F=0}$ between surface molecules indicating the equilibrium of molecular attraction and repulsion forces. The adhesion force F_{H0} (the so-called jump in force) is force defined at the zero-point of this diagram. Theoretical evaluation of the adhesion force F_{H0} is basically relevant for calculating the adhesion between perfectly stiff and smooth surfaces corrected, however, by the influence of nanoscale asperities.

When the particle reaches the plane surface at point L, the contact is formed and elastically deformed as a response to the attraction force. Due to the action of kinetic energy of the particle, the force-displacement curve may go further to the point U, while the particles are more strongly elastically deformed. Consequently, normal adhesive sphere-plane contact L-Y is governed by an extension of the Hertz theory that is equivalent to the DMT model.

Finally, nonlinear elastic-plastic contact force above the yield point Y is described by superposition of all components as follows Y-U. Loading path is well described in numerous references.

The particle reaches the maximal overlap at displacement h_U, and the contact is elastically unloaded at the point U until the deformation path achieves the adhesion limit at the point A. the unloading of the elastic-plastic contact between h_U and h_A is governed by Hertz theory. Finally, for the following expression of the resultant force depending on residual displacement is developed:

$$\boldsymbol{F}^{N}(t) = \frac{2}{3} \cdot \frac{E}{1-\nu^2} \cdot R^{1/2} \cdot (h(t) - h_A)^{3/2} - \Delta F(h_U) - F_{H0} - F_{diss}(t) \cdot \tag{4}$$

Here, $\Delta F(h_U)$ is a residual adhesion force, reflecting the elastic-plastic deformation history, ν – Poisson ratio, R – particle radius, E – modulus of elasticity The force F_{diss} is included to capture additional dissipation mechanisms which will be considered below.

When particle reach overlap corresponded to adhesion limit at point A with displacement h_A, it loses touch with target. Adhesion limit additionally depends on dissipated energy. Detachment path between $-h_D \le h(t) \le h_A$ is denoted in Fig. 1 by A-D. For characterisation of force driving detachment behaviour of particle, the following expression was elaborated:

$$\boldsymbol{F}^{N}(t) = -\frac{\left(F_{H0} + F_{diss,adh}\right)\cdot a_{F=0}^{2}}{\left(a_{F=0} + h_A - h(t)\right)^2} - \frac{F_{el-pl}\left(h_A\right)}{\left(a_{F=0} + h_A - h(t)\right)^3}\cdot a_{F=0}^{3}\cdot \qquad (5)$$

Here, $F_{el\text{-}pl}$ – elastic-plastic force The above expressions along with normal contact forces form the base of constitutive interaction model.

Energy Dissipation Mechanism, Related to Adhesion. Dissipation of energy is important feature of particle behaviour. Generally, various mechanisms may be responsible for energy dissipation during interaction, therefore almost routine characterisation of amount of dissipated energy by single parameter – coefficient of restitution (COR) – remains unsatisfactory. Consequently, evaluation of separate dissipation mechanisms is problematic and presents significant part of current work.

The above constitutive interaction model demonstrates the dominant role of hysteric dissipation mechanism related to plastic deformation. For micron-sized ultrafine particles, the interfacial adhesion within the contact area between the two surfaces presents another significant energy dissipation mechanism. It is assumed that adhesion dictated energy dissipation is independent on other dissipation mechanisms and it is characterised by fixed value of energy dissipation related to adhesion $W_{diss,adh}$. for the case of Van der Waals attraction it is obtained in terms of model parameters: $W_{diss,adh} = F_{H0} \cdot a_{F=0}$.

Adhesive dissipation in combination with the elastic contact is illustrated in Fig. 2. It should be noted that the elastic contact presents particular case of the elastic-plastic contact if initial kinetic energy is not sufficient to reach the yield point. The entire interaction path is indicated by the diagram (S-L-U-A-D).

During elastic contact denoted by L-U the particle reaches the maximal overlap h_U at the point U and it starts to unload. It is known that unloading path U-A-D is observed experimentally and should satisfy energy balance. Energy balance of the elastic adhesive contact during the entire approach-rebound cycle is characterized by the mechanical work $W_{tot} = \int \boldsymbol{F}^{N}(h)\mathrm{d}h$, which is equal to the closed area between the loading and unloading curves (Fig. 1 and 2). For the dissipative contact backward path U-A-D is predefined by the dissipated energy $W_{tot} = -W_{diss}$. For the elastic, non-adhesive and non-dissipative contact, this work is simply zero, $W_{tot} = 0$.

Explicit description of unloading and detachment applicable to DEM simulations on the basis of the single parameter is complicated and still not resolved problem. Solution elaborated below assumes dissipation force as constituent of general model defined by (4) for unloading and by (5) for detachment.

Numerical implementation of the above dissipation mechanism requires that prescribed portion of dissipated energy $W_{diss,adh}$ continuously contribute to the particle motion.

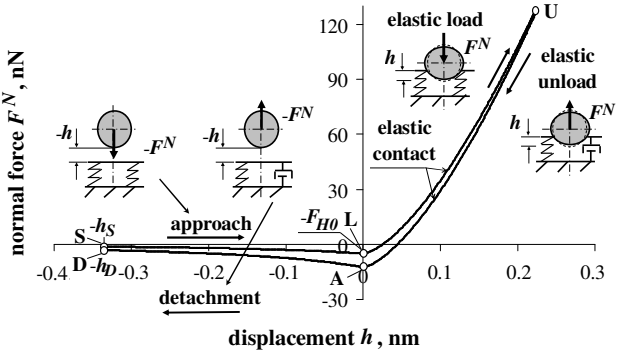

Fig. 2. Adhesive elastic interaction. Energy dissipation related to adhesion

Consequently, new expression of the time-dependent dissipation force is suggested:

$$F_{diss,adh}(t) = F_{diss,adh,W} \cdot \bar{h}(t). \tag{6}$$

The resulting dissipative force is calculated as:

$$F_{diss,adh,W} = 2 \cdot W_{diss,adh} \cdot (a_{F=0} + h_U - h_A)^{-1}. \tag{7}$$

The elaborated linear displacement-dependent dissipation mechanism is characterized by the normalized displacement:

$$\bar{h}(t) = \begin{cases} \dfrac{h_U - h(t)}{h_U - h_A}, & h_U > h(t) > h_A \\ 1, & h_A > h(t) > -h_D \end{cases}. \tag{8}$$

This function allows us to achieve the final energy balance during the interaction that is satisfied by the routine integration of the particle motion between h_U and $-h_D$. It automatically reflects the fact, that the point of unloading h_U is not constant and depends on impact velocity.

Energy Dissipation by Viscous Damping. Dissipation of energy by viscous damping is certainly the most known dissipation mechanism employed in multi-body dynamics and particulate solids. It is velocity-dependent phenomenon and

results into dissipative force. Combined with contact forces, viscous damping yields to hysteric force-displacement behaviour. In our case, viscous damping described by the nonlinear Tsuji model is incorporated by coupling with the elastic and elastic-plastic contact. Consequently, the normal dissipative force for ultrafine particle is expressed as:

$$F_{diss,viscous} = \alpha_d \cdot (m_{eff} \cdot K^N)^{1/2} \cdot h'(h_U) \cdot (\mathrm{d}h/\mathrm{d}t). \quad (9)$$

Here, K^N – nonlinear particle stiffness; $\mathrm{d}h/\mathrm{d}t$ – displacement rate; $h'(h_U)$ – depending on history relative contact displacement; α_d – damping coefficient, m_{eff} – effective mass.

It was earlier observed, that for the nonlinear non-adhesive contact hysteric loop my lead to artificial attractive force which exceeds adhesion limit. The developed viscous damping model is physically correct, after particle detachment it does not form residual displacement, also the adhesion limit not exceeded.

3. Numerical Investigation of Elastic Particle Interaction

The main attention focused on examination of different energy dissipation mechanisms numerical simulation when interaction has elastic contact manner.

The emphasis of this section is to illustrate of the interaction behaviour of elastic particle in of presents adhesion related energy dissipation.

Investigation of Energy Dissipation Mechanisms. The characteristic sample of particle-substrate impact illustrates influence of adhesion related to energy dissipation. Numerical simulations deals with the silica particle $R = 0.6$ μm impact by applying the elastic contact model. The total dissipated energy W_{diss} is assumed to be proportional to absorption energy $W_{diss,abs}$ and controlled by the factor k_H.

This fixed value of dissipated energy $W_{diss,adh,0} = 1.68 \cdot 10^{-18}$ J is defined analytically by $W_{diss,adh} = k_H \cdot F_{H0} \cdot a_{F=0} = k_H \cdot W_{diss,adh,0}$, and is set constant in all simulations. If kinetic energy is not sufficient for the particle rebound, it remains adhered to the substrate. In this case, the dissipated energy determines the threshold of critical sticking velocity v_{cr}. The selected results of the numerical simulation are presented in Fig. 3 by four curves 1–4, corresponding to additional different proportionality factors k_H equal to 10, 100 and 1000, respectively. All curves exhibit similar tendency – with increasing initial interaction velocity the kinetic energy increases, diminishing the influence of absorption energy, while coefficient of restitution converges to $e = 1$ in the limit denoted by the line EL. In summary, the increase of dissipated energy W_{diss} can shift the coefficient of restitution e profile, retaining practically identical

shapes. All the curves are characterised by critical sticking velocities $v_{cr,j}$. Final values of critical velocity also can be obtained analytically $v_{0,cr} = (2 \cdot k_H \cdot W_{diss,adh,0} / m_{eff})^{1/2}$, here $W_{diss,adh,0} = F_{H0} \cdot a_{F=0}$.

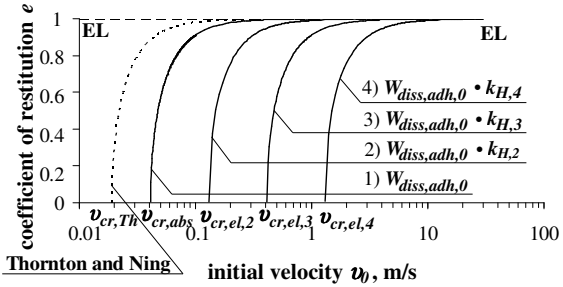

Fig. 3. Variations of coefficient of restitution e depending on initial velocity v_0 at adhesive elastic silica interaction with various values of energy absorption

Additionally, the analytical solution of Thornton and Ning (1998) is shown by the dashed line. The difference between the analytical and numerical solutions stems from the difference in the absorbed energy because Thornton and Ning (1998) used JKR model assuming a lower value of the absorbed energy compared to that of DMT model. Thus, the presented results prove correctness of the suggested dissipation model.

4. Numerical Investigation of Elastic-Plastic Particle Interaction

The main attention focused on examination of different energy dissipation mechanisms numerical simulation of the physical experiment.

Elastic-plastic interaction is considered in the first to illustrate first sample to illustrate contribution of two energy dissipation mechanisms, while the second sample present numerical simulation of the physical impact experiment.

Investigation of Energy Dissipation Mechanisms. The characteristic sample of particle-substrate impact illustrates influence of adhesion and elastic-plastic deformation related to energy dissipation. Numerical simulations deals with the silica particle $R = 0.6$ μm impact by applying the elastic-plastic contact model.

The plasticity properties are defined by the assumed value of plastic micro-yield strength $p_f = 650$ MPa. The simulations are performed similar to those used in elastic calculations with the same elasticity data while the influence of the energy absorption $W_{diss,abs}$ is examined. Numerical results presented in Fig. 4 by four plotted curves 1–4, corresponded to different values of the

adhesive related dissipation energy, additionally defined by factors $k_H = 10, 100, 1000$. Since the particle starts to rebound with purely elastic contact (curve 1 and 2), their values respond to the elastic solution. In other curves 3 and 4, the sticking velocity is affected by plastic deformation.

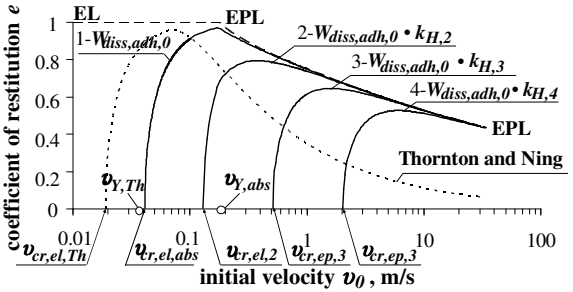

Fig. 4. Adhesive elastic-plastic interaction. Variations of coefficient of restitution e depending on initial velocity v_0 with different absorption energy values

The descending branches of the whole family of curves with increasing values of the absorbed energy converge to a single curve, denoted by the capital letters EPL. This curve related to the specified value of micro-yield strength p_f will be considered as the elastic-plastic limit curve, bounding the values of coefficient of restitution. Curve EPL depends on micro-yield strength and here particle can start to rebound to initial position with restitution $e = 1$ with high p_f and $e = 0$ with small p_f. Whereas additionally dissipation receives from elastic-plastic contact and coefficient of restitution e is smaller, than elastic one. It is observe, that coefficient of restitution decreasing when dissipation increasing.

The analytical solution of Thornton and Ning (1998) is shown by the dashed line just for the sake of comparison. It is obtained using the same data as those used for obtaining curve 1, with the same value of plasticity constant p_f. The shift between the analytical solution and numerically obtained curve 1 is characterised by different velocities $v_{cr,Th}$ and $v_{cr,abs}$, obtained basing on JKR and DMT model respectively.

It is obvious that the numerical results obtained by applying the DMT theory yield higher values of coefficient of restitution e. The difference in the slope of the coefficient of restitution e of the descending part may be explained by the differences in adhesion forces, although plasticity assumptions are not identical either.

Comparison of Numerical and Physical Experiment Results. The developed models were employed for reasonable explanation (Fig. 5) of the impact experiment, conducted with identical silica particles. The collisions

between the silica particles and the fixed silica flat target are observed by optical imaging of the particle trajectories. The values of the coefficient of restitution e extracted from measurements against initial interaction velocities v_0 are taken from Poppe, Blum and Henning (2000, Fig. 5). The rebound of the particles was detected in the range from 0.7 to 40 m/s.

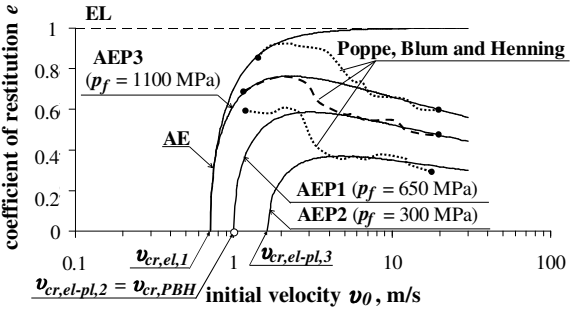

Fig. 5. The variation of coefficient of restitution e versus the initial velocity v_0 in interpreting the experimental results (Poppe, Blum and Henning 2000)

The processed results are presented graphically in terms of three curves. The curves are plotted in the range between 1 up to 30 m/s. the mean values are denoted by a thin dashed line while the lower and upper bounds are shown by dotted lines. The lowest sticking velocity $v_{cr,PBH}$ was equal to 1 m/s.

Conceptually, the numerical experiments described thereafter combine two initially independent dissipation mechanisms related to absorbed energy and plastic deformation. The fixed amount of absorption energy obtained by $W_{diss,adh} = k_H \cdot F_{H0} \cdot a_{F=0}$ is used to envelope the coefficient of restitution e with elastic solution. This specified energy yields the final value $W_{diss,adh} = 0.5 \cdot 10^{-15}$ J elaborated in the below simulations. The solid curve AE in Fig. 5 presents elastic the solution which is interpreted as the envelope of experimental results is converging to elastic limit EL with $e = 1$. It corresponds to minimal rebound velocity $v_{cr,el,1} = 0.71$ m/s and converges to the upper bound of coefficient of restitution with $e = 1$ denoted by line EL.

Elastic-plastic results are illustrated by considering three specified values of the micro-yield strength $p_{f1} = 300$ MPa, $p_{f2} = 650$ MPa and $p_{f3} = 1100$ MPa, respectively. Three solids curves, AEP1, AEP2 and AEP3, present the elastic-plastic solutions. The values of micro-yield strength were selected to illustrate the best fit of experiment at higher initial interaction velocities. It is easy to notice that the character of coefficient of restitution, numerically obtained by

applying the elastic-plastic model, well agrees with the trend observed in experimental results, especially at high velocities.

The obtained sticking velocities also seem to be meaningful. At $p_f = 1100$ MPa, the sticking velocity is the same as elastic $v_{cr,el,1} = 0.71$ m/s, implying that first curve branch is elastic, while the contact is becoming elastic-plastic. The smaller values of plasticity constant leads to increase of dissipation due to plastic deformation and results in increase of the sticking velocity, $v_{cr,el\text{-}pl} \geq v_{cr,el}$.

The developed DEM technique and the results of the numerical tests confirm quantitatively that energy absorption is a dominant source of energy dissipation at lower initial interaction velocities. The plastic deformation-induced dissipation prevails with the increase of initial interaction velocities. It has been proved numerically that the elastic-plastic contact model is formally able to envelope the values of the coefficient of restitution e at higher initial interaction velocities. Enhancing of the knowledge on particle parameters accounting surface roughness or material porosity is necessary to assess the uncertainty of the impact behaviour.

5. Investigation of Sticking Process of Particle System

Investigation of Sticking of Particles System at Adhesive Viscous Elastic-Plastic interaction. Here was investigated cohesive particle system normal interaction with background. Normal interaction investigated without tangential forces and model chosen thread shape.

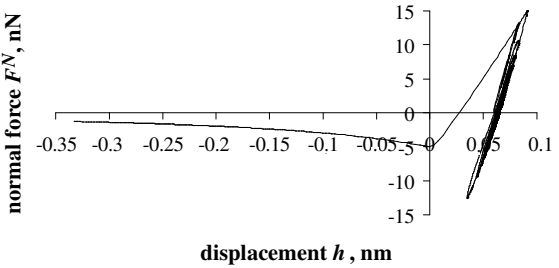

Fig. 6. Adhesive viscous elastic-plastic interaction. Normal force F^N versus displacement h. Micro-yield strength $p_f = 200$ MPa. Damping coefficient $\alpha_d = 2.5$

At initial moment, particles are located at $-a_{F=0}$ distance, while distance between particles are zero and surfaces are in touch. Attraction influence of force at interaction is reason of particle agglomeration, and it is important characteristic of particle mechanical behaviour.

For investigation of particle sticking process was chosen model of 10 particles interaction with background. Mechanical behaviour of adhesive particles basically is different from non cohesive granular material. Because of influence of attractive force at interaction particles stick and form agglomerate.

This is important characteristic of cohesive particles behaviour. Investigated 10 particle system normal interaction model with background. Interacting particles has same characteristics. Particles with initial velocity υ_0 moving toward background. Here for yarn model in Fig. 6 are shown sticking of 10 particles with viscous damping mechanism.

There is shown influence of viscous damping model at elastic interaction. It needed $30 \cdot 10^3$ ns for particle stick. For elastic-plastic model ($p_f = 200$ MPa), duration of sticking process is 10 time longer than elastic interaction.

General Conclusions

1. A theoretical model assessing the specific small-size body effects is proposed and developed for the description of normal interaction between ultrafine spherical particles. The model, employing a concept of the stiff particle with a soft contact, involves adhesive interaction coupled with elastic and elastic-plastic deformation, as well as characteristic energy dissipation mechanisms. Their performance was proved by various numerical experiments and the comparison with the well-known experiment results.

2. Based on the results obtained by numerical testing of three dominant energy dissipation mechanisms, it can be concluded that energy dissipation associated with adhesion becomes decisive at lower initial interaction velocities and predefines particle sticking, while the role of dissipation caused by the accumulation of elastic-plastic deformations grows with the increase of the initial interaction velocity, and this defines the maximum achieved values of the coefficient of restitution.

3. The adhesive elastic interaction of ultrafine particles is characterized by dissipation associated with adhesion governed by a single parameter, as well as by the specified amount of the absorbed energy related to adhesion. In the examination of the results of the numerical impact experiment, it was observed that the value of this parameter predefines the value of the critical sticking velocity. The profile of the ascending branch of the coefficient of restitution, varying against the velocity in the range from 0 to 1 remains of the fixed shape.

4. The adhesive elastic-plastic interaction of ultrafine particles is governed by an additional parameter, the value of micro-yield strength, and is characterized by the coupling of dissipation mechanisms. The increase of the initial interaction velocity results in the occurrence of the descending branch of

the coefficient of restitution. The family of the descending curves, defined for different values of the absorbed energy related to adhesion, converge to a single curve, bounding the values of the coefficient of restitution. By examining the results of the numerical impact experiment of 1.2 μm particle and comparing them with the elastic solution, we could observe that the maximal value of the coefficient of restitution with micro-yield strength 650 MPa was reduced from 1 to 0.95, while, with micro-yield strength 300 MPa, it was reduced even from 1 to 0.6.

5. By considering energy dissipation, related to the adhesion mechanism during the adhesive elastic-plastic interaction, it was observed that when a particle detached with residual displacement, energy dissipation related to adhesion also increased. This shows that the adhesion influence during adhesive elastic-plastic interaction of the particle is stronger than at adhesive elastic interaction.

6. The created viscous damping model is physically correct. After particle detachment it does not form any residual displacement, and the adhesion limit is not exceeded either. It confirms the assumption that the residual displacement may occur only under the influence of the elastic-plastic properties of the particle.

7. In the numerical study of particle's sticking, it was observed that when energy dissipation mechanism related to viscous damping model was applied, particle oscillation had a tendency to decrease. The particles stick together with an overlap, when the normal force and velocity are zero. It could be observed that when viscous damping mechanism was applied to the interaction model, overlap of the stick was independent of the initial velocity during the adhesive elastic interaction, while for the particles with elastic-plastic properties the overlap of the stick increased with the increase of the initial velocity.

8. The simulation approach developed in the present work was employed for reasonable explanation of the results of a physical experiment conducted by Poppe, Blum and Henning (2000) to investigate the impact of the silica particles on the flat silica target. It has been numerically proved that the adhesive elastic-plastic interaction model is able to envelope the scattering of the coefficient of restitution values. Consequently, plastic deformation behaviour of ultrafine silica particles has been confirmed.

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List of Published Works on the Topic of the Dissertation

In the Reviewed Scientific Periodical Publications

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About the Author

Raimondas Jasevičius was born in Širvintos, on 1981.

First degree at Vilnius Gediminas Technical University in Industrial Engineering, Faculty of Mechanics in 2004 and Master of Science in 2006, while in 2006–2010 – PhD student. Raimondas Jasevičius in 2007–2008 was on internship at Otto von Guericke University in Magdeburg, Germany. At present – work in Department of Strength of Materials as research fellow.

ULTRASMULKIŲ DALELIŲ NORMALINĖS SĄVEIKOS SKAITINIS MODELIAVIMAS

Mokslo problemos aktualumas. Ultrasmulkios dalelės yra chemijos, farmacijos, maisto ir kitų pramonės šakų produktų sudėtinė dalis. Tiriant šių produktų technologinius procesus, reikia turėti teorinių žinių apie ultrasmulkias daleles. Fundamentalus supratimas įmanomas atlikus įvairius tyrimus. Pastaruoju metu milteliai, klasifikuojami kaip ultrasmulkios ($0{,}1\ \mu m < d < 10\ \mu m$) dalelės, tapo plačiai naudojami pramoniniuose procesuose, todėl suprasti dalelių elgsenos fundamentalumą miltelių technologijoje yra labai svarbu. Mikroskopinis tyrimas remiasi dalelės sąveika su pagrindu, suvokiant dalelę kaip kūną, turintį mechaninių savybių.

Modeliuojamai ultrasmulkiai dalelei adhezijos poveikis yra reikšminis. Taikant skaitinius modelius bei dalelės judėjimą aprašančias jėgų lygtis, sąveikos modelis apima adhezinę, klampią, tamprią bei tampriai plastinę sąveikas. Dalelės elgsena sąveikos metu priklauso ir nuo sąveikos istorijos. Tokių modelių suvokimas ir pritaikymas šiuolaikinėje mechanikoje yra itin aktualus.

Ultrasmulki dalelė yra itin maža, todėl su ja labai sunku atlikti fizinį eksperimentą, kuris reikalauja specialios įrangos bei žinių. Tokiu atveju dažniausiai naudojamas skaitinis eksperimentas, kurį galima atlikti virtualiai. Toks eksperimentas svarbus tiriant ultrasmulkios dalelės dinamines savybes bei dinaminį uždavinį.

Mikroskopinis adhezinės sąveikos modeliavimas yra aktualus mechanikos mokslo uždavinys. Taikant minėtus modelius, svarbu pritaikyti ir diskrečiųjų elementų metodą. Norint aprašyti ir suprasti dalelių elgseną, reikia tiksliai suvokti ir aprašyti dalelės modelį. Dalelės elgsenos skaitiniam modeliavimui siūlomi teoriniai modeliai leidžia tirti dalelės sąveiką su dalele ar tampria puserdve bei sąveikos dinamiką. Ultrasmulkios dalelės modeliai gali būti pritaikyti ir nano dalelėms modeliuoti.

Ultrasmulkios dalelės tyrimas galėtų būti aktualus sparčiai besivystančiame ultrasmulkių dalelių technologijos (UDT) bei nanotechnologijos moksle (NT), tuo pačiu tai yra indėlis į kontakto mechanikos mokslą.

Tyrimų objektas. Ultrasmulkių dalelių normalinės sąveikos teorinis modelis ir jo taikymas diskrečiųjų elementų metode.

Mokslinis naujumas

Rengiant disertaciją buvo gauti šie mechanikos inžinerijos mokslui nauji rezultatai:

1. Ultrasmulkių sferinių dalelių normalinės sąveikos modelis apimantis adhezinį tamprųjį bei tampriai plastinį kontaktą su šiai sąveikai būdingais energijos sklaidos mechanizmais.

2. Adhezijos mechanizmo, turinčio energijos sklaidos, susietos su poveikio istorija pobūdį, sukūrimas ir realizavimas DEM. Klampaus slopinimo mechanizmo, susieto su poveikio istorija, taikymas dalelės sulipimo procesui aprašyti bei realizavimas DEM.

3. Dalelių sulipimo ir atšokimo sąlygų ir procesų nustatymas, įvertinimas bei aprašymas.

4. Ultrasmulkios silicio dioksido dalelės smūgio į plokščią pagrindą žinomo fizinio eksperimento interpretavimas ir jos savybių apibūdinimas.

Darbo tikslas ir uždaviniai. Suformuluoti ir skaitiškai ištirti ultrasmulkios adhezinės dalelės normalinio sąveikos modelį.

Darbo tikslui pasiekti darbe sprendžiami šie uždaviniai:

1. Suformuluoti ir aprašyti dalelių normalinės adhezinės tamprios bei tampriai plastinės sąveikos fizinius modelius.

2. Įvertinti normalinei adhezinei sąveikai būdingus energijos sklaidos mechanizmus.

3. Taikant sukurtą teorinį modelį, ištirti dalelės atšokimo ir sulipimo procesus ir sąlygas šiems procesams įvykti.

4. Sukurti programinę įrangą ultrasmulkių dalelių normalinei sąveikai tirti DEM.

Tyrimų metodika. Darbe taikomi analiziniai ir skaitiniai metodai. Skaitiniai eksperimentai atlikti taikant diskrečiųjų elementų metodą.

Praktinė reikšmė. Pasiūlytas teorinis modelis parodo galimybę apimti įvairius ultrasmulkių sferinių dalelių normalinei sąveikai būdingus efektus. Sukurta programinė įranga yra skaitinis įrankis tinkamas modeliuoti diskrečiųjų elementų metodu. Jis gali būti panaudotas, kaip didelių sistemų modeliavimui ir technologinės įrangos projektavimui.

Ginamieji teiginiai

1. Sudarytas ultrasmulkių dalelių normalinės sąveikos modelis, kuris įvertina adhezinę tamprią bei tampriai plastinę elgseną, su šiai sąveikai būdingais energijos sklaidos mechanizmais.

2. Paaiškintas atskirų energijos sklaidos mechanizmų vaidmuo, ultrasmulkios dalelės sąveikos metu, kuri apima jos artėjimą ir susidūrimą su pagrindo paviršiumi, esant įvairiems pradiniams sąveikos greičiams.

3. Skaičiavimai parodė, kad fizinio eksperimento su SiO_2 dalelėmis rezultatai galimi tik dalelėms deformuojantis plastiškai.

Darbo rezultatų aprobavimas. Disertacijos tema perskaityti septyni pranešimai Lietuvos bei kitų šalių konferencijose ir paskelbti septyni straipsniai.

Darbo struktūra ir apimtis. Darbą sudaro įvadas, 5 skyriai, išvados, literatūros sąrašas, autoriaus publikacijų sąrašas. Bendra disertacijos apimtis – 124 puslapiai, 102 numeruotos formulės, 48 iliustracijos ir 2 lentelės. Pirmasis skyrius skirtas literatūros apžvalgai. Jame pateikti disertacijos tema atliktų mokslininkų darbai. Skyriaus pabaigoje formuluojamos išvados ir disertacijos uždaviniai. Antrajame skyriuje pateikiami sudaryti ultrasmulkios dalelės teoriniai sąveikos modeliai. Taikant šiuos modelius, trečiajame ir ketvirtajame skyriuose aprašomas tamprios bei tampriai plastinės dalelės normalinės sąveikos skaitinis eksperimentas, tiriami energijos sklaidos mechanizmai, taikant diskrečiųjų elementų metodą. Penktame skyriuje tiriama dalelių sistemos normalinė sąveika.

Bendrosios išvados

1. Ultrasmulkių dalelių normalinei sąveikai aprašyti pasiūlytas naujas standžios dalelės su minkštu kontaktu teorinis modelis, kuris įvertina mažų matmenų kūnui būdingus efektus. Šis modelis apima adhezinę sąveiką su tampriu ir tampriai plastiniu deformavimu bei energijos sklaidos mechanizmus. Jo veikimas patikrintas, atliekant įvairius skaitinius eksperimentus ir palygintas su žinomais rezultatais.
2. Skaitiškai ištyrus energijos sklaidai būdingus mechanizmus, galima teigti, jog energijos sklaida, siejama su adhezija, lemia dalelės prilipimą prie pagrindo bei dalelių sulipimą tarpusavyje. Dalelės plastinės savybės lemia energijos sklaidos didėjimą, taip pat atsistatymo koeficiento mažėjimą didėjant pradiniam greičiui bei apibrėžiant didžiausias pasiektas atsistatymo koeficiento reikšmes.
3. Energijos sklaida, esant tampriam dalelės kontaktui, apibrėžiama tik vienu rodikliu – adhezinės sąveikos metu sugertu energijos kiekiu. Skaitiniai eksperimentai parodė, kad būtent šio rodiklio reikšmė lemia kritinį sulipimo greitį. Tuo tarpu atsistatymo koeficiento priklausomybės nuo pradinio sąveikos greičio pobūdis visame intervale nuo 0 iki 1 nuo išsklaidytos energijos kiekio nepriklauso.
4. Adhezinė tampriai plastinė sąveika apibūdinama dviejų energijos sklaidos mechanizmų sąsaja, kurią lemia dalelės mikrotakumo įtempis. Priklausomybė nuo pradinio sąveikos greičio, esant skirtingos sudėties energijoms, konverguoja į ribinę kreivę, kurios pobūdį lemia mikrotakumo įtempio reikšmės. Didėjant pradiniam sąveikos greičiui atsistatymo koeficientas pradeda mažėti. Lyginant su tampriąja sąveika pastebėta, kad kai mikrotakumo

įtempio reikšmė yra 650 MPa, maksimali atsistatymo koeficiento reikšmė sumažėja nuo 1 iki 0,95, o esant mikrotakumo įtempio reikšmei 300 MPa, atsistatymo koeficiento reikšmė sumažėja nuo 1 iki 0,6.

5. Taikant sudarytą energijos sklaidos, siejamos su adhezija, mechanizmą esant tampriai plastinei sąveikai, pastebėta, jog lyginant su adhezine tampria sąveika, dalelei atsiskyrus su liekamuoju poslinkiu ir padidėjus atsiskyrimo atstumui, su adhezija siejama energijos sklaida yra didesnė. Liekamasis poslinkis ir su adhezija siejama energijos sklaida didėja, didėjant pradiniam sąveikos greičiui. Tai įrodo, jog adhezijos poveikis plastinių savybių turinčiai dalelei yra stipresnis.

6. Pasiūlyta sąveika papildomai veikiant klampiajam slopinimui yra suderinta su adhezinėmis savybėmis, kadangi adhezijos riba neviršijama, o atsiskyrusios dalelės liekamasis poslinkis susidaro tik dėl plastinio deformavimo.

7. Skaitiškai ištyrus dalelės sulipimo procesą pastebėta, jog įvertinus energijos, siejamos su klampiu slopinimu, sklaidą sulipimo proceso metu, dalelės svyravimai yra gęstančio pobūdžio. Dalelė prilimpa prie pagrindo bei dalelės sulimpa tarpusavyje su persiklojimu, kai sąveikos metu normalinė jėga ir greitis yra lygūs nuliui. Pastebėta, jog įvertinus klampų slopinimą, esant tampriai sąveikai, sulipimo poslinkis nuo pradinio greičio nepriklauso. Tuo tarpu tampriai plastinių savybių turinčios dalelės sulipimo persiklojimas turi tendenciją didėti, mažėjant mikrotakumo įtempiui bei didėjant pradiniam sąveikos greičiui.

8. Sudarytas modelis buvo pritaikytas žinomam silicio dalelės smūgio į pagrindą eksperimento (Poppe, Blum, Henning 2000) rezultatų išsibarstymui paaiškinti: eksperimento skaitinis modeliavimas parodė, kad eksperimento rezultatų gaubtines galima sudaryti kombinuojant įvairius sudarytus energijos sklaidos mechanizmus. Interpretuojant rezultatus galima teigti, kad atsistatymo koeficiento mažėjimą, esant dideliam sąveikos greičiui, nulemia plastinių deformacijų silicio dioksido dalelėje susidarymas.

Trumpos žinios apie autorių

Raimondas Jasevičius gimė 1981 m. Širvintose. 2004 m. įgijo pramonės inžinerijos bakalauro laipsnį, 2006 m. įgijo pramonės inžinerijos mokslo magistro laipsnį Vilniaus Gedimino technikos universiteto Mechanikos fakultete, 2006–2010 m. – universiteto doktorantas. Raimondas Jasevičius 2007–2008 m. stažavosi Otto von Guericke Magdeburgo universitete Vokietijoje. Šiuo metu dirba VGTU jaunesniuoju mokslo darbuotoju Medžiagų atsparumo katedroje.

Raimondas JASEVIČIUS

THE NUMERICAL MODELLING OF NORMAL INTERACTION OF ULTRAFINE PARTICLES

Summary of Doctoral Dissertation
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Vilniaus Gedimino technikos universiteto
leidykla „Technika“,
Saulėtekio al. 11, LT-10223 Vilnius,
http://leidykla.vgtu.lt
Spausdino UAB „Ciklonas“,
J. Jasinskio g. 15, 01111 Vilnius,
http://www.ciklonas.lt