JOURNAL OF THEORETICAL AND APPLIED MECHANICS
44, 3, pp. 637-648, Warsaw 2006

INNOVATIVE MODELING METHODS IN DAMAGE ASSESSMENT: APPLICATION OF DISSIPATIVE PARTICLE DYNAMICS TO SIMULATION OF DAMAGE AND SELF-HEALING OF POLYMER-COATED SURFACES

Aleksandar S. Jovanovic

University of Stuttgart/Steinbeis University Berlin, Germany
e-mail: jovanovic@risk-technologies.com

Nenad Filipovic

University of Kragujevac, Serbia
e-mail: filipovic@risk-technologies.com

The paper presents an exemplary application of an innovative modeling technique (Dissipative Particle Dynamics – DPD) as a possible tool for multi-scale modeling of the behavior of advanced engineering materials (e.g. coated materials and/or multi-materials). The multi-scale modeling of the behavior of advanced engineering materials is primarily related to development of new techniques and methods needed to bridge the gap between the atomistic scale and macro applications. The presented example of examination of the applicability of the DPD to damage assessment dealing with the problem of interaction of particles, polymers and surfaces, is an issue concerning many applications in the colloid science. It has confirmed the applicability of the DPD as a method for linking the macro and atomistic scales. The imminent application of the method and the example are in the area of "self-healing" advanced engineering materials, thus in line with the objectives of EuMaT (cf. Appendix).

Key words: modeling, engineering materials, self-healing

1. Introduction

Many practical issues in the colloid science concern interactions of particles, polymers, and surfaces. The technique of Dissipative Particle Dynamics (DPD) has been initially implemented to problems of controlling the effects of soot

and deposition (e.g. in diesel engine lubricants or surface fouling in chemical reactors), but now it is also a suitable alternative technique for simulating hydrodynamic behavior of other colloid-polymer-solvent systems. Hoogerbrugge and Koelman (1992) suggested a new Dissipative Particle Dynamics (DPD) approach to simulate flow fields of incompressible complex fluids. A fluid is divided into mesoscale particles so that each particle contains a large number of molecules but is still much smaller than dimensions of the containing vessel. Based on concepts prevalent in Molecular Dynamics (MD) theory, a Langevin equation was postulated by which motion of the fluid particles can be calculated. The forces exerted on every particle by its neighbors that are within a prescribed distance r_c (radius of influence) from it, are normally divided into three categories; conservative repulsive forces that can be derived from a potential function, dissipative forces that stem from viscous friction generated by relative translational motion of adjacent particles, and random forces that may be significant due to the mesoscale dimension of the particles.

One of the controversial, unsettled aspects in DPD modeling relates to the formulation of proper no-slip conditions near a rigid wall. The Lees-Edwards method (Lees and Edwards, 1972) in essence, circumvented the problem of how to avoid particles that can both penetrate and slide along rigid walls. Their ingenious suggestion that worked quite well for Couette flows, in which particles penetrating one wall should be reintroduced at the other wall, can hardly be qualified as a condition that should be applied *locally* at any rigid wall in more complex flow systems. A more advanced suggestion was to freeze the regions of fluid near the rigid wall (Hoogerburgge and Koelman, 1992; Boek *et al.*, 1996). This, however, resulted in possible particle penetration through the walls due to a 'soft' conservative potential (Revenga *et al.*, 1998). To avoid such non-physical results, various methods were suggested that combine the freezing particle layer near the wall with specular, bounce-back or Maxwellian reflection of a particle reaching a rigid wall (e.g., Hoogerburgge and Koelman, 1992; Revenga *et al.*, 1998). More recently, Pivkin and Karniadakis (to be published) suggested combining the above with an augmented conservative force at the rigid wall.

Flekkoy and Coveney (1999), and in particular Flekkoy *et al.* (2000) suggested linking DPD and Molecular Dynamics (MD) equations that govern motion of mesoscopic and molecular size particles, respectively (a bottom-up strategy). However, reaching closure still required defining constitutive relations prevailing at the continuum level (top-down strategy). Thus, the friction coefficient was linked to the dynamic viscosity η of a Newtonian fluid perceived as a continuum and the ratio between the intersection length and

distance between two interacting Voronoi cells. In this article, we adopt the strategy initiated by Hoogerbrugge and Koelman (1992) and further developed by Espanol and Warren (1995) and Espanol (1998), namely, that the DPD equations governing motion of identical mesoscopic particles, are postulated.

2. DPD model

During more than a decade, a considerable number of articles focused on the proper formulation of constitutive equations governing different forces and how their *a priori* unknown parameters are related to known phenomenological coefficients of a given fluid. A widely accepted formulation for equations of motion of a DPD particle (e.g. Espanol and Warren, 1995; Groot and Warren, 1997; Novik and Coveney, 1997; Besold *et al.*, 2000; Pivkin and Karniadakis, to be published) has the following form

$$\begin{aligned} d\boldsymbol{r}_i &= \boldsymbol{v}_i dt \\ d\boldsymbol{v}_i &= \sum_{j\neq i} \boldsymbol{F}_{ij} dt = \sum_{j\neq i} (\boldsymbol{F}^C_{ij} dt + \boldsymbol{F}^D_{ij} dt + \boldsymbol{F}^R_{ij} d\sqrt{t}) \end{aligned} \tag{2.1}$$

where $d\boldsymbol{r}_i$ and $d\boldsymbol{v}_i$ are infinitesimal displacement and velocity changes measured relative to a Galilean coordinate system, that the particle i undergoes during the time increment dt. The forces $\boldsymbol{F}^C_{ij}$, $\boldsymbol{F}^D_{ij}$ and $\boldsymbol{F}^R_{ij}$ are conservative (repulsive), dissipative and random forces (per unit mass of particle i) that the particle j exerts on the particle i, respectively, provided that the particle j is within the radius of influence r_c of the particle i

$$\begin{aligned} &\boldsymbol{F}^C_{ij} = a_{ij}\Big(1 - \frac{r_{ij}}{r_c}\Big)\boldsymbol{e}_{ij} \qquad\qquad \boldsymbol{F}^D_{ij} = -\gamma\Big(1 - \frac{r_{ij}}{r_c}\Big)^2 (\boldsymbol{v}_{ij}\cdot\boldsymbol{e}_{ij})\boldsymbol{e}_{ij} \\ &\boldsymbol{F}^R_{ij} = \sqrt{2k_B T\gamma}\, m_i \Big(1 - \frac{r_{ij}}{r_c}\Big)\xi_{ij}\boldsymbol{e}_{ij} \end{aligned} \tag{2.2}$$

Here, a_{ij} is the maximum repulsion force per unit mass, r_{ij} is the distance between the particles i and j, $\boldsymbol{e}_{ij}$ is a unit vector pointing in the direction from j to i, $\boldsymbol{v}_{ij} = \boldsymbol{v}_i - \boldsymbol{v}_j$ is the velocity of the particle i relative to that of the particle j, m_i is the mass of the particle i, γ stands for the friction coefficient, k_B is the Boltzmann constant, T is the equilibrium temperature and ξ_{ij} is a random number with zero mean and unit variance. In the case $r_{ij} > r_c$, the particle j is assumed to exert no force on the particle i. Notice

that the conservative, dissipative and random forces that the particle j exerts on the particle i were assumed to depend upon the distance between these particles. The dissipative force also depends upon a single component of the relative velocity between the particles $(\boldsymbol{v}_{ij} \cdot \boldsymbol{e}_{ij})$, and that the direction of all the foregoing forces is along the line connecting the centers of two particles.

If we define the following dimensionless variables

$$\widehat{\boldsymbol{r}}_i = \frac{\boldsymbol{r}_i}{r_c} \qquad \widehat{r}_{ij} = \frac{r_{ij}}{r_c} \qquad \widehat{\boldsymbol{v}}_{ij} = \frac{\boldsymbol{v}_{ij}}{v_T} \qquad \widehat{t} = \frac{t v_T}{r_c} \tag{2.3}$$

where $v_T = \sqrt{k_B T / m_i}$ is the thermal velocity of the particle i, equation (2.1) can thus be expressed in the following dimensionless form

$$\begin{aligned} d\widehat{\boldsymbol{r}}_i &= \widehat{\boldsymbol{v}}_i d\widehat{t} \\ d\widehat{\boldsymbol{v}}_i &= \sum_{j \neq i} \frac{a_{ij} r_c}{v_T^2}(1 - \widehat{r}_{ij}) \boldsymbol{e}_{ij} d\widehat{t} - \frac{\gamma r_c}{v_T}(1 - \widehat{r}_{ij})^2 (\widehat{\boldsymbol{v}}_{ij} \cdot \boldsymbol{e}_{ij}) \boldsymbol{e}_{ij} d\widehat{t} + \\ &\quad + \sqrt{\frac{2\gamma r_c}{v_T}}(1 - \widehat{r}_{ij}) \xi_{ij} \boldsymbol{e}_{ij} d\sqrt{\widehat{t}} \end{aligned} \tag{2.4}$$

In the case when all particles have identical masses and all coefficients a_{ij} are equal, Eq. (2.4) depends on two dimensionless numbers only

$$\widehat{a} = \frac{a_{ij} r_c}{v_T^2} \qquad \widehat{\gamma} = \frac{\gamma r_c}{v_T} \tag{2.5}$$

Thus, there is no need to assume that the trio; i.e. the mass of a particle m, $k_B T$ and r_c are all unity, which has been an assumption made in many previous studies. It is sufficient to assume that v_T and r_c are equal to one and to vary γ and a_{ij} in order to obtain different DPD fluids. This would be equivalent to setting numerical values to the dimensionless variables $\widehat{a}$ and $\widehat{\gamma}$.

The boundary conditions would introduce at least two additional dimensionless parameters

$$\widehat{L} = \frac{L}{r_c} \qquad \widehat{V}_W = \frac{V_W}{v_T} \tag{2.6}$$

where L and V_w scale the macroscopic size of the system and the velocity of its wall, respectively.

More recently, Espanol (1998) suggested that additional components to dissipative and concomitant random forces be added. These included force components perpendicular to $\boldsymbol{e}_{ij}$ and the effect of particle rotation. The former is a natural extension based on simple tensorial considerations and the

latter stems from the finiteness of the particles. Based on MD theory, Flekkoy and Coveney (1999) and Flekkoy *et al.* (2000) concluded that forces which are not collinear with $\boldsymbol{e}_{ij}$ exist at the DPD mesoscale. These modifications, however, have not thoroughly been tested, and their contribution to the solution accuracy is awaiting further exploration.

3. DPD simulation model

The simulations are conducted in a three-dimensional simulation box, as shown in Fig. 1. A wall of frozen particles is created at one end providing the surface.

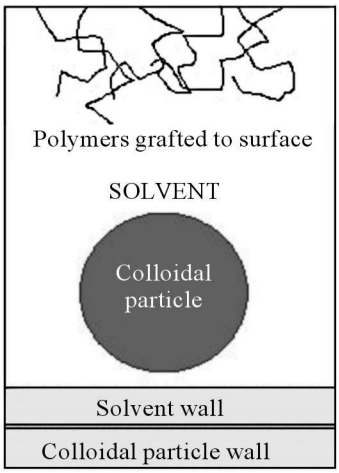

Fig. 1. DPD model for adsorption of colloidal particles

Although the surface of the wall is square, the periodic boundary conditions make it appear infinite. Polymers are then attached, effectively "chemically grafted," to this wall. A rough spherical object is created at a given distance from the wall to simulate a colloidal particle. The box is filled with DPD particles which represent the solvent. The wall is divided into two ones along a plane parallel to the wall-fluid interface. The half to which the polymers are attached is made up of particles identical to those which make up the colloidal particle, while the other half is made up of solvent particles. These solvent particles ensure that the colloidal particle can only reach the wall, and hence adsorb onto its surface by traveling through the layer of polymers. Another type of the structure is a polymer (Fig. 2). Here, a bead-and-spring type model

is used to provide an additional force between adjacent particles in the chain. A Fraenkel spring is mainly used

$$\boldsymbol{F}_{ij}^{p} = k(r_{ij} - r_{eq})\widehat{\boldsymbol{e}}_{ij} \tag{3.1}$$

where k is the spring constant and r_{eq} is the equilibrium spring length.

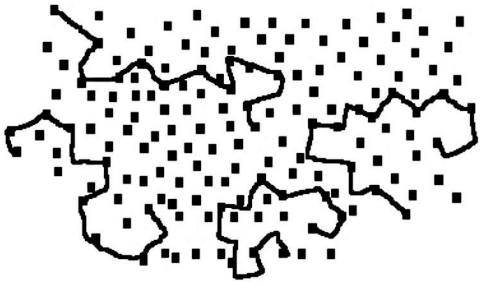

Fig. 2. Example of polymer chains

4. Results

The adsorption has been defined with the spring constant $k = 50\,\mathrm{N/m}$. The snapshot with the distribution of colloidal particles and solvent particles after 0.1 s is presented in Fig. 3. Grey dots represent colloidal Voronoi elements, darker dots represent solvent Voronoi elements. Our results closely matched those experimentally and numerically recorded by Gibson *et al.* (1998) as it is shown in Fig. 4.

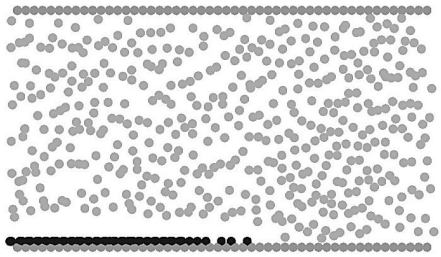

Fig. 3. Snapshot after 0.1 s of colloidal particle adsorption

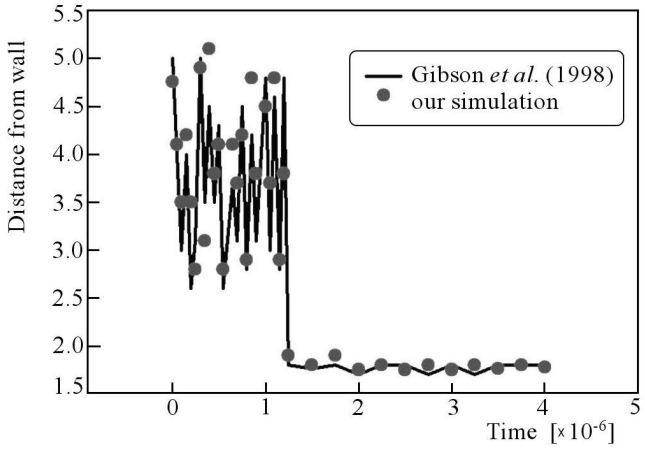

Fig. 4. Comparison of results for colloidal particle adsorbtion

5. Discussion and conclusions

The simulation and modeling of material behavior and degradation mechanisms, dependence of material structure on manufacturing methods and manufacturing processes, is a prerequisite for the design of materials and manufacturing method as well as for the evaluation of life cycle performance. The simulation example presented here shows that the DPD model is potentially a very useful tool for simulation of the adsorption process on coated surfaces.

The imminent application of the method and the example are in the area of "self-healing" advanced engineering materials. The method presented in the paper allows doing it up to the point of calculating the probability of deposition as a function of a system of interaction of particles, polymers and surfaces. In that sense, the DPD modeling can be used for non-invasive repair of damaged coatings (Fig. 5).

A significant step and the desirable direction of further work in the area of DPD-based damage modeling and analysis would be the research on "intelligent repair materials" (Jovanovic and Jovanovic, 2006). Corresponding theoretical considerations are already available (Zomaya, 2006), and when combined with the available modeling techniques (Fig. 6) could significantly improve the current practice in terms of (a) costs, (b) reduced total effort of repair and (c) significantly less intrusive character of the repair, which can be decisive for certain types of applications.

The ideal situation would be simulation of the total life cycle. This requires a combination of several research activities which are separated today. For

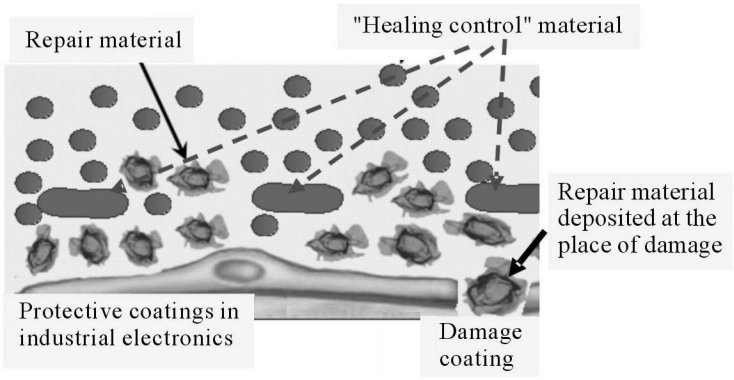

Fig. 5. Deposition of the repair material at the damaged coating

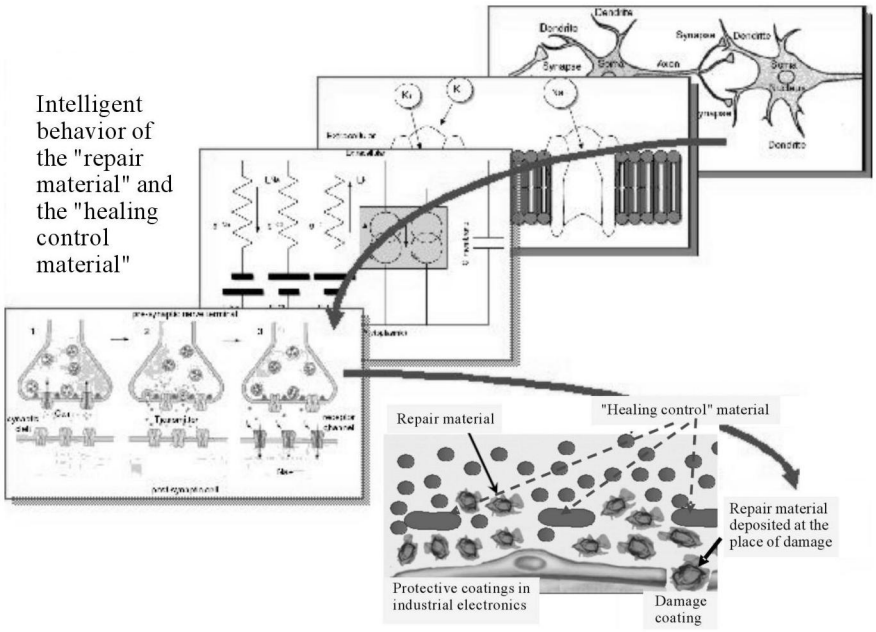

Fig. 6. Practical steps in the development of intelligent repair materials (Jovanovic and Jovanovic, 2006; Zomaya, 2006)

many engineering materials, the correlation of a microstructure with technical properties, e.g. creep, is known. However, the modeling of a manufacturing process to achieve the optimum microstructure is in infancy. Engineers use material data to predict lifetime of components. However, because of non-existing correlation between the microstructure and material data, safety factors are

included which will not exploit the potential of engineering materials. Therefore, the vision is to develop a virtual manufacturing chain with an optimized technology of materials and low scatter output.

Appendix – Mesoscale damage analysis and modeling in the future European research (EuMaT)

The main practical policy objective of EuMaT (European Technology Platform of Advanced Engineering Materials and Technologies) is to assure optimum involvement of industry and other important stakeholders in the process of establishing European R&D priorities in the area of advanced engineering materials and technologies (Jovanovic, 2005). EuMaT should improve coherence in existing and forthcoming EU projects, and introduce "Radical Changes" and assure "Sustainable Development" in the sector of advanced engineering materials and related technologies (Jovanovic, 2006). Damage analysis and damage modeling, including their application to phenomena of self-healing materials and structures are among the key factors for achieving some of the main overall performance targets of EuMaT envisaged for 2030, like for instance:

- helping to reduce life-cycle costs of the process equipment and infrastructure by 30% and energy consumption by 50% (more efficient materials)
- increase productivity of assets by reducing downtime by 25% (more reliable materials)
- protect the environment by containing processes (e.g. by recycling 95% of metallic and 70% on average of other advanced engineering materials at the end of their useful life)
- capture the existing knowledge and effectively train a future workforce and develop capability and capacity to develop a new generation of materials.

Innovative damage assessment and modeling of advanced engineering materials are important also for EuMaT "horizontal" and "life-cycle issues" (Fig. 7) like simulation, testing, inspection, monitoring, characterization, standardization and qualification of materials and manufacturing processes, prediction of in-service behavior/characteristics and failure criteria, risk and impacts of new materials, training and education issues.

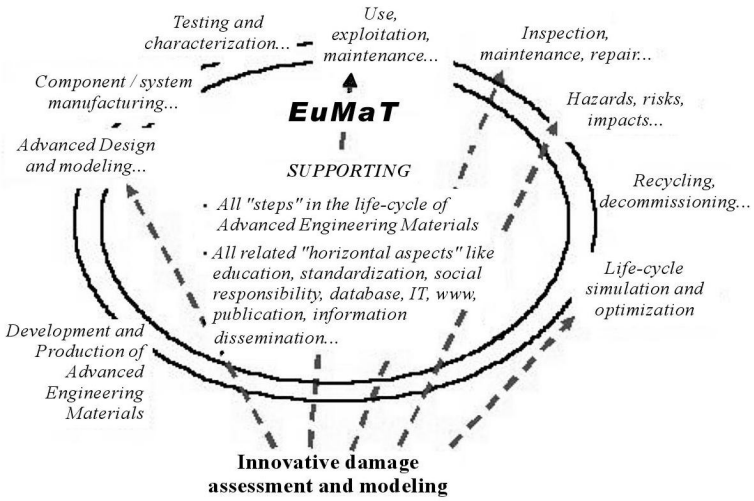

Fig. 7. Place of innovative damage assessment and modeling for advanced engineering materials in the EuMaT "life cycle oriented" approach

The multi-scale modeling of the behavior of advanced engineering materials is one of the five "pillars" of EuMaT (Fig. 8). In EuMaT it is primarily related to development of new techniques and methods needed to bridge the gap between the atomistic scale and macro applications.

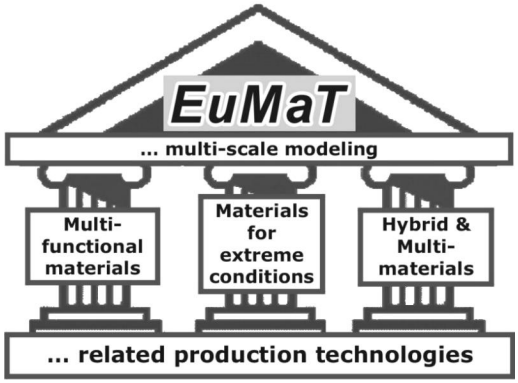

Fig. 8. Five priorities ("pillars") of EuMaT

Acknowledgement

This study was partly supported by the Humboldt Fellowship Program IV – SER/1114337 STP hosted by Steinbeis University Berlin/Stuttgart.

References

1. BESOLD G., VATTULAINEN I., KARTTUNEN M., POLSON J.M., 2000, Toward better integrators for dissipative particle simulations, *Phys. Rev. E*, **62**, 6, R7611-R7614
2. BOEK B., COVENEY P., LEKKERERKER H., VAN DER SCHOOT P., 1997, Simulating the rheology of dense colloidal suspensions using dissipative particle dynamics, *Phys. Rev. E*, **55**, 3124- 3133
3. ESPANOL E., 1998, Fluid particle model, *Phys. Rev. E.*, **57**, 2930-2948
4. ESPANOL E., WARREN P., 1995, Statistical mechanics of dissipative particle dynamics, *Europhys. Lett.*, **30**, 4, 191-196
5. FLEKKOY E.G., COVENEY P.V., 1999, From molecular dynamics to dissipative particle dynamics, *Phys. Rev. Lett.*, **83**, 1775-1778
6. FLEKKOY E.G., COVENEY P.V., DE FABRITIIS G., 2000, Foundations of dissipative particle dynamics, *Phys. Rev. E.*, **62**, 2140-2157
7. GIBSON J.B., ET AL., 1998, Simulation of particle adsorption into a polymer-coated surface using the Dissipative Particle Dynamics Method, *J. Colloid Interface Sci.*, **206**, 464-482
8. GROOT R.D., WARREN P.B., 1997, Dissipative particle dynamics: bridging the gap between atomistic and mesoscopic simulation, *J. Chem. Phys.*, **107**, 4423-4435
9. HOOGERBURGGE P.J., KOELMAN J.M., 1992, Simulating microscopic hydrodynamic phenomena with dissipative particle dynamics, *Europhys. Lett.*, **19**, 3, 155-160
10. JOVANOVIC A., 2005, EuMaT: The European technology platform for advanced engineering materials and technologies – status and prospects, *Plenary lecture at the E-MRS Conference 2005*, Strasbourg, France
11. JOVANOVIC A., 2006, *EuMaT – Materials for Life Cycle, The Roadmap document of the European Technology Platform for Advanced Engineering Materials and Technologies*, EuMaT Consortium, Published by MPA Stuttgart, Germany
12. JOVANOVIC A., JOVANOVIC S., 2006, Needs of industry in the area of technology transfer and practical implementation, *Plenary lecture at the NiSIS* (Nature-Inspired Smart Information Systems), Brainstorming meeting June 2006, NiSIS Consortium, www.nisis.de
13. LEES A.W., EDWARDS S.F., 1972, The computer study of transport processes under extreme conditions, *J. Phys. C*, **5**, 1921-1926
14. NOVIK K.E., COVENEY P.V., 1997, Using dissipative particle dynamics to model binary immiscible fluids, *Int. J. Mod. Phys. C*, **8**, 4, 909-918

15. REVENGA M., ZUNIGA I., ESPANOL P., PAGONABARRAGA I., 1998, Boundary models in DPD, *Int. J. Mod. Phys. C*, **9**, 1319-1331

16. PIVKIN I.V., KARNIADAKIS G.E., 2005, A New Method to Impose No-Slip Boundary Conditions in Dissipative Particle Dynamics, www.dam.brown.edu/scicomp/publications/Reports/Y2005/BrownSC-2005-02.pdf

17. ZOMAYA A.Y. (EDIT.), 2006, *Handbook of Nature-Inspired and Innovative Computing Integrating Classical Models with Emerging Technologies*, Springer Science, Business Media, Inc.

Innowacyjne metody modelowania w szacowaniu zniszczenia. Zastosowanie dynamiki dyssypatywnego układu punktów materialnych do symulacji zniszczenia samonaprawiających się powierzchni pokrywanych polimerami

Streszczenie

W artykule zaprezentowano przykładową aplikację innowacyjnej techniki modelowania DPD (*Dissipative Particle Dynamics* – dynamika dyssypatywnego układu punktów materialnych) jako możliwego narzędzia do wielo-skalowego modelowania zachowania się zaawansowanych materiałów inżynierskich (z pokryciami wierzchnimi, lub wieloskładnikowych). Modelowanie wielo-skalowe jest związane głównie z rozwojem nowych metod badawczych potrzebnych w opisie zjawisk przy przechodzeniu od poziomu atomistycznego do makroskali. Przedstawiona analiza przydatności metody DPD w szacowaniu zniszczenia zawierającego problem oddziaływania cząstek materiału, polimerów i powierzchni elementów stanowi przykład aplikacji nauki o koloidach. W pracy potwierdzono stosowalność DPD w efektywnym łączeniu makroskali z poziomem atomistycznym. Spodziewane zastosowania zaprezentowanej metody i omówiony przykład wchodzą w zakres zaawansowanych technologii samonaprawiających się materiałów, których rozwój jest konsekwencją wytycznych EuMat (w Dodatku).

Manuscript received May 10, 2006; accepted for print June 2, 2006