# COMPUTER-AIDED SIMULATION OF MATERIAL LOCAL FRACTURE EFFECTS AT THE AREA OF TRIBOLOGICAL CONTACTS ON THE BASE OF METHODS OF DISCRETE APPROACH

H.Kloss[1], E.Santner[1], A.I.Dmitriev[2], E.V.Shilko[2]
[1]Federal Institute of Materials Testing and Researching, D-12203, Berlin Germany
[2]Institute of Strength Physics and Materials Science SB RAS, Tomsk, 634021 Russia

## ABSTRACT

For deep understanding of elementary acts of friction and wear of mechanical systems it is necessary to have an ability to precisely describe material behaviour under external tangential and normal forces. Methods of computer-aided simulation can be useful for this aim. Due to choosing of methods of numerical approach it is necessary to take into account that friction and wear are accompanied by intensive processes of discontinuity formation, damage generation and accumulation. Moreover contact formation its development and fracture are taking place at nano and micro levels. In the paper modelling of contact area at atomic- and meso-scale levels was carried out on the base of discrete computational approach (method of particles). Molecular dynamic method was used at micro level, movable cellular automata method – at nano-scale level. Movable cellular automata (MCA) method provides the necessary information about response of different homo- and heterogeneous materials, composites and layers under uniaxial compression, indentation and sliding conditions. Due to mobility of the separate automata the MCA method allows to simulate different processes ongoing in the real materials during impact, beam bending, friction and wear, e.g. formation and accumulation of damages, grinding and penetration effects, fracture processes, fragmentation, formation of pores and cracks. Because of the possibility of the MCA method to choose the scale of simulation, the results of MCA simulation can help to understand elementary processes under impaction of normal and tangential forces.

In the paper using metallic and ceramic bulk materials two-dimensional and three-dimensional computer simulations in framework of MCA based software for indentation and sliding (scratch) tests was carried out. Results of simulation have shown quite good agreement with experimental data and analytical solutions. Computer simulation has shown that MCA method is applicable for investigation of indentation, sliding, friction and wear phenomena. Note, that some results are more qualitatively and be use as a way to improve the MCA method in future. For that propose also more experimental test of material response on varying scales of stress and contact dimensions are needed.

## 1 INTRODUCTION

Tribology is an interdisciplinary and relative complex science and its basics are still under development and discussion. In general, surface interactions are associated with material properties, contact conditions and are resulting in energy dissipation (friction) and material loss (wear). The use of simulation techniques (FEM, MD, MCA), interest in new nanotechnologies and the development of scanning probe techniques has led to a renaissance in fundamental areas of tribology. It became possible to study surface interactions, friction and wear at atomic-scale on the basis of elementary processes.

The understanding of the elementary processes at friction and wear is one aspect of modern tribology. The choice, development and improvement of materials for advanced applications by modelling and experimental testing is an other aspect.

Experimental testing is often material and time consuming and very expensive. Theoretical modeling can be used instead as a helpful tool for material choice and performance prediction. In the present paper the potential of the MCA method as a simulation tool is described (Psakhie [1 – 3], Kloss [4]). According to this method, a medium is represented as an ensemble of discrete elements – movable cellular automata – characterized by continuous variables such as mass centre, value of plastic deformation, rotation pseudo-vector as well as by the discrete variables characterizing strength of cohesion between the neighbouring automata. The principles of derivation of the equation of motion for system of cellular automata and prescribing interactions between them are described in Popov [5]. Due to unique capabilities MCA method allows one to simulate formation and accumulation of damages, grinding and penetration effects, fracture processes, fragmentation, formation of pores and cracks, simulation of friction and wear.

MCA simulations of indentation and sliding phenomena are presented in this paper to test this new software for the prediction of tribological behavior.

## 2 INDENTATION, BENDING AND IMPACT

Fig. 1 shows 3D simulation results from circular punch indentation tests. Material properties for specimen and task geometry are summarised in Fig. 2.

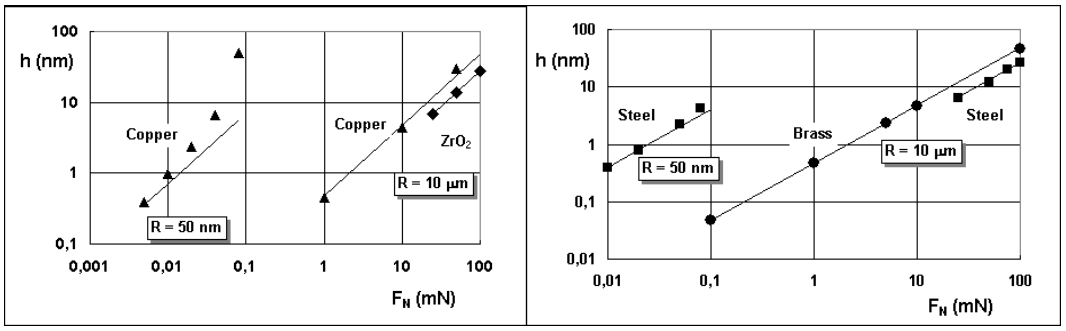



Figure 1: 3D simulation: circular punch (diamond, E = 1140 GPa, ν = 0,07) radius of punch: 50 nm and 10 µm, lines: analytical solution

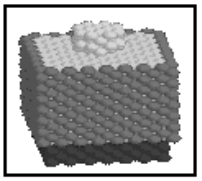
| | $ZrO_2$ | Copper | Steel | Brass | Geometry |
|---|---|---|---|---|---|
| E (GPa) | 200 | 107,6 | 206 | 104 |  |
| ν | 0,3 | 0,254 | 0,28 | 0,32 | |
| $\sigma_y$ (MPa) | 1000 | 34,5 | 541 | 393 | |
| $\sigma_t$ (MPa) | 1000 | 423,5 | 920 | 552 | |
| ε_t | 0,005 | 0,033 | 0,097 | 0,081 | |

Figure 2: Material properties und 3D task geometry

The selected materials are different in young modulus E, yield stress $\sigma_y$, tensile stress $\sigma_t$ and tensile strain ε_t. The indentation depth – force curves are linear in the elastic part. Therefore, the relationship relating to the curves is given by Sneddon [6]:

$$h = \frac{F_N}{2E^* R} \qquad \text{with} \qquad \frac{1}{E^*} = \frac{1-n_1}{E_1} + \frac{1-n_2}{E_2}, \tag{1}$$

were $F_N$ is the normal force, $E^*$ is the reduced young modulus, $R$ is the radius of contact area and $h$ is the indentation depth.

The MCA simulation results shoe a good agreement with the analytical solution. At higher loads, elastic-plastic deformations and cracks determine the non-linear behaviour, which are not treatable analytical.

The simulation of beam deflection by external force was carried out as the next step of the MCA method test (Fig. 3.). Such simulations are important for the investigation the mechanical properties of materials on the nano- and micro-scale and therefore for the understanding of the behaviour of microsystems under mechanical load or stress. The results shoe good agreement with the analytical solution by beam theory. Higher deflections at higher forces are caused by plastic deformation and cracks inside the beam. For this processes no analytical approaches exist.

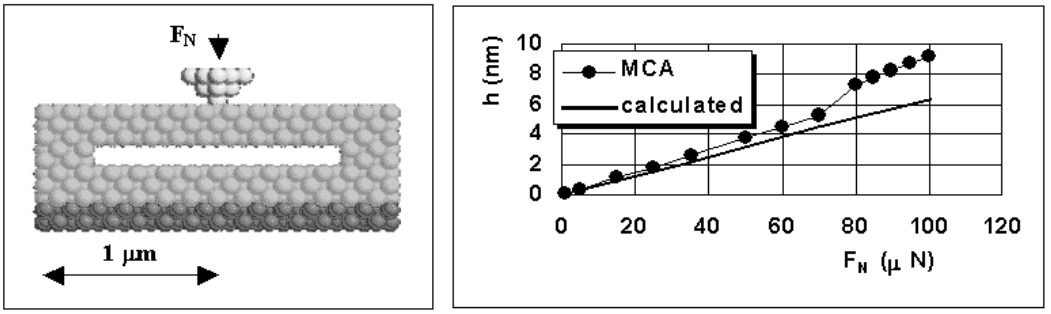



Figure 3: Beam deflection: 3D simulation and analytical solution indenter: diamond, beam: $ZrO_2$

Thin hard coatings on highly loaded components are today the measure of choice to reduce friction and especially wear in technical products. To simulate such film properties and to make the improvement of coatings more systematically, indentation and micro membrane deflection can be used. As an example, deflection of different structures made of $ZrO_2$ and diamond was investigated in the paper. With higher young modulus and strength of diamond in comparison to $ZrO_2$, diamond shows a lower deflection and no destruction of the membrane. The $ZrO_2$ membrane failed at 1.2 mN for the chosen geometry.

## 3 FRICTION SIMULATION

Atomic force microscope (AFM) is used today for surface analysis on atomic scale. Stick-slip behavior is a unique friction process at this level (Mate [7], Carpick [8]). Molecular dynamics simulations have been performed by Shimizu [9] to clarify the contact mechanism between specimen surfaces and AFM-tip. Fig. 4 shows the MD-simulation model and the variation of forces as function of position in x direction, using a copper specimen and a diamond tip.

The qualitative same behaviour was found with MCA simulation on nano-scale (Fig. 5.). A diamond cone (tip radius: 50 nm) moves in x direction over a copper specimen. Both simulations show two-dimensional stick-slip behaviour and the period of the waveform is determined by the lattice geometry. The advantage of MCA simulation compared with MD is the more realistic time and dimension scale, which can be treated. Elementary atomic interactions and deformation of

topography structures are the main mechanism of friction. Simulations with well-defined topography are helpful to understand second one.

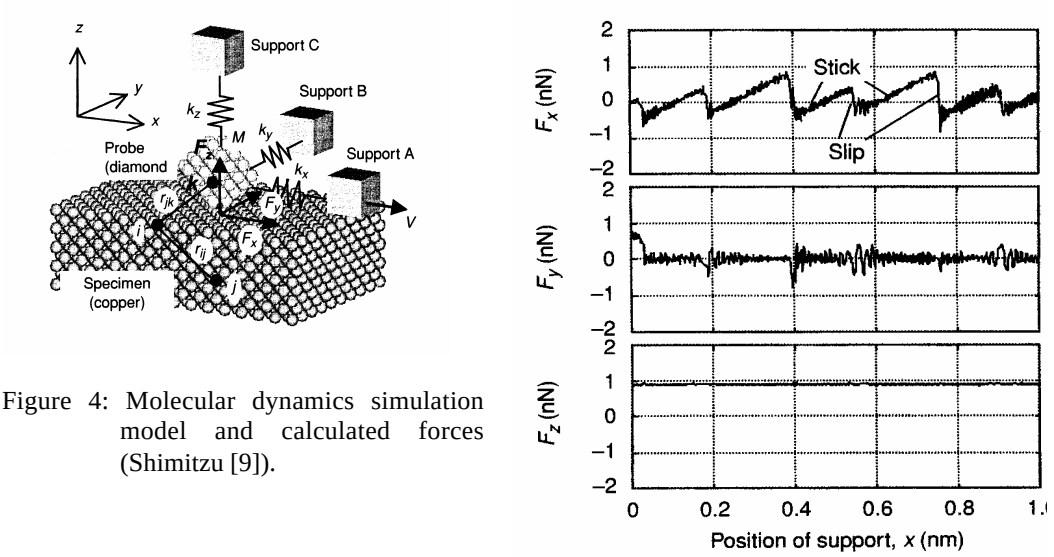



Figure 4: Molecular dynamics simulation model and calculated forces (Shimitzu [9]).

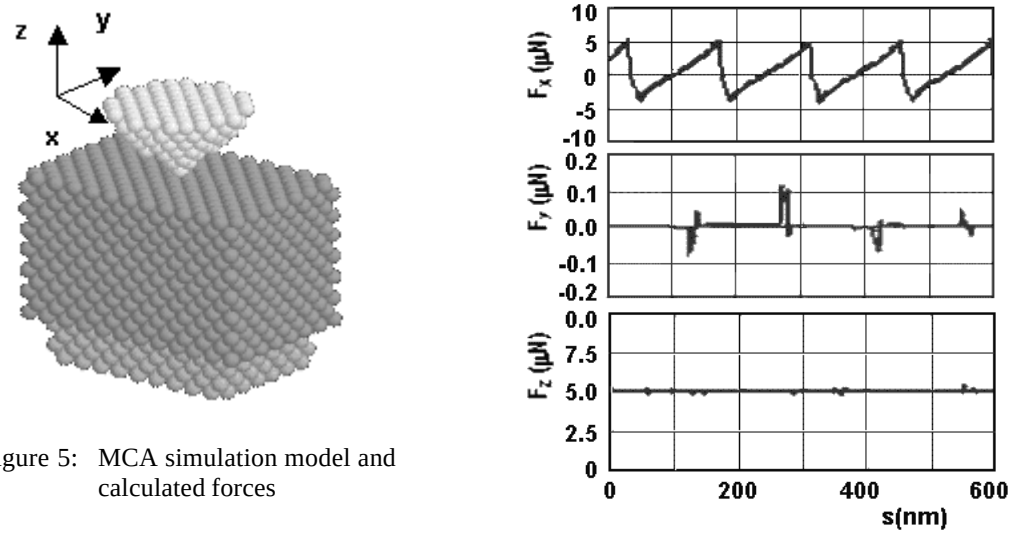



Figure 5: MCA simulation model and calculated forces

## 4 WEAR SIMULATION

As the next step of the MCA method test the scratch test was used. These tests are often used for the characterisation of wear behaviour of materials, especially for hard coatings. These investigations take place on a micro and nano-scale. One test method is the use of the atomic force microscope as scratch tester. Miyamoto [10] used a sharp diamond tip to scratch a single-crystal silicon surface, Fig.6.

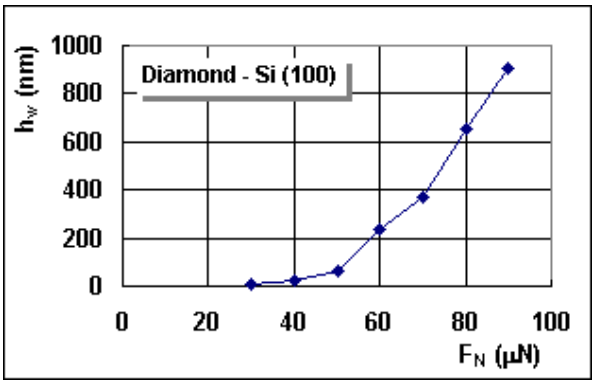



Figure 6: Mean wear depth as function of normal force, $s$ = 30 µm; $v$ = 1,62 µm/s

At low loads are the deformation elastic and no wear take place. At higher loads plastic deformation and fracture caused wear. Fig. 7 shows 3D MCA simulation results for $ZrO_2$ wear by a diamond tip. Here, at loads below 0,1 mN the contact is elastic and no wear takes place. At higher loads wear is caused by brittle fracture of $ZrO_2$.

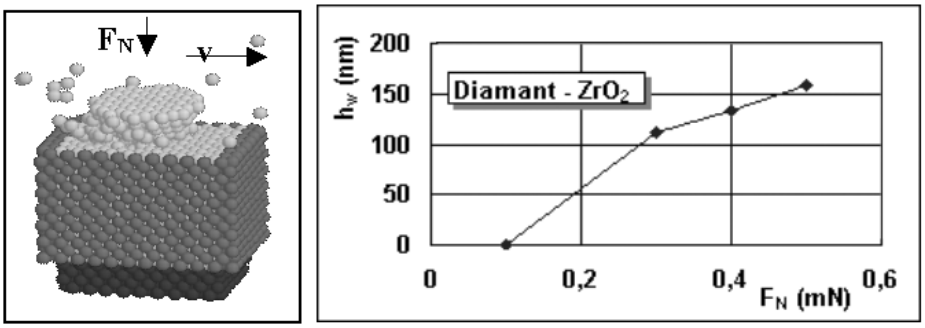



Figure 7: MCA simulation model and mean wear depth as function of normal force, v = 10 m/s, tip radius: 50 nm

## 5 SUMMARY

The results of MCA simulations in this paper are applicable on indentation, sliding, friction and wear phenomena. Because of the possibility of the MCA method to choose the scale of simulation, the results of MCA simulation can help to understand elementary processes under the action of normal and tangential forces. Friction and wear are results of such processes and can be simulated from nano- to macro-scale.

Some of the results until now are more qualitatively and improvements of the MCA method are planed for the future. For that propose also more experimental test of material response on varying scales of stress and contact dimensions are needed.

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