MOLECULAR DYNAMICS SIMULATION OF MECHANICAL PROPERTIES FOR POLYCRYSTAL MATERIALS

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Abstract. The lack of continuity conditions of the rock materials presents a serious challenge for the continuum mechanics approach, hindering the effective use of the well-established methods such as the finite element method and the boundary element methods. In the presented paper a discrete technique based on molecular dynamics approach is used for computer constructing of polycrystal materials. On the first step material grains are obtained from condensation of vaporised mixture of particles. Then the grains are compressed to obtain the material with the desirable porosity. Another variant for obtaining polycrystals is melting of the grain mixture with the consequent cooling. Uniaxial compressive loading tests for the obtained computer materials are presented, where the stress-strain relationships for mono and polycrystal specimens are compared. Influence of porosity on elastic and strength properties of the material is investigated. Applications for sandstone materials with different porosity are considered. Use of the described technique for simulation of percussive drilling in hard rock formations is discussed.

1. INTRODUCTION

Current and future demands on the effectiveness, reliability, safety and adaptivity of existing geotechnical ground penetration processes, such as downhole drilling, require the development of generic methods capable of a robust characterisation and analysis of the complex machine-ground interactions involved. Such methods need to incorporate not only machine/soil and inter-particle interaction but also secondary structures such as fissures. The lack of continuity conditions of the material being penetrated presents a serious challenge for the continuum mechanics approach, hindering the effective use of the well-established methods such as the finite element method or (and) the boundary element methods. This necessitates an introduction of complementary conditions, creation of heavily complex models, leading eventually to a cumbersome non-uniform approach. Particularly the continuum mechanics approach in civil engineering applications fails when the dynamic modelling of

ground penetration requires the soil porosity to be accounted for in order to predict correctly the dynamic system behaviour. The optimal design of a whole range of machines, where there is significant element of nonlinearity, cannot therefore be properly undertaken due to the inadequacy of the existing models of machine-ground interaction.

The relative maturity of the computer simulation methods using particulate mechanics means that real engineering systems/processes can be now modelled more accurately, and at the same time preserving simplicity by using a coherent theory. An attractive way forward is to apply an approach initially borrowed from chemical physics, where a material is represented as a set of interacting particles. The concept is close to the Molecular Dynamics method (MD) [1,2], where the material is modelled by a large number of particles interacting with each other via the prescribed nonlinear force laws; trajectories of each particle are followed through time by integrating the classical equations of motion. The interaction forces usually contain potential and

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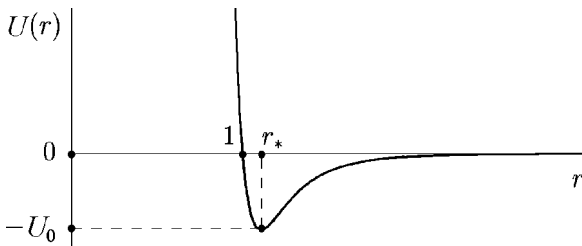Corresponding author: A.M. Krivtsov, e-mail: krivtsov@AK5744.spb.edu

Fig. 1. Lennard-Jones potential modelling the interaction forces between two particles.

dissipative components. One of the simplest examples of interparticle potential is the Lennard-Jones potential, depicted in Fig. 1. This potential has an r^{-6} attraction at long range and a r^{-12} repulsion at short range. For simulation of rock materials more complicated spline potentials can be used to give the best agreement with the elastic and strength constants of the materials. The dissipative components of the interaction forces are intended to describe viscose and dry friction between the material grains.

In the last decade MD has become one of the most powerful methods for studying condensed matter systems. It has been successfully applied to a wide variety of problems, including simulation of liquid crystals [3]; shock waves, fracture and plas-

tic flow in solids [4], material modelling [5], to name a few. Recently an interest to simulation of polycrystal materials was highly increased; let us note the important results on plasticity in nanocrystals obtained by molecular dynamics simulation [6]. In many works on MD the particles cannot be considered as real atoms or molecules, but the term MD is used historically. It has been proven that in the current advancement of the computer technology, mesoscopic particle models can be effectively used. This is due to the fact that they can represent well the material at the grain level, whilst the computational complexity is still manageable.

2. METHODS

The research programme into the application of novel nonlinear dynamics methods to percussive drilling of hard rock formations [7-9] has led the development of the special MD simulation methods. The first step in this process is to model the mechanical properties of the rock. The following idea of creating computer model for rock materials is used. Initially particles are randomly distributed in a rectangular area – Fig.2a. Then the simulation is started (integration of classical equations of motion) and due to attraction forces the particles start to coalesce forming grains. Fig.2a,b,c show sequen-
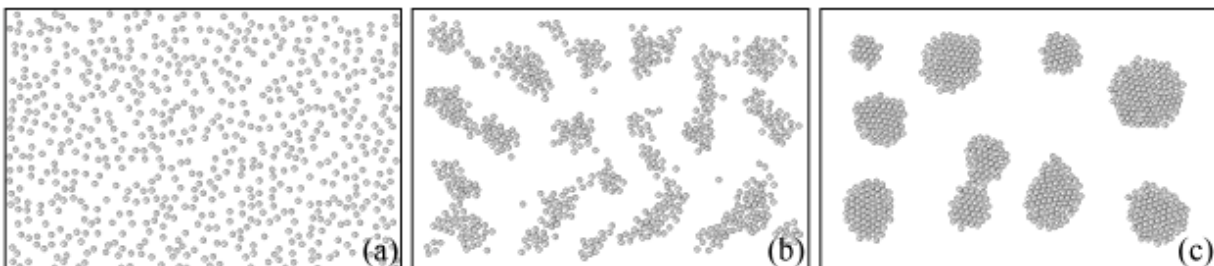

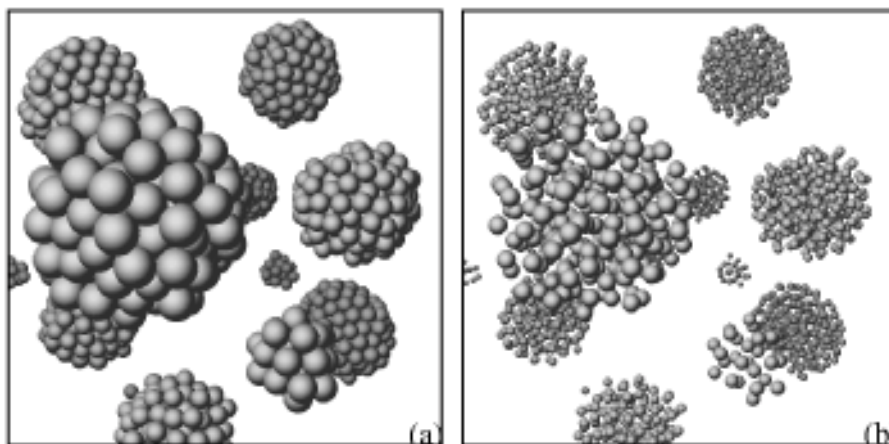**Fig.2.** Particles coalescing in fluidised mixture, 2D computer simulation.

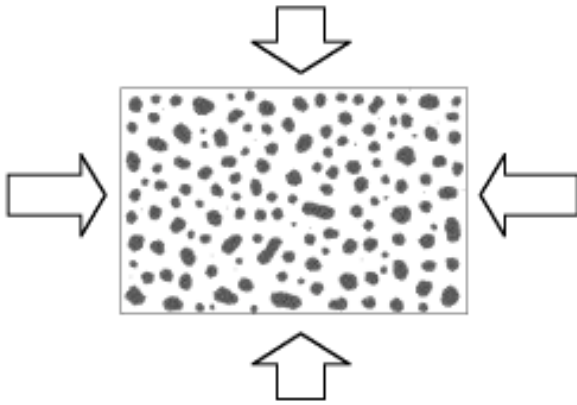**Fig.3**. Grains combined from particles, 3D simulation.

Fig.4. Compression of the grain mixture

tial moments of time while grain formation. Figs.2 correspond to 2D simulation, results of 3D simulation are depicted in Fig.3. In Fig.3b, to visualise better the inner structure of the grains, the radiuses are shown as if they were two times smaller then in Fig.3a.

The next stage of the material preparation is obtaining the polycrystal material from the grains. This can be done differently. The main variants are compression or melting techniques. In the

compression method the mixture of the obtained grains is being compressed uniformly in all directions – Fig.4. Under compression the grains consolidate and form a porous material. In the melting method the grain mixture is being melted with consequent cooling down to the zero temperature. The melting means that a random component is added to the velocities of all particles, and these additional velocities are high enough to break the crystal structure of the grains.

Examples of the polycrystal computer materials with different porosity are shown in Fig.5, where for better visibility negative colouring is used – white for material and black for voids. Each 2D pattern consists of approximately 100 thousand particles. Zoom-up enlargement of a small area inside each pattern is provided to visualise the material structure, where individual particles can be identified. After the material with the required porosity is prepared it is used in various computer tests to determine its elastic and strength properties.

Fig.6a shows density of the material plotted against applied pressure (quantities are given in percents to their maximum value) for the compression technique. The graph clearly shows
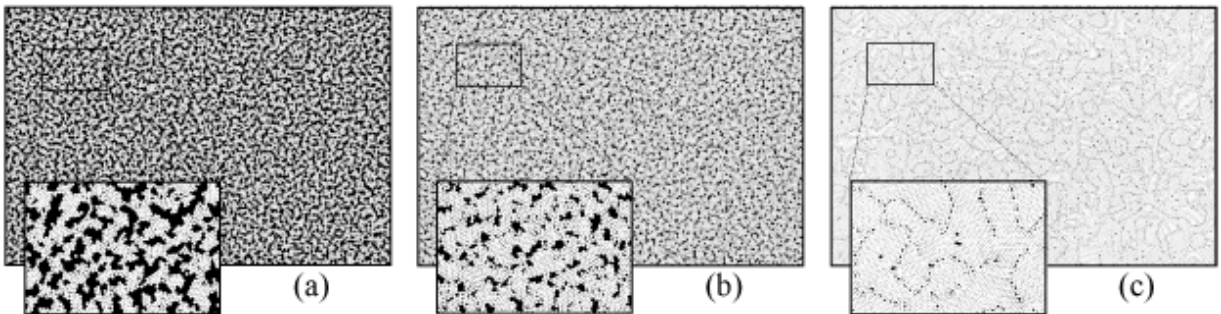

Fig. 5. Material patterns with different porosity, simulation using 100 thousands particles; (a) 20% porosity, (b) 10% porosity, (c) 1% porosity.
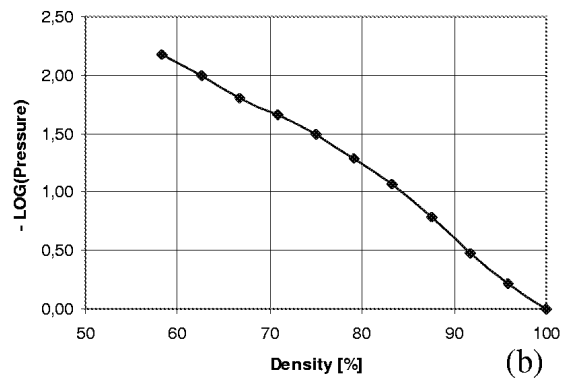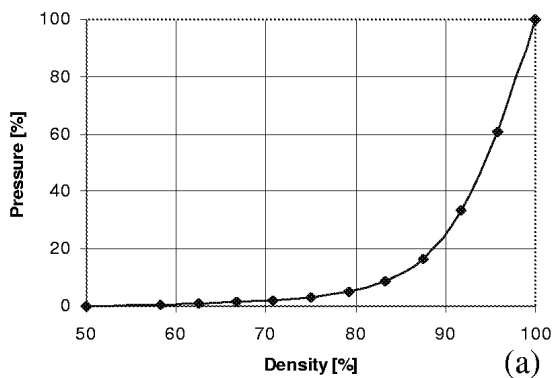

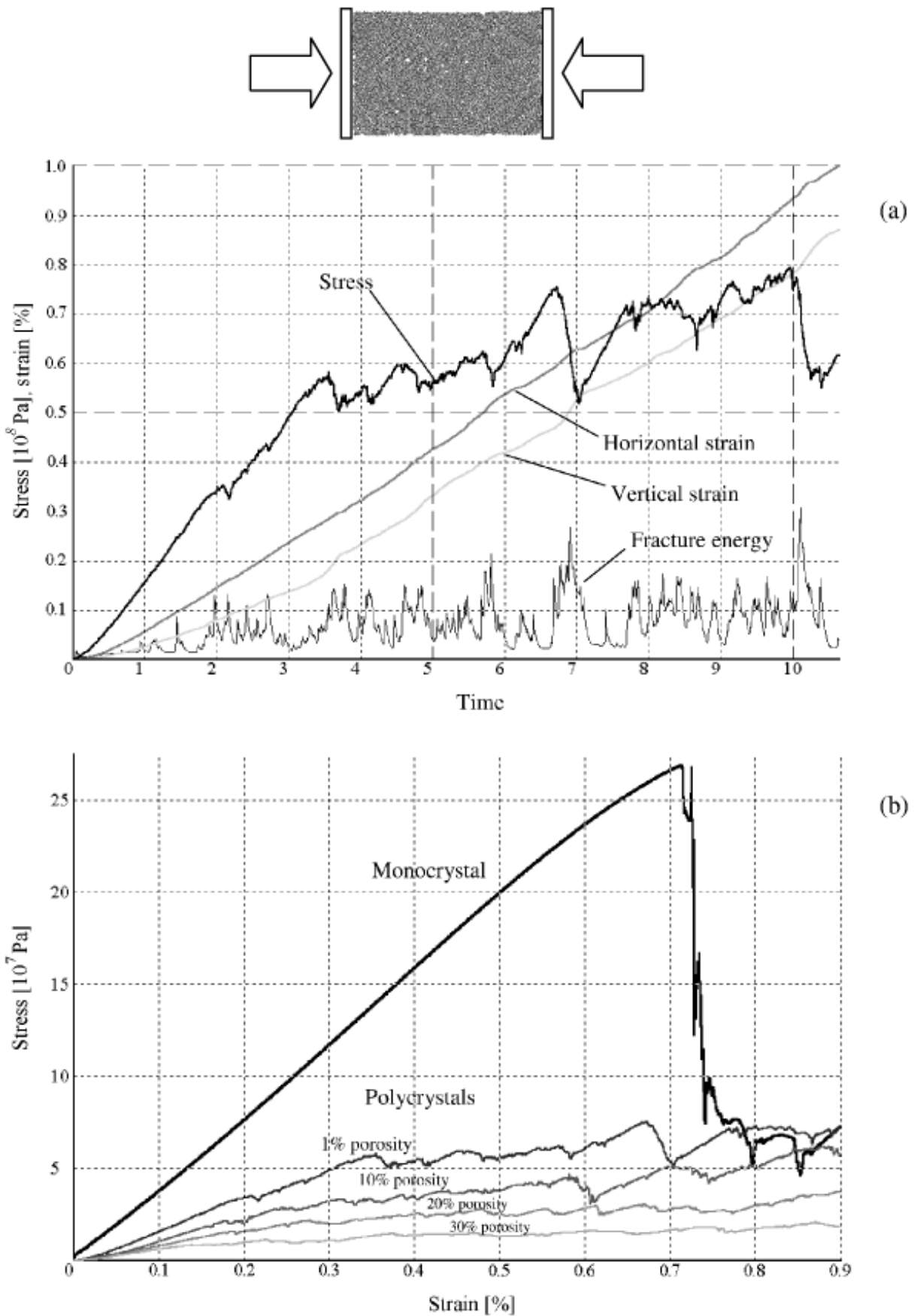**Fig.6.** Pressure versus density during compression.

Fig. 7. Results of computer compression tests; (a) loading diagram for polycrystal material, (b) stress-strain diagrams for monocrystal and polycrystals with different porosity.
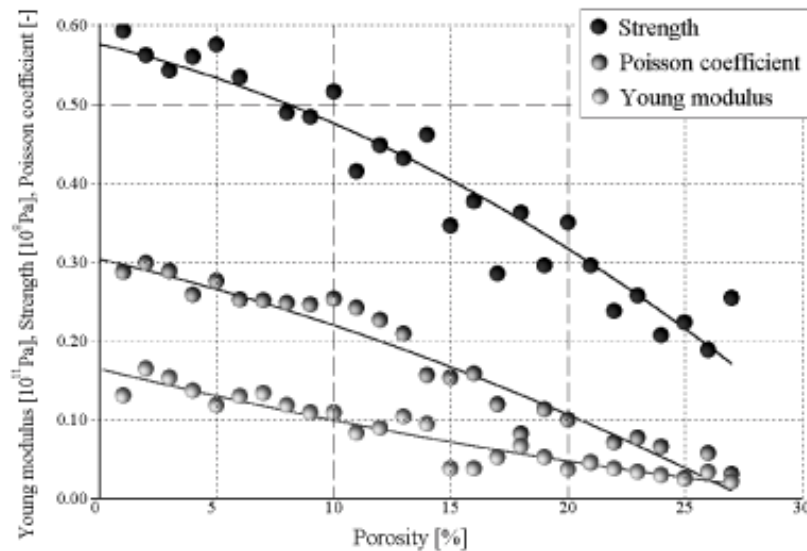
Fig. 8. Results of computer compression tests: polycrystal properties versus porosity.

exponential relation — logarithm of the pressure is nearly linear function of the density (Fig.6b), which is in a good agreement with experimental results [10].

3. RESULTS AND DISCUSSION

Let us consider uniaxial compressive loading tests with the computer specimens possessing different porosity (Fig. 7). The parameters of the interparticle interaction are such that the specimens approximately show the mechanical properties of sandstone. The specimens used in the later computer experiments were obtained by the melting technique. The loading is stiff, i.e. the deformation (not the pressure) is being set during the loading. Fig. 7a shows the loading diagram for the polycrystal material. The horizontal axis is dimensionless computer time. The stress and strain in the direction of loading (horizontal direction in the figure) are measured during the computer experiment and they are plotted against the vertical axis in Fig. 7a. These quantities allow obtaining stress-strain relations, such as depicted in Fig. 7b. Strain in the direction orthogonal to the loading (vertical direction in the figure) is also measured and plotted. This allows calculating Poisson coefficient for the material.

The last quantity, which is plotted in Fig. 7a, is energy of the chaotic oscillations of the particles (further: fracture energy), which are initialised by the inelastic deformation in the specimen. The graphs in Fig. 7a clearly show that when the stress of the loading is dropping down, then immediately the fracture energy is sharply increasing. Thus we can see

transfer of the mechanical energy of loading to the heat energy of the chaotic oscillations. During the experiment the heat is continuously removed from the specimen by means of small dissipative forces acting on each particle. That is why the fracture energy is not accumulated in the specimen, but each time after the increase it is slowly decreasing until the next inelastic jump.

Stress-strain relations for mono and polycrystal specimens are compared in Fig. 8a. From the graphs it is clearly visible that strength for the monocrystal material is much higher then for the polycrystal ones. Moreover, monocrystal material shows brittle behaviour, the polycrystal specimens are more ductile. Strength, Poisson coefficient, and Young modulus of the polycrystals as functions of porosity are depicted in Fig. 8b. Values of all these mechanical properties decrease when the porosity of the material increases.

4. CONCLUDING REMARKS

For the simulation of granular, polycrystal materials, such as rocks and soils the following two mesoscopic scale levels can be considered.

- Sub-grain level. The material grains are perfect crystals made of a number of the simple representative particles. On this level mainly the laws of interaction between grains are examined.
- Grain level. Each grain is modelled by a single particle represented as a rigid body, which can vary in shape and level of interaction potentials. This model is used for simulation of machine-rock interaction involved with percussive drilling.
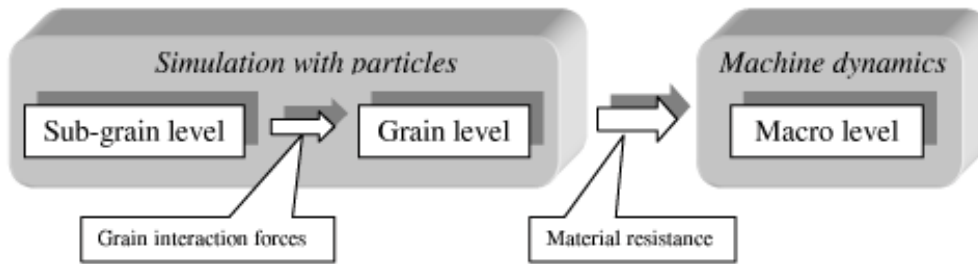
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Fig. 9. Interrelationships between the models of different scales.
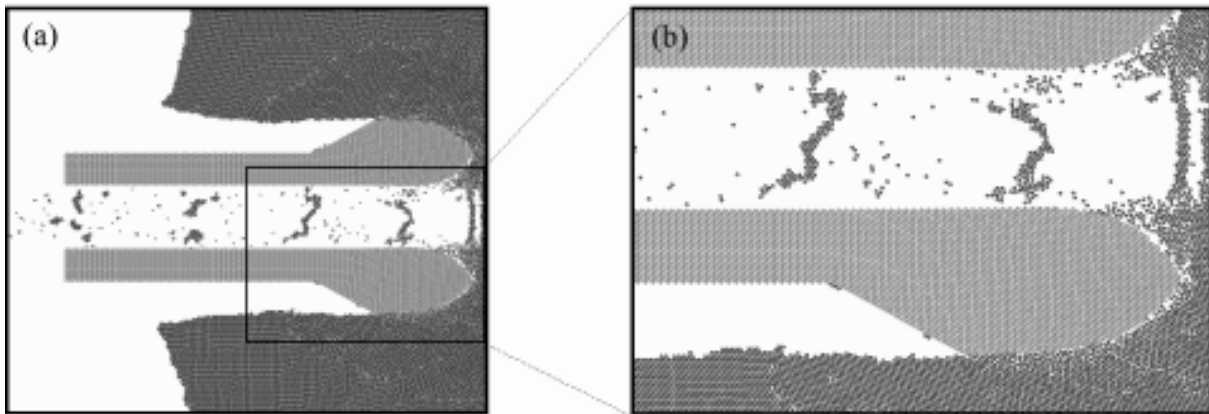

Fig. 10. Particle simulation of downhole percussive drilling; (a) propagation of the drillbit, (b) zoom-up of (a).

Interrelationships between the models on the different scale levels is depicted in Fig. 9 indicating the coupling between the "micro" and "macro" mechanics necessary to appropriately model the dynamic interactions during drilling process.

Computation on the sub-grain level involves many more degrees of freedom, since each material grain contains hundreds of particles, but this level can be studied with relatively simple interparticle potentials. For example according to [11] for brittle materials even the simplest Morse and Lennard-Jones potentials can give reasonable approximation, while ductile materials required many body potentials.

On the grain level more complex models of particle interactions are required, where not only forces but also moments have to be accounted for. These interaction laws are to be taken from the sub-grain level simulations. The grain-level models are used to obtain resistive forces, which then can be fed in the overall dynamics model of the percussive drilling devices.

To illustrate the practical application of the described above methods a slide from a computer simulation showing a downhole tool penetrating rock is depicted in Fig. 10. The drilling is performed by a traditional hammer bit, but with percussive enhancement. From the simulation it can be clearly seen, how periodic impacts increase the material fracture. The light grey colour specifies cross-section of the hammer bit, which has an axial channel used for debris removal; dark grey colour specifies the rock being drilled. The simulation itself can be found at the Vibration Enhanced Drilling Research Group web site [12], where the majority of physical phenomena such as wave propagation, compaction, development of cracks and forming the debris, and dynamic progression of the tool in the drilled rock can be visually examined.

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