

## MOLECULAR MODELLING OF STRESSES AND DEFORMATIONS IN NANOSTRUCTURED MATERIALS

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A molecular dynamics approach to the deformation and stress analysis in structured materials is presented. A new deformation measure for a lumped mass system of points is proposed. In full consistency with the continuum mechanical description, three kinds of stress tensors for the discrete system of atoms are defined. A computer simulation for a set of  $10^5$  atoms forming a sheet undergoing tension (Case 1) and contraction (Case 2) is given. Characteristic microstress distributions evoked by a crack propagation illustrate the mechanical problem considered.

**Keywords:** molecular modelling, deformation and stress analysis, nanostructured materials

### 1. Introduction

Nanotechnology, which is a new field of engineering, constitutes a challenge for the modelling of deformations and stresses in the range of nanoscale dimensions, i.e., in the range of  $10^{-9}$  to  $10^{-7}$  m. The design and manufacturing of new kinds of materials and devices like NanoElectroMechanicalSystems, intermetallics, nanotubes, quantum dots, quantum wires, etc. (Cleland, 2003; Nalva, 2000) need new ideas for the analysis of mechanical processes in nanosize domains.

The classical description based on continuum mechanics must be supplemented by molecular dynamics and quantum mechanical approaches. This means that the natural notions of stresses and deformations based on the hypothesis of a material continuum must be extended to the case of the discrete structure of atoms and molecules.

In the present paper a molecular dynamics approach to the description of stresses and deformation in structured materials will be considered. Although the notion of stresses was used in the papers (Egami and Srolovitz, 1982; Parrinello and Rahman, 1980) and especially in the papers (Ribarsky and Landman, 1988; Singer and Pollock, 1992), we present here an independent approach to derive the stress and strain tensors for a collection of atoms (molecules) as a set of lumped material points. A comparison with Parrinello and Rahman's idea and Cauchy and Born's rule is made, too.

To illustrate the specific circumstances of the molecular system from a numerical point of view as well, a computational simulation problem will be demonstrated. The paper is organized as follows: we start with the derivation

of stress tensors in Section 2. Then in Section 3 a plane problem is considered with numerical analysis. We finish with some conclusions in Section 4.

### 2. Modelling of Stresses at the Molecular Level

Let us consider a system of dense discrete material points  $A_1, \dots, A_N$  with masses  $m_i$ . Its localization is described by the position vectors  $\mathbf{r}_i$ ,  $i = 1, \dots, N$ , in a fixed Cartesian frame  $\{Ox^\alpha\}$ ,  $\alpha = 1, 2, 3$ . The intermolecular reactions result from a potential  $U(\mathbf{r}_1, \dots, \mathbf{r}_N) = U(r_{ij})$ , where the distance is  $r_{ij} = |\mathbf{r}_j - \mathbf{r}_i| = |\mathbf{r}_{ij}|$ . Thus the global force acting on point  $A_i$  has the form

$$\begin{aligned} \mathbf{f}_i &= \sum_j \mathbf{f}_{ij} = \sum_j \frac{\partial U}{\partial \mathbf{r}_{ij}} = \sum_j \frac{\partial U}{\partial r_{ij}} \frac{\partial r_{ij}}{\partial \mathbf{r}_{ij}} \\ &= \sum_j \frac{1}{r_{ij}} \frac{\partial U}{\partial r_{ij}} \mathbf{r}_{ij} = \sum_j X_{ij} \mathbf{r}_{ij}, \end{aligned} \quad (1)$$

where

$$X_{ij} = \frac{1}{r_{ij}} \frac{\partial U}{\partial r_{ij}}.$$

The governing system of motion equations takes the classical Newtonian form

$$m_i \ddot{\mathbf{r}}_i = \sum_j X_{ij} \mathbf{r}_{ij}, \quad i = 1, 2, \dots, N. \quad (2)$$

This system must be considered together with the initial conditions  $\mathbf{r}_i(t_0) = \mathbf{r}_{i0}$ ,  $\dot{\mathbf{r}}_i(t_0) = \mathbf{v}_{i0}$ .

Note that, in contrast to the formulation of an initial problem in the macro dimension range, the setting of the initial quantities  $\mathbf{r}_{i0}$  and  $\mathbf{v}_{i0}$  cannot be prescribed arbitrarily. This results from the fact that a discrete placement of the molecules violates the intrinsic interactions of the system. Thus the assumption of initial values must be physically admissible. Therefore, the equilibrium state assumed at the beginning of the process needs an equilibration procedure. It will be described in the next section.

To introduce the notion of stresses, consider a mapping from the initial (reference) state  $B_0$  onto the current configuration  $B_t$  at instant  $t$ . Denoting by  $\mathbf{R}_i = \mathbf{r}_{i0}$  the position vectors at the configuration  $B_0$ , we introduce the following relations for any pair of points  $A_i$  and  $A_j$ :

$$\begin{aligned} \mathbf{R}_{ij} &= \mathbf{R}_j - \mathbf{R}_i, & \mathbf{r}_{ij} &= \mathbf{r}_j - \mathbf{r}_i, \\ \mathbf{u}_{ij} &= \mathbf{u}_j - \mathbf{u}_i, & \mathbf{r}_{ij} &= \mathbf{R}_{ij} + \mathbf{u}_{ij}. \end{aligned}$$

Here  $\mathbf{u}_i$  and  $\mathbf{u}_j$  denote the displacements of the points  $A_i$  and  $A_j$ , respectively. The current distance vector  $\mathbf{r}_{ij}$  can be constructed as a composition of the translation of  $\mathbf{R}_{ij}$ , the elongation (shortening) by  $\mathbf{u}_{ij}^s$  and next by the rotation of  $\mathbf{u}_{ij}^s$  (cf. Fig. 1). This operation is

$$\mathbf{r}_{ij} = \mathbf{R}_{ij} + \mathbf{Q}_{ij} \mathbf{u}_{ij}^s,$$

where  $\mathbf{Q}_{ij}$  is an orthogonality tensor,  $\mathbf{Q}_{ij} \mathbf{Q}_{ij}^T = \mathbf{1}$  (1 stands for the identity matrix).

The elongation vector  $\mathbf{u}_{ij}^s$  can be expressed in the form

$$\begin{aligned} \mathbf{u}_{ij}^s &= u_{ij}^s \mathbf{e}_0 = \text{sign}(\mathbf{u}_{ij} \cdot \mathbf{e}_0) |\mathbf{u}_{ij}| \mathbf{e}_0 \\ &= \text{sign}(\mathbf{u}_{ij} \cdot \mathbf{e}_0) \frac{|\mathbf{u}_{ij}|}{|\mathbf{R}_{ij}|} \mathbf{R}_{ij} = w_{ij}^s \mathbf{R}_{ij}. \end{aligned}$$

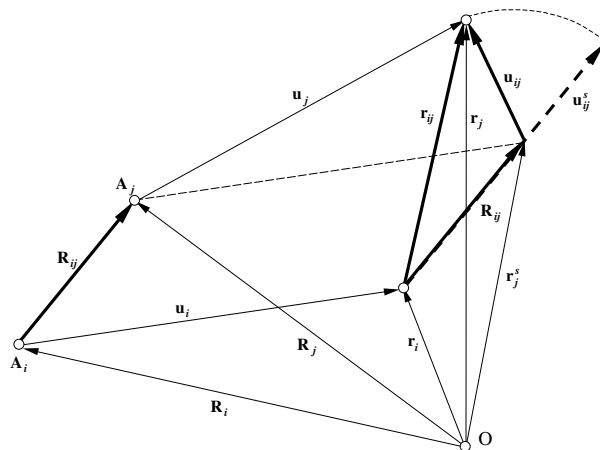


Fig. 1. Construction of the current distance vector.

Here  $\mathbf{e}_0$  is the unit vector in the direction determined by  $\mathbf{R}_{ij}$ , and the scalar  $w_{ij}^s$  is equal to

$$w_{ij}^s = \text{sign}(\mathbf{u}_{ij} \cdot \mathbf{e}_0) \frac{|\mathbf{u}_{ij}|}{|\mathbf{R}_{ij}|} = \frac{u_{ij}^s}{|\mathbf{R}_{ij}|}.$$

Thus

$$\mathbf{r}_{ij} = \mathbf{R}_{ij} + \mathbf{Q}_{ij} w_{ij}^s \mathbf{R}_{ij} = (1 + w_{ij}^s \mathbf{Q}_{ij}) \mathbf{R}_{ij}.$$

Introducing the tensor

$$\Delta_{ij} = w_{ij}^s \mathbf{Q}_{ij}$$

as a measure of deformation, we can finally write

$$\mathbf{r}_{ij} = (1 + \Delta_{ij}) \mathbf{R}_{ij} = \mathbf{F}_{ij} \mathbf{R}_{ij}. \quad (3)$$

The tensor  $\mathbf{F}_{ij} = 1 + \Delta_{ij}$  plays a similar role as the deformation gradient in continuum mechanics. It maps the initial placement set  $B_0$  of the points onto the deformed configuration  $B_t$  described by the positions  $\mathbf{r}_i = \mathbf{F}_{ij} \mathbf{R}_i$ . It is easy to verify that the matrix

$$\mathbf{C}_{ij} = \mathbf{F}_{ij}^T \mathbf{F}_{ij} = (1 + w_{ij}^s \mathbf{Q}_{ij})^T (1 + w_{ij}^s \mathbf{Q}_{ij})$$

is symmetric and therefore constitutes an object analogous to the known Cauchy right deformation tensor. One also sees that the tensor

$$\mathbf{E}_{ij} = \frac{1}{2} (\mathbf{C}_{ij} - 1)$$

can be interpreted as the strain tensor since by calculating the difference  $|\mathbf{r}_{ij}|^2 - |\mathbf{R}_{ij}|^2$  we obtain

$$\begin{aligned} \mathbf{r}_{ij} \mathbf{r}_{ij} - \mathbf{R}_{ij} \mathbf{R}_{ij} &= \mathbf{F}_{ij} \mathbf{R}_{ij} \mathbf{F}_{ij} \mathbf{R}_{ij} - \mathbf{R}_{ij} \mathbf{R}_{ij} \\ &= (\mathbf{F}_{ij}^T \mathbf{F}_{ij}) : \mathbf{R}_{ij} \otimes \mathbf{R}_{ij} - \mathbf{R}_{ij} \mathbf{R}_{ij} \\ &= 2 \left( \frac{\mathbf{F}_{ij}^T \mathbf{F}_{ij} - 1}{2} \right) : \mathbf{R}_{ij} \otimes \mathbf{R}_{ij} \\ &= 2 \mathbf{E}_{ij} : \mathbf{R}_{ij} \otimes \mathbf{R}_{ij}, \end{aligned}$$

which is fully consistent with the suitable formula known in continuum mechanics.

Above, the symbol ‘:’ denotes the double contraction of rank-two tensors, whereas the symbol ‘ $\otimes$ ’ denotes the dyadic multiplication of vectors.

The potential  $U(\mathbf{r}_{ij})$  is then equal to  $U(\mathbf{F}_{ij}) = U(\Delta_{ij})$ . Thus let us define the matrix

$$\begin{aligned} T_{\alpha\beta} &= \frac{1}{V_0} \sum_j \frac{\partial U}{\partial \Delta_{\alpha\beta}^{ij}} = \frac{1}{V_0} \sum_j \frac{\partial U}{\partial r_{ij}} \frac{\partial r_{ij}}{\partial r_{ij\alpha}} \frac{\partial r_{ij\alpha}}{\partial \Delta_{\alpha\beta}^{ij}} \\ &= \frac{1}{V_0} \sum_j X_{ij} r_{ij\alpha} R_{ij\beta} = \frac{1}{V_0} \sum_j f_{ij\alpha} R_{ij\beta}, \end{aligned}$$

$$\alpha, \beta = 1, 2, 3.$$

In the absolute notation, it will be

$$\mathbf{T}_R = (T_{\alpha\beta}) = \frac{1}{V_0} \sum_j \mathbf{f}_{ij} \otimes \mathbf{R}_{ij} = \frac{1}{V_0} \sum_j \mathbf{T}_{ij}. \quad (4)$$

This dyadic product is called the Piola-Kirchhoff microstress tensor for the set of molecules. Above,  $V_0$  is the volume of a presumed calculational cell which, after deformation, takes the value  $V$ .

Analogously to the known formula in continuum mechanics, we obtain the Cauchy stress tensor

$$\begin{aligned} \boldsymbol{\sigma} &= J^{-1} \sum_j \mathbf{T}_{ij} \mathbf{F}_{ij} = \frac{1}{V} \sum_j \mathbf{f}_{ij} \otimes (\mathbf{1} + \boldsymbol{\Delta}_{ij}) \mathbf{R}_{ij} \\ &= \frac{1}{V} \sum_j \mathbf{f}_{ij} \otimes \mathbf{r}_{ij}, \end{aligned} \quad (5)$$

where  $J = V/V_0$ , and the second Piola-Kirchhoff tensor

$$\begin{aligned} \mathbf{S} &= \sum_j \mathbf{F}_{ij} \mathbf{T}_{ij} = \frac{1}{V_0} \sum_j (\mathbf{1} + \boldsymbol{\Delta}_{ij}) \mathbf{f}_{ij} \otimes \mathbf{R}_{ij} \\ &= \frac{1}{V_0} \sum_j X_{ij} \mathbf{R}_{ij} \otimes \mathbf{R}_{ij}. \end{aligned} \quad (6)$$

The tensors (5) and (6) are symmetric. All the tensors coincide with suitable objects considered by Parrinello and Rahman and those which are based on the Cauchy-Born hypothesis known in crystal elasticity (Ortiz and Phillips, 1999). For periodic structured materials, Andersen (1980) and then a number of authors (Parrinello and Rahman, 1980; Ray, 1983; Ribarsky and Landman, 1988) introduced a calculational cell  $\Omega$  constructed from three vectors  $\mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3$  which span the edges of  $\Omega$ . Forming a matrix  $\mathbf{H} = (H_{\alpha\beta})$  whose columns are vectors  $\mathbf{H}_\alpha$ ,  $\alpha = 1, 2, 3$ , we can express the position vectors  $\mathbf{r}_i$  in terms of this matrix and scaled coordinates ( $s_{i\alpha}$ )  $r_{i\beta} = \sum_{\alpha=1}^3 H_{\alpha\beta} s_{i\alpha}$ . The volume of the cell is given by  $V = \det \mathbf{H}$ . Regarding the components of  $\mathbf{H}$  as generalized variables, we calculate the derivative

$$\begin{aligned} \frac{\partial U}{\partial H_{\alpha\beta}} &= \sum_j \frac{\partial U}{\partial r_{ij}} \frac{\partial r_{ij}}{\partial r_{ij\alpha}} \frac{\partial r_{ij\alpha}}{\partial H_{\alpha\beta}} = \sum_j X_{ij} r_{ij\alpha} s_{ij\beta} \\ &= \sum_j X_{ij} r_{ij\alpha} r_{ij\gamma} H_{\beta\gamma}^{-1} \\ &= \frac{1}{V} \sum_j X_{ij} r_{ij\alpha} r_{ij\gamma} A_{\beta\gamma}, \end{aligned}$$

where  $A_{\beta\gamma} = V H_{\beta\gamma}^{-1}$  are components of the area tensor  $\mathbf{A} = \partial V / \partial \mathbf{H}$ . Hence the tensor  $\boldsymbol{\sigma} = (1/V) \sum_j X_{ij} \mathbf{r}_{ij} \otimes \mathbf{r}_{ij}$  coincides with (5). The same formula results from the Cauchy-Born hypothesis, which

states that for a homogenous deformation the particle motion follows the continuum displacement field through the continuum deformation gradient  $\mathbf{F} = \nabla \mathbf{x} = (\partial x^i / \partial X^K)$ , where the vector  $\mathbf{x} = (x^i)$  stands for the spatial configuration  $B_t$  and the gradient is calculated with respect to the material coordinates  $X^K$ ,  $K = 1, 2, 3$ . Thus  $\mathbf{r}_{ij} = \mathbf{F} \mathbf{R}_{ij}$  and  $U = U(\mathbf{F})$ , from which

$$\mathbf{T}_R = \frac{1}{V_0} \frac{\partial U}{\partial \mathbf{F}} = \frac{1}{V_0} \sum_j X_{ij} \mathbf{r}_{ij} \otimes \mathbf{R}_{ij},$$

i.e., we get the formula (4).

Consequently, all the three different approaches to molecular dynamics description of deformation (through  $\mathbf{F}_{ij}$ ,  $\mathbf{H}$  and  $\mathbf{F}$ ) lead to the same forms of stress tensors (4)–(6).

Like in continuum mechanics, an extension of kinematics by using the so-called second gradient theory (Sunyk and Steinmann, 2001) can be applied, too. Thus, according to this idea, the mapping from the initial state onto the current one follows not only through the deformation gradient  $\mathbf{F}$  but also through its gradient  $\nabla \mathbf{F} = (\partial^2 x^i / \partial X^K \partial X^L)$ . In that case, the arrangement of molecules becomes

$$\mathbf{r}_{ij} = \mathbf{F} \mathbf{R}_{ij} + \frac{1}{2} \nabla \mathbf{F} : \mathbf{R}_{ij} \otimes \mathbf{R}_{ij}, \quad (7)$$

by analogy to the continuum formulation

$$\Delta \mathbf{x} = \mathbf{F} \cdot d\mathbf{X} + \frac{1}{2} \nabla \mathbf{F} : d\mathbf{X} \otimes d\mathbf{X}.$$

Hence  $U = U(r_{ij}) = U(\mathbf{F}, \nabla \mathbf{F})$ , which leads to the expressions

$$\begin{aligned} \mathbf{T}_R &= \frac{1}{V_0} \frac{\partial U}{\partial \mathbf{F}} = \frac{1}{V_0} \sum_j \mathbf{f}_{ij} \otimes \mathbf{R}_{ij}, \\ \mathbf{T}_R^H &= \frac{1}{V_0} \frac{\partial U}{\partial \nabla \mathbf{F}} = \frac{1}{2V_0} \sum_j \mathbf{f}_{ij} \otimes \mathbf{R}_{ij} \otimes \mathbf{R}_{ij}. \end{aligned} \quad (8)$$

The last quantity constitutes a third-order tensor of hyperstresses whose components describe the intrinsic reaction of the particle system on the nonhomogenous deformation field  $\nabla \mathbf{F}$ .

In the present paper we focus our attention on microstresses  $\boldsymbol{\sigma}$  only. This will be done in the next section.

### 3. Numerical Analysis of Molecular Microstresses

To investigate the behaviour of the material at the nanoscale range, let us consider a typical problem discussed in damage mechanics, namely, the state of stresses

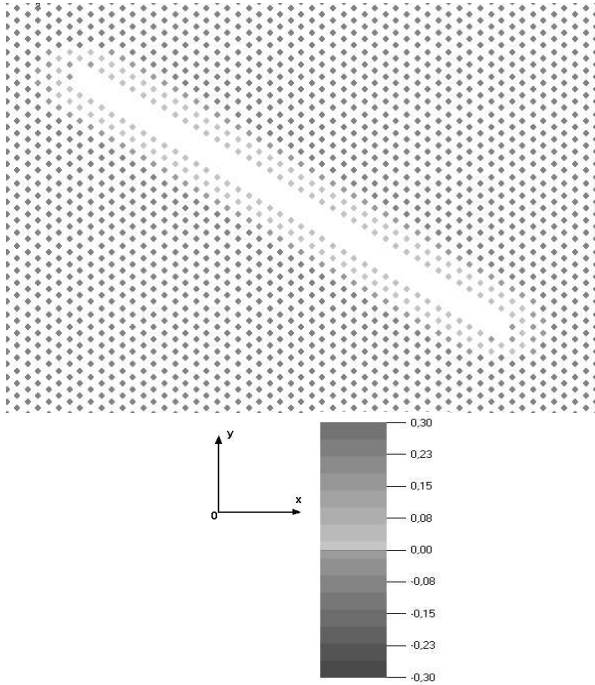


Fig. 2. Sheet with a crack (bottom of the scale – tension, top of the scale – compression).

in the neighbourhood of a crack. To simplify the calculations, let a collection of about 100,000 atoms be arranged on a plane as shown in Fig. 2 (there are exactly 93,847 atoms, which results from the geometry of the sheet). The sheet is stretched (Case 1) or compressed (Case 2) in the  $x$ -direction by applying external displacements on the vertical edges. Using the Lennard-Jones potential

$$U = -4\varepsilon \left[ \left( \frac{r_0}{r_{ij}} \right)^{12} - \left( \frac{r_0}{r_{ij}} \right)^6 \right]$$

and copper as an example, the data will be the following:  $m_i = 6.772 \cdot 10^{-9}$  g,  $\varepsilon = 0.345 \cdot 10^{-19}$  J,  $r_0 = 2.1 \text{ \AA}$ ;  $\Delta v_x^{\text{ext}} = 1.2 \cdot 10^{-5}$  nm/ $\Delta t$ ,  $\Delta t = 7.41$  ns. Since for sufficiently large distances the interactions between points vanish, we cut the interatomic actions outside a circle with a radius of  $r_c = 4$  neighbours. To solve Eqns. (2), Verlet's method (Heermann, 1997) was used. It is based on the difference scheme

$$\begin{aligned} \ddot{r}_i &= \frac{r_i^{n+1} - 2r_i^n + r_i^{n-1}}{h^2} = \frac{f_i^n}{m_i}, \\ r_i^{n+1} &= 2r_i^n - r_i^{n-1} + f_i^n \frac{h^2}{m_i}, \\ v_i^n &= \frac{1}{2h} (r_i^{n+1} - r_i^{n-1}), \end{aligned}$$

where  $h$  stands for the integration step and  $f_i$  is defined by (1).

As has been mentioned earlier, the initial conditions must be physically admissible. Thus the initial arrangement of the atoms cannot be arbitrary. The interatomic distances evoke forces and hence the motion of the system whose kinetic energy determines the temperature. When the temperature is assumed to be fixed, a proper localization of atoms must be found. Assuming that the system is in equilibrium at the beginning, e.g., at the temperature of  $20^\circ \text{C}$ , an equilibrium procedure must be applied (Heermann, 1997). It consists in performing the following steps: (a) start with a prescribed initial localization, (b) randomly choose velocities, (c) perform simulation, and (d) apply velocity scaling to control the temperature. For this reason, we compute the kinetic energy  $E_K$ . Then we determine the temperature  $T_K = 2E_K/3Nk_B$ , where  $k_B$  is the Boltzmann constant and  $N$  stands for the number of particles, and the velocity  $v_i^{\text{new}} = \beta v_i^{\text{old}}$ , where  $\beta = T_{\text{demand}}/T$ . This procedure should be repeated until an equilibrium state is achieved.

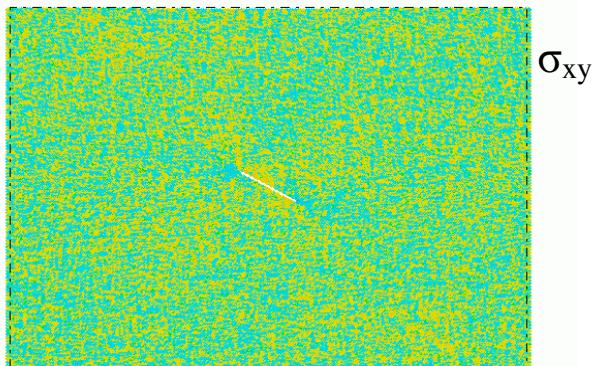
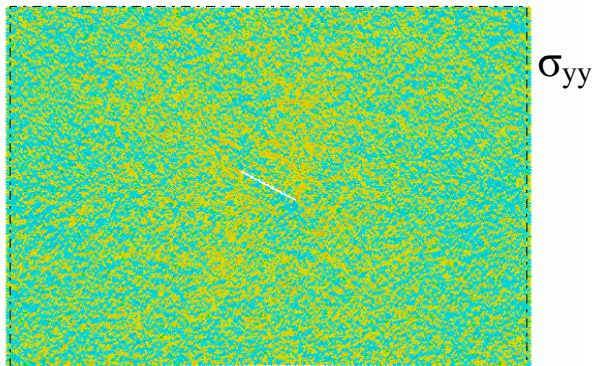
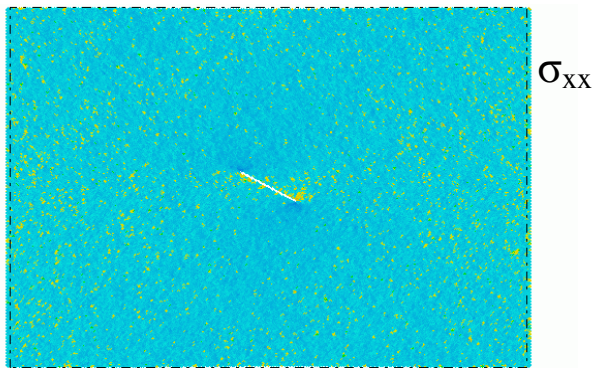
Using the above procedures, the results presented in Figs. 1–10 were obtained. For Case 1 (stretching), the stress distributions  $\sigma_{xx}$ ,  $\sigma_{yy}$  and  $\sigma_{xy}$  are presented in Figs. 3–6. Characteristic stress concentration zones and a typical kink phenomenon are evidently observed. Triangular concentration zones propagate from the tip of the crack up to the edge until a failure takes place. The stress evolution along the side lines of the triangle has a visible undulate character (dark regions).

Another kind of behaviour is observed in Case 2 (compression). The crack tends to be closed as expected. Compressive stress concentration zones occur but with quite different shapes (see Figs. 7–10). A characteristic diagonal effect is observed. The normal stresses  $\sigma_{xx}$  and  $\sigma_{yy}$  concentrate in a diagonal strip perpendicular to the initial crack, whereas visible triangular shapes with small shear stresses  $\sigma_{xy}$  are created. The time instants  $t$  marked in the figures mean the numbers of snapshots. One snapshot interval is  $1000\Delta t$ .

## 4. Conclusions

A molecular description of the states of stresses and deformations in nanostructured materials was presented. It complements the classical continuum mechanical approach. Three kinds of stress tensors corresponding to those known in continuum mechanics were defined.

As a numerical example of the effectiveness of this kind of analysis, a stress evaluation process in the neighbourhood of a crack in a copper sheet was considered. It should be emphasized that the stress distribution around the crack in a discrete lattice differs from the elastic continuum description, as there is no singularity at the crack tip.

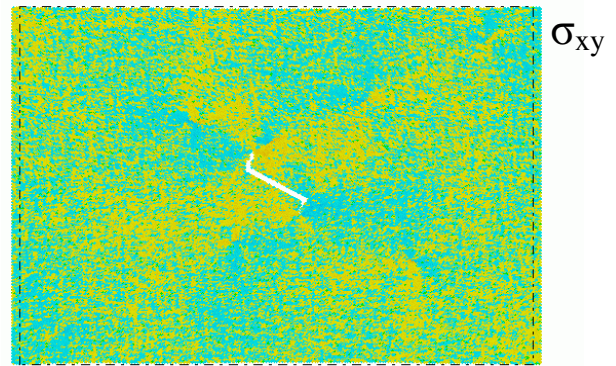
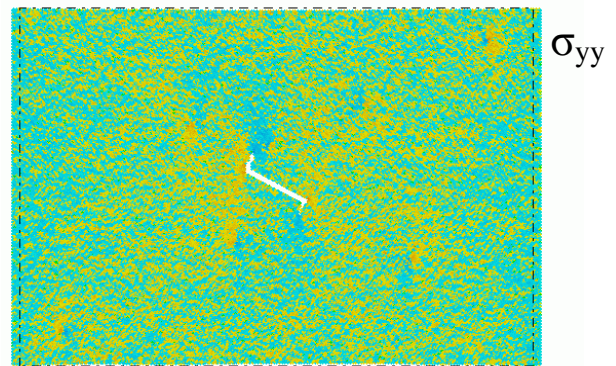
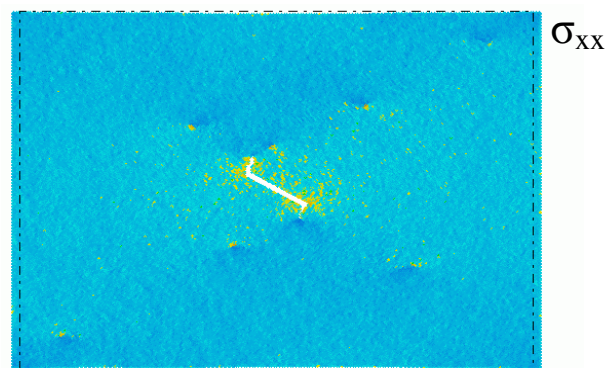
Fig. 3. Crack state at  $t = 10$ .

The calculations were limited to the Lennard-Jones interatomic forces only. More realistic for solids are intrinsic forces induced by metallic, ionic, covalent and van der Waals bonds. They will be considered during further research.

The molecular dynamics combined with a continuous description in the framework of the so-called multi-scale modelling become an effective and promising field of investigation in mechanics, materials science and engineering.

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Fig. 4. Crack state at  $t = 19$ .

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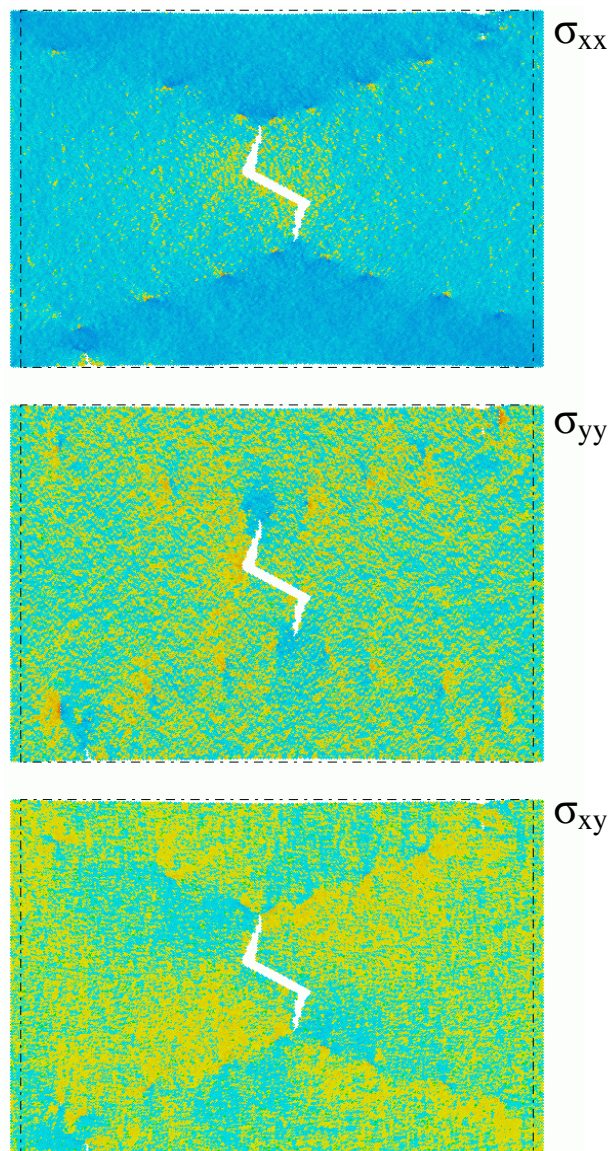


Fig. 5. Crack state at  $t = 22$ .

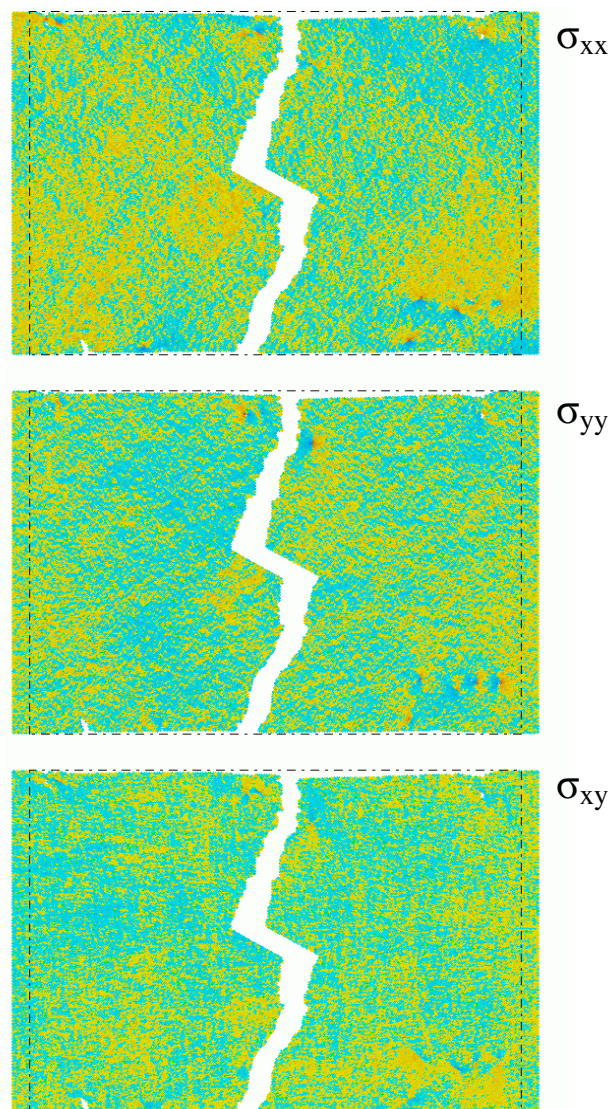


Fig. 6. Crack state at  $t = 39$ .

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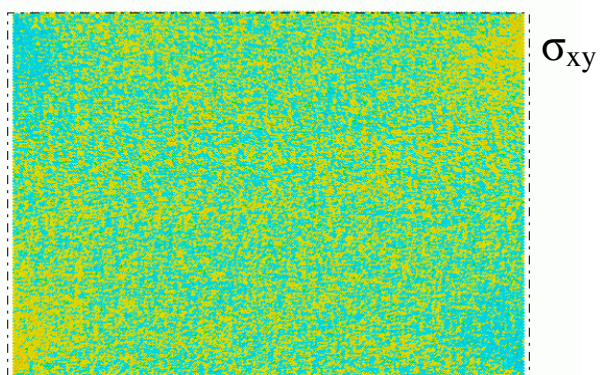
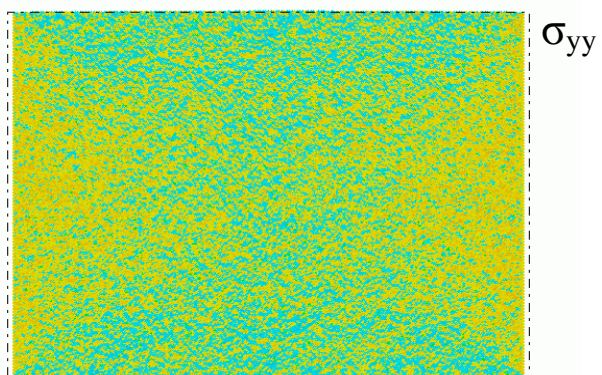
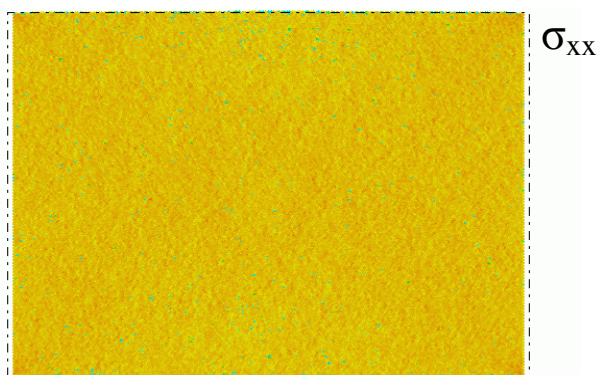


Fig. 7. Crack state at  $t = 10$ .

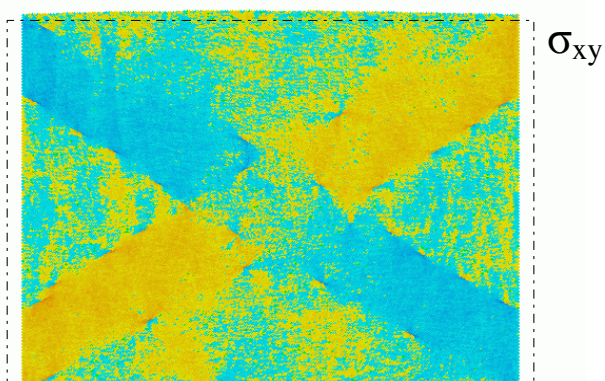
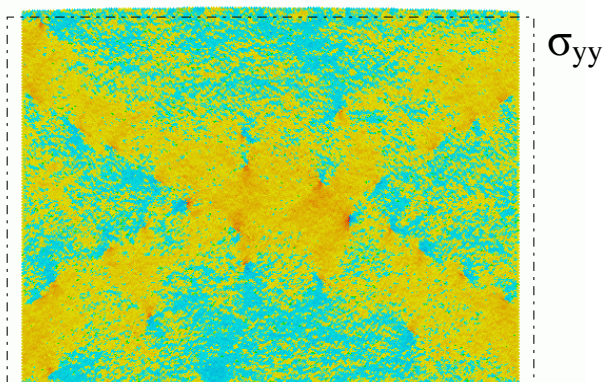
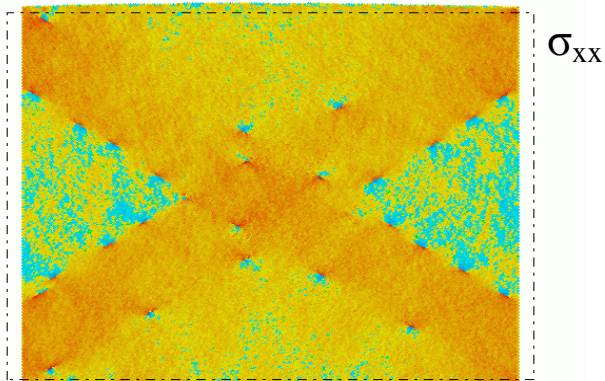
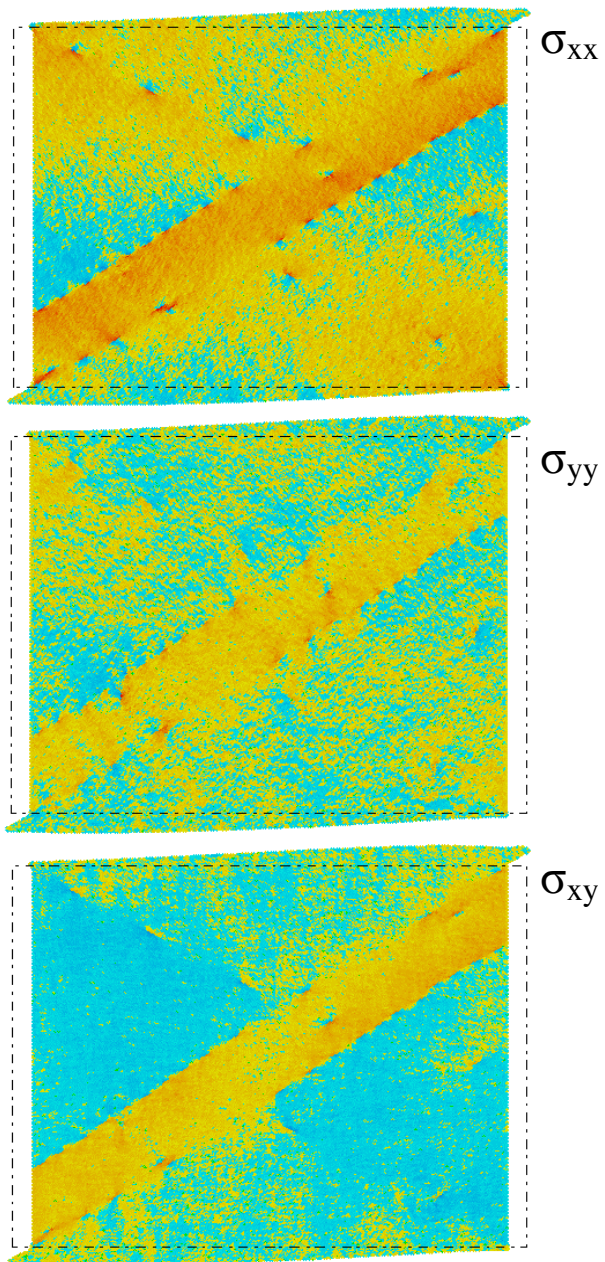
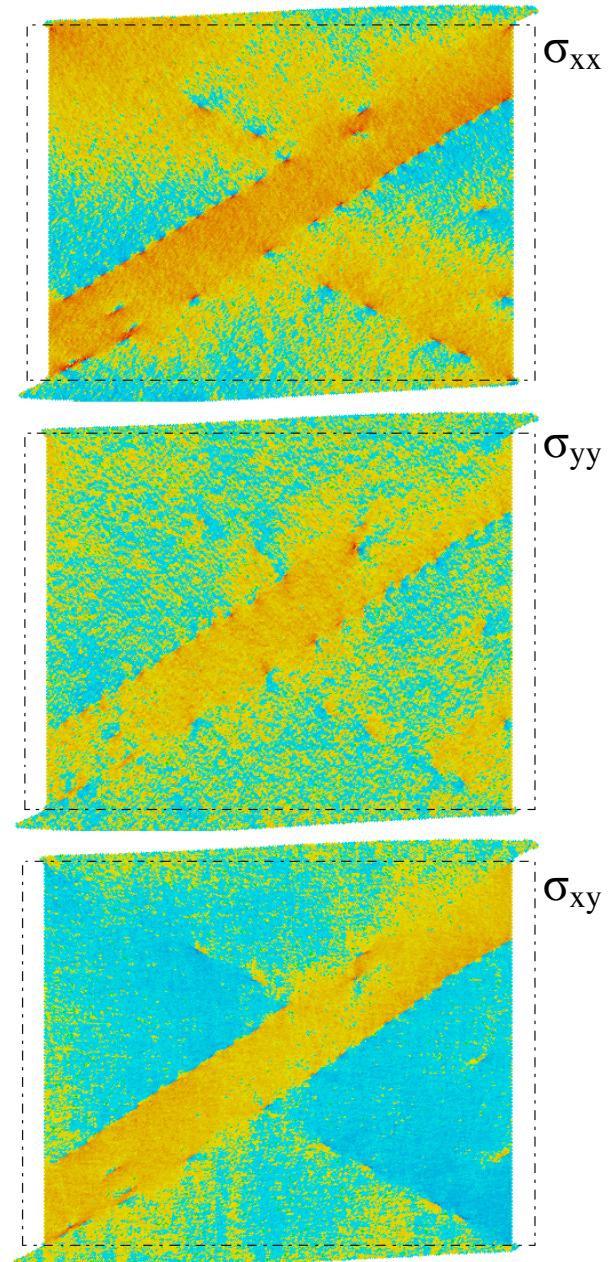


Fig. 8. Crack state at  $t = 30$ .

Fig. 9. Crack state at  $t = 40$ .Fig. 10. Crack state at  $t = 45$ .