Computer Assisted Mechanics and Engineering Sciences, 2: 141–148, 1995.


# Finite element simulation of dislocation field movement[1]

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(Received November 23, 1994)

The problem of dislocation motion in monocrystals is faced in the framework of the continuum theory of dislocations. The presented approach is based on the defects balance law. A constitutive model is formulated which relates the driving forces with the dislocation velocity. The model makes use of the relations between the plastic deformation tensor and the tensor of dislocation density. Given a crystal under certain boundary and initial conditions, the evolution of both dislocation field and elastic-plastic deformations is obtained by solving the coupled system of equations resulting from the equilibrium equation and the dislocation balance for each time step. The set of equations is discretized by the finite element method. As an example the movement of an edge dislocation field inducing shear band deformation in a monocrystal is considered.

## 1. Introduction

In spite of the discrete character of the atomic structure of metals, the continuum theories still remain the main tool to predict the strain and force distributions in deformed crystals and polycrystals.

The foundations of the continuum theory of dislocations have been formulated, among others, by Kondo [5], Kröner [6], Mura [9] and Bilby [2]. It is worth emphasizing that many papers written in that period were devoted mainly to the geometry and kinematics. We can say that there is a real fascination about geometry of defects in that period. In some sense this fascination lasts till now, cf. [4]. In spite of that, many problems in the domain of defect geometry and finite deformations have not been solved as yet, e.g. although there have been many attempts, a general, continuum theory of defects does not seem to have been satisfactorily formulated in finite deformations. On the other hand, any theory, in order to be applied to the solution of a given engineering problem, should involve not only geometry and kinematics but dynamics or thermodynamics as well, as required to determine the forces. Moreover, such a theory should include suitable constitutive equations relating the defect velocities to the driving forces.

In this paper our interest is focused on modelling the dislocation field movement in the elastic-plastic continuum. The linear theory used here includes the elements of kinematics as well as thermodynamics and constitutive modelling.

In the next section we consider the fundamental relations in the continuum theory of dislocations. The field of driving forces acting on the dislocations is determined as being energetically conjugated to the dislocation velocity field. In Sections 3 and 4 the problem discretization by the finite element method is presented and illustrated with an example of edge dislocation propagation inducing shear band deformation in a monocrystal.

[1]The paper has been presented at Japan–Central Europe Joint Workshop on Advanced Computing in Engineering, Pułtusk, Poland, September 26–29, 1994.

## 2. CONTINUUM THEORY OF DISLOCATIONS

Let us consider a dislocated crystal described in terms of the linear continuum theory of dislocations, in which it is assumed that the displacement gradient can be decomposed in the following way,

$$\nabla \mathbf{u} = \mathbf{w} + \boldsymbol{\varepsilon}_{\mathrm{e}} + \boldsymbol{\varepsilon}_{\mathrm{pl}}\,, \tag{1}$$

where $\mathbf{w}$ is the antisymmetric tensor of crystal lattice rotation, $\boldsymbol{\varepsilon}_{\mathrm{e}}$ is the tensor of elastic strain of the lattice, while $\boldsymbol{\varepsilon}_{\mathrm{pl}}$ is the (generally nonsymmetric) tensor of plastic deformation. This tensor is often called the plastic distortion tensor, cf. e.g. [6, 7, 8, 9]. As a quantity related to it we define the dislocation density tensor as

$$\boldsymbol{\alpha}_{\mathrm{d}} \stackrel{\mathrm{df}}{=} \operatorname{rot} \boldsymbol{\varepsilon}_{\mathrm{pl}}\,. \tag{2}$$

In the index notation this equation reads $\alpha_{\mathrm{d}\,ij} = \varepsilon_{\mathrm{pl}\,im,n} e_{jmn}$, where $e_{jmn}$ is the respective representation of the alternating tensor. For clarity, while using the index notation we write the subscript of global quantities in parentheses.

Using the Stokes' theorem it is easy to show that the total Burgers vector of dislocations piercing the surface region $\Delta S$ bounded by a given Burgers circuit $C$ satisfies the following relations,

$$\mathbf{b} \stackrel{\mathrm{df}}{=} \oint_C \boldsymbol{\varepsilon}_{\mathrm{pl}}\,\mathrm{d}\boldsymbol{r} = \int_{\Delta S} \operatorname{rot} \boldsymbol{\varepsilon}_{\mathrm{pl}}\,\mathrm{d}\boldsymbol{S} = \int_{\Delta S} \boldsymbol{\alpha}_{\mathrm{d}}\,\mathrm{d}\boldsymbol{S}\,. \tag{3}$$

In the continuum theory of dislocations it is also assumed that the rate of plastic deformation satisfies the following kinematic relation,

$$\dot{\boldsymbol{\varepsilon}}_{\mathrm{pl}} = \boldsymbol{\alpha}_{\mathrm{d}} \times \mathbf{v}_{\mathrm{d}}\,, \tag{4}$$

where $\mathbf{v}_{\mathrm{d}}$ is the local dislocation velocity and $\times$ denotes the cross product. $\mathbf{v}_{\mathrm{d}}$ is defined as relative to the material, so that if $\mathbf{v}$ is the material velocity, then the total velocity of dislocations will be $\mathbf{v} + \mathbf{v}_{\mathrm{d}}$.

For dislocated crystals, the balance laws for mass, momentum, moment of momentum, energy and the inequality of entropy, respectively, can be stated in the same form as for the ordinary continuum, namely:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_v \rho\,\mathrm{d}v = 0\,, \tag{5}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_v \rho\mathbf{v}\,\mathrm{d}v = \int_s \boldsymbol{\sigma}\,\mathrm{d}\mathbf{s} + \int_v \rho\mathbf{j}\,\mathrm{d}v\,, \tag{6}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_v \mathbf{x}\times\rho\mathbf{v}\,\mathrm{d}v = \int_s \mathbf{x}\times\boldsymbol{\sigma}\,\mathrm{d}\mathbf{s} + \int_v \mathbf{x}\times\rho\mathbf{j}\,\mathrm{d}v\,, \tag{7}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_v \left(\rho u + \frac{1}{2}\rho\mathbf{v}\mathbf{v}\right)\mathrm{d}v = \int_s \mathbf{v}\boldsymbol{\sigma}\,\mathrm{d}\mathbf{s} + \int_v \rho\mathbf{j}\mathbf{v}\,\mathrm{d}v - \int_s \mathbf{q}_{\mathrm{T}}\,\mathrm{d}\mathbf{s} + \int_v \rho h\,\mathrm{d}v\,, \tag{8}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_v \rho\eta\,\mathrm{d}v \geq -\int_s \frac{\mathbf{q}_{\mathrm{T}}}{T}\,\mathrm{d}\mathbf{s} + \int_v \frac{\rho h}{T}\,\mathrm{d}v\,, \tag{9}$$

where $\rho$, $\boldsymbol{\sigma}$, $\mathbf{j}$, $\mathbf{v}$, $\mathbf{x}$, $u$, $\mathbf{q}_{\mathrm{T}}$, $h$, $\eta$, $T$ denote the mass density, Cauchy stress tensor, body force density, velocity, position vector, internal energy density, heat flow, heat source density, entropy density and temperature. The above integral equations lead to the following field equations

$$\dot{\rho} + \rho\,\operatorname{div}\mathbf{v} = 0\,, \tag{10}$$

$$\operatorname{div}\boldsymbol{\sigma} + \rho\mathbf{j} - \rho\dot{\mathbf{v}} = \mathbf{0}\,, \tag{11}$$

$$\boldsymbol{\sigma} - \boldsymbol{\sigma}^{\mathrm{T}} = \mathbf{0}\,, \tag{12}$$

$$-\rho\dot{u} + \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}_{\mathrm{e}} + \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}_{\mathrm{pl}} - \operatorname{div}\mathbf{q}_{\mathrm{T}} + \rho h = 0\,, \tag{13}$$

$$\rho\dot{\eta} + \operatorname{div}\left(\frac{\mathbf{q}_{\mathrm{T}}}{T}\right) - \frac{\rho h}{T} \geq 0\,, \tag{14}$$

where $\operatorname{div}\boldsymbol{\sigma} = \sigma_{ij,j}\mathbf{e}_i$ while $\mathbf{e}_i$ denotes the $i$-th base vector. If we assume that the plastic deformation is induced by the dislocation field motion, then, using (4) and (13) the inequality of entropy (14) can be rewritten in the form

$$-\rho\dot{\psi} - \rho\eta\dot{T} + \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}_e + \mathbf{f}_d \cdot \mathbf{v}_d - \frac{\mathbf{q}_T}{T}\operatorname{grad} T \geq 0 \tag{15}$$

where

$$\psi = u - \eta T, \tag{16}$$

$$\mathbf{f}_d = \boldsymbol{\sigma} \dot{\times} \boldsymbol{\alpha}_d, \tag{17}$$

$$\boldsymbol{\sigma} = \mathbf{D} : \boldsymbol{\varepsilon}_e. \tag{18}$$

In the latter equations $\psi$, $\mathbf{D}$ and $\mathbf{f}_d$ denote, respectively, the free energy density, elastic modulus tensor and the vector of the driving force acting on dislocations per unit material volume, while $\dot{\times}$ denotes the double product: the scalar one over the first subscripts and the cross one over the second ones, i.e. $f_{di} = \sigma_{jk}\alpha_{djl}e_{ikl}$. Equation (17) is a counterpart of the Peach-Koehler formula in the notation used here, cf. [3, 11, 13]. According to the thermodynamic restriction (15), the constitutive equations for the movement of the dislocation field can be stated in the following form,

$$\mathbf{v}_d = \mathbf{v}_d\left(\frac{\mathbf{f}_d}{\rho_d}\right), \tag{19}$$

where $\rho_d$ is the scalar density of dislocation determined as the total length of dislocations per unit volume. Additionally, $\rho_d$ is related to the dislocation density tensor by

$$\boldsymbol{\alpha}_d = \rho_d \boldsymbol{\alpha}_o \tag{20}$$

where $\boldsymbol{\alpha}_o = \mathbf{b} \otimes \mathbf{n}_3$ is the tensor describing geometry of unit density dislocation, $\mathbf{b}$ is the Burgers' vector and $\mathbf{n}_3$ is the unit vector normal to the plane. A detailed discussion of various tensor, vector and scalar dislocation measures has been presented by Dłużewski in [4].

## 3. Computer algorithm

Let us consider the dislocation motion in the elastic-plastic continuum at constant temperature. Usually such motion is induced by the stress field. On the basis of the set of equations presented in the previous section we may build a numerical model which will allow us to simulate the behaviour of a dislocated crystal under given imposed loads and boundary conditions. Discretization of the resulting set of equations by the finite element method yields to an algebraic equation system. By solving this system we obtain the values of displacements and dislocation density at the nodes and, from them, the problem dependent variables (strains, stresses) can be calculated.

The set of equations to be discretized consists of the rate form of the momentum equation (11), and a balance equation for the dislocations. Neglecting the change of configuration (small deformation approach) the material derivative of Eq. (2) takes the form

$$\dot{\boldsymbol{\alpha}}_d = \operatorname{rot}\dot{\boldsymbol{\varepsilon}}_{pl}. \tag{21}$$

Using Eq. (4), Eq. (21) can be rewritten as[2]

$$\dot{\alpha}_{dkl} = -(\alpha_{dkl}v_{dn})_{,n} + \alpha_{dkn,n}v_{dl} + \alpha_{dkm}v_{dl,m}. \tag{22}$$

Let us discuss the role of the sequential terms on the right hand side of (22).

[2]The following transformations have been applied:

$$\dot{\alpha}_{din} = (\alpha_{dij}e_{kjl}v_{dl})_{,m}e_{nkm} - \varepsilon_{plim,r}v_{dr,k}e_{nmk} = (\alpha_{dij}v_{dl})_{,m}e_{kjl}e_{kmn}.$$
$$= (\alpha_{dij}v_{dl})_{,m}(g_{jm}g_{ln} - g_{jn}g_{lm}) = (\alpha_{dim}v_{dn})_{,m} - (\alpha_{din}v_{dm})_{,m}.$$

- We can notice that the first term represents the effect of the dislocation transport.
- In the dislocation theory it is assumed that single dislocations cannot end within the crystal lattice. According to Nye [10] this corresponds to the following condition,

$$\operatorname{div} \boldsymbol{\alpha}_{\mathrm{d}} = \mathbf{0}\,, \tag{23}$$

from which results that the second term on the right hand of (22) always vanishes.

- The third term represents the effect of the reorientation of existing dislocations. In this paper our interest is focused on the plane problem of the plastic deformation induced by the movement of straight line dislocations in a crystal. Therefore, the third term also vanishes, since $\alpha_{\mathrm{d}\,k1} = 0$, $\alpha_{\mathrm{d}\,k2} = 0$ and $v_{\mathrm{d}\,n,3} = 0$ where the third coordinate is, by assumption, perpendicular to the plane problem and is parallel to the direction of the assumed dislocation lines.

In other words, for plain problems formulated in small deformations, we can assume that the dislocation velocity is governed by the following equation,

$$\dot{\boldsymbol{\alpha}}_{\mathrm{d}} + \operatorname{div}(\boldsymbol{\alpha}_{\mathrm{d}} \otimes \mathbf{v}_{\mathrm{d}}) = \mathbf{0}\,. \tag{24}$$

Summing up, after neglecting dynamic terms from the rate form of (11), replacing (20) in (24) and considering that $\boldsymbol{\alpha}_{\mathrm{o}}$ is constant, we conclude that, from the mathematical point of view, the solution procedure is equivalent to the solution of the following differential equation set

$$\begin{cases} \operatorname{div} \dot{\boldsymbol{\sigma}} = \mathbf{0}\,, \\ \dot{\rho}_{\mathrm{d}} + \operatorname{div}(\rho_{\mathrm{d}} \mathbf{v}_{\mathrm{d}}) = 0\,. \end{cases} \tag{25}$$

The concept of transporting a given material in terms of a scalar field has been successfully applied to other problems, e.g. to metal forming processes [1]. After application of the weighted residual method, the weak form of the differential equation set (25) yields

$$\begin{bmatrix} \mathbf{C}_u & \mathbf{0} \\ \mathbf{0} & \mathbf{C}_\rho \end{bmatrix} \begin{bmatrix} \dot{\mathbf{a}}_u \\ \dot{\mathbf{a}}_\rho \end{bmatrix} + \begin{bmatrix} \mathbf{P}_u \\ \mathbf{P}_\rho \end{bmatrix} = \begin{bmatrix} \dot{\mathbf{f}}_u \\ \mathbf{f}_\rho \end{bmatrix} \tag{26}$$

where $\mathbf{a}_u$ and $\mathbf{a}_\rho$, $\mathbf{f}_u$ and $\mathbf{f}_\rho$ are the nodal displacement vector, a defect density tensor, force vector and defect velocity vector, respectively, while

$$\mathbf{C}_u = \int_v \nabla^{\mathrm{T}} \mathbf{W}_u \, \mathbf{D} \, \nabla \mathbf{N} \, \mathrm{d}v\,, \tag{27}$$

$$\mathbf{C}_\rho = \int_v \mathbf{W}_\rho \otimes \mathbf{N} \, \mathrm{d}v\,, \tag{28}$$

$$\mathbf{P}_u = -\int_v \nabla^{\mathrm{T}} \mathbf{W}_u \mathbf{D} \dot{\boldsymbol{\epsilon}}_{\mathrm{pl}} \, \mathrm{d}v\,, \tag{29}$$

$$\mathbf{P}_\rho = \int_v (\nabla^{\mathrm{T}} \mathbf{W}_\rho \mathbf{v}_{\mathrm{d}}) \boldsymbol{\alpha}_{\mathrm{d}} \, \mathrm{d}v\,. \tag{30}$$

In Eq. (28), $\otimes$ denotes the dyadic product while $\mathbf{W}_u$ and $\mathbf{W}_\rho$ are the weighting functions for the momentum and defects balances, respectively and $\mathbf{N}$ are the shape functions. Equation (26) can be considered as the set of first order differential equations nonlinear with respect to $\mathbf{a}$,

$$\mathbf{C}\dot{\mathbf{a}} + \mathbf{P}_{\mathbf{a}} = \mathbf{f}\,. \tag{31}$$

Time discretization of (31) by the backward Euler scheme yields

$$\frac{1}{\Delta t}\mathbf{C}(\mathbf{a}_{n+1} - \mathbf{a}_n) + \mathbf{P}_{\mathbf{a}_{n+1}} = \mathbf{f} \tag{32}$$

from which the solution for time $t_{n+1}$, $\mathbf{a}_{n+1}$ is obtained. Equation (32) is solved by the Newton Raphson method, from which results the tangent matrix (cf. [12])

$$\mathbf{K}_{\mathrm{T}}^{(i)} = \mathbf{K}_{\mathrm{T}}^{L} + \mathbf{K}_{\mathrm{T}}^{NL} = \frac{\mathbf{C}}{\Delta \mathbf{t}} + \frac{\partial \mathbf{P}}{\partial \mathbf{a}_{n+1}^{(i)}}. \tag{33}$$

Up to now we have considered a general FEM algorithm which can be applied to the computer simulation of the motion of an arbitrarily chosen defect field. In accordance to the kind of defects, the above set can be supplemented by the respective kinematic equation relating the defect motion with the plastic deformation of crystals. For the case of dislocation motion, we substitute (4) into (29) and next to (33) to obtain the tangent stiffness matrix, which reads

$$\mathbf{K}_{\mathrm{T}}^{NL} = \begin{bmatrix} \displaystyle\int_{v_{\mathrm{el}}} \nabla^{\mathrm{T}} \mathbf{W}_u \mathbf{D} \left( \boldsymbol{\alpha}_{\mathrm{d}} \times \frac{\partial \mathbf{v}_{\mathrm{d}}}{\partial \mathbf{a}_u} \right) \mathrm{d}v & \displaystyle\int_{v_{\mathrm{el}}} \nabla^{\mathrm{T}} \mathbf{W}_u \mathbf{D}(-\mathbf{v}_{\mathrm{d}} \times \mathbf{N}) \, \mathrm{d}v \\ \displaystyle\int_{v_{\mathrm{el}}} \nabla^{\mathrm{T}} \mathbf{W}_\rho \left( \frac{\partial \mathbf{v}_{\mathrm{d}}}{\partial \mathbf{a}_u} \otimes \boldsymbol{\alpha}_{\mathrm{d}} \right) \mathrm{d}v & \displaystyle\int_{v_{\mathrm{el}}} (\nabla^{\mathrm{T}} \mathbf{W}_\rho \mathbf{v}_{\mathrm{d}}) \mathbf{N} \, \mathrm{d}v \end{bmatrix}. \tag{34}$$

It is worth pointing out that the last dependency is still general with respect to the choice of constitutive equations governing the dislocation motion.

## 4. Numerical example

In order to test the present formulation we consider a monocrystal in a square domain, where a shear tensile state is induced by external forces.

The following assumptions have been made:

1. Plane motion of monomial edge dislocation field is considered. These dislocations are directed perpendicular to the considered plane, while the Burgers' vector is deviated 20° from the horizontal direction on this plane, i.e. $\mathbf{b} = b\,(\cos 20° \mathbf{n}_1 + \sin 20° \mathbf{n}_2)$, where the mutually orthogonal vectors $\mathbf{n}_1$ and $\mathbf{n}_2$ lay on the considered plane while $\mathbf{n}_3$ is perpendicular to it.
2. The dislocations are in conservative motion, i.e. $\dot{\boldsymbol{\varepsilon}}_{\mathrm{pl}} = \rho_{\mathrm{d}} v_{\mathrm{d}} \boldsymbol{\varepsilon}_{\circ}$, where $\boldsymbol{\varepsilon}_{\circ} = \mathbf{b} \otimes (\mathbf{n}_3 \times \mathbf{b})$, and $\mathbf{v}_{\mathrm{d}} = v_{\mathrm{d}} \frac{\mathbf{b}}{|\mathbf{b}|}$,
3. The dislocation velocity is proportional to the Peach-Koehler force. This means that for the conservative motion, we have $v_{\mathrm{d}} = m\boldsymbol{\sigma} : \boldsymbol{\varepsilon}_{\circ}$ or, equivalently, $\mathbf{v}_{\mathrm{d}} = \mathbf{m}(\boldsymbol{\sigma} \dot{\times} \boldsymbol{\alpha}_{\circ})$, where $\mathbf{m} = m\mathbf{b} \otimes \mathbf{b}$ and $\boldsymbol{\alpha}_{\circ} = \mathbf{b} \otimes \mathbf{n}_3$.

It can be shown that, under the above assumptions, the tangent stiffness matrix for an element, (34), takes the form

$$\mathbf{K}_{\mathrm{T}}^{NL} = \begin{bmatrix} \displaystyle\int_{v_{\mathrm{el}}} \nabla^{T} \mathbf{W}_u \mathbf{D} \boldsymbol{\varepsilon}_{\circ} \rho_{\mathrm{d}} m \boldsymbol{\varepsilon}_{\circ} \mathbf{D} \nabla \mathbf{N} \, \mathrm{d}v & \displaystyle\int_{v_{\mathrm{el}}} \nabla^{T} \mathbf{W}_u \mathbf{D} \boldsymbol{\varepsilon}_{\circ} v_{\mathrm{d}} \mathbf{N} \, \mathrm{d}v \\ \displaystyle\int_{v_{\mathrm{el}}} (\nabla^{\mathrm{T}} \mathbf{W}_\rho \mathbf{b}) \rho_{\mathrm{d}} m \boldsymbol{\varepsilon}_{\circ} \mathbf{D} \nabla \mathbf{N} \, \mathrm{d}v & \displaystyle\int_{v_{\mathrm{el}}} (\nabla^{\mathrm{T}} \mathbf{W}_\rho \mathbf{b}) v_{\mathrm{d}} \mathbf{N} \, \mathrm{d}v \end{bmatrix} \tag{35}$$

where $v_{\mathrm{el}}$ denotes the volume of the finite element. In the discussed example the Galerkin method has been applied, i.e. $\mathbf{W}_\rho = \mathbf{W}_u = \mathbf{N}$.

As a basis for computer analysis we have used the finite element code FEAP (see [12]). In order to simulate the dislocation motion, the additional finite element procedures have been inserted. Since the problem is formulated in rate form, it is necessary to store not only the nodal dislocation densities, but the total plastic deformations for the Gauss points inside the elements as well. In our approach the plastic deformations are relatively large in magnitude with respect to the (small) elastic deformations considered. For this reason small time steps have to be taken. The step size in the present work has been such chosen so that the plastic deformation increment would be of

Table 1. Material constants

| | Notation | Value |
|---|---|---|
| Kirchhoff modulus | G | $0.3 \times 10^5$ MPa |
| Young modulus | E | $0.7 \times 10^5$ MPa |
| Burgers vector | b | 3Å |
| Dislocation mobility | m | $1 \times 10^{13} \frac{\text{m}}{\text{s·MPa}}$ |

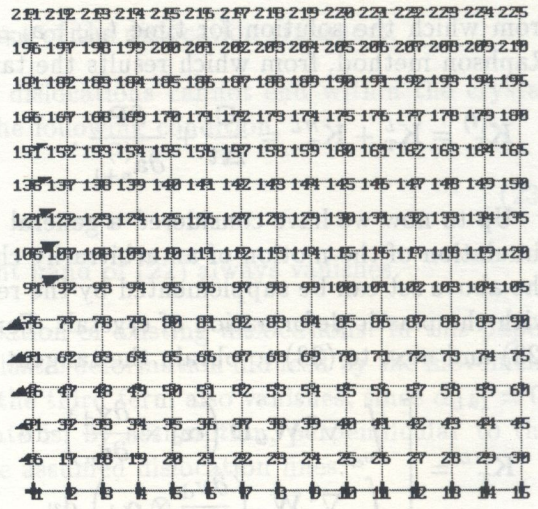

Fig. 1. Discretization data and loading

the same range as the elastic one. When dealing with elastic-plastic deformations, an elastic-plastic stiffness matrix is used. Usually, this leads to difficulties to correctly predict the unloading process. In our calculation, the stress increment was not determined on the basis of the strain increment, but on the basis of the stored total strain value at the Gauss points. Such approach allows to avoid elastic spring back problems.

In our calculations a square region $0.7\mu\text{m} \times 0.7\mu\text{m}$ of a crystal has been divided into 196 bilinear elements. The assumed material constants for this crystal are shown in Table 1. The external loading applied to this region together with the mesh and node numbering are presented in Fig. 1.In what concerns the kinematics, the domain is simply supported by constraining the displacements in the left lower corner (node 1) and the vertical displacement in the rest of the lower boundary (nodes 2 to 15). The applied loads change sign between nodes 76 and 91. These nodes have been assumed to be a source of edge dislocations with the following components of the Burgers' vector $b_x = b\cos 20°$ and $b_y = b\sin 20°$. The boundary conditions for the dislocations are as follows: a dislocation flux value of $f = 6\times10^5/(\text{m·s})$ has been assumed both in nodes 76 and 91, whereas in the rest of the left, upper and lower boundaries zero dislocation flux (natural boundary conditions) have been adopted. On the right boundary zero dislocation density has been imposed. Therefore, the dislocation flux is found there as a solution of such stated boundary value problem. In Fig. 2 the shear stress contours are shown at the deformed configuration. The considered deformation–flux process has

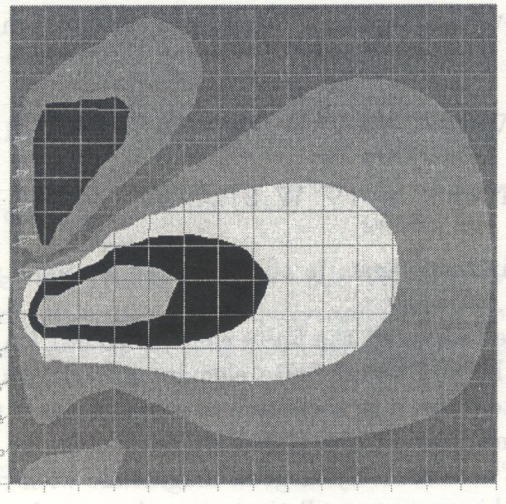


Fig. 2. Shear stress contours at initially deformed configuration and loading

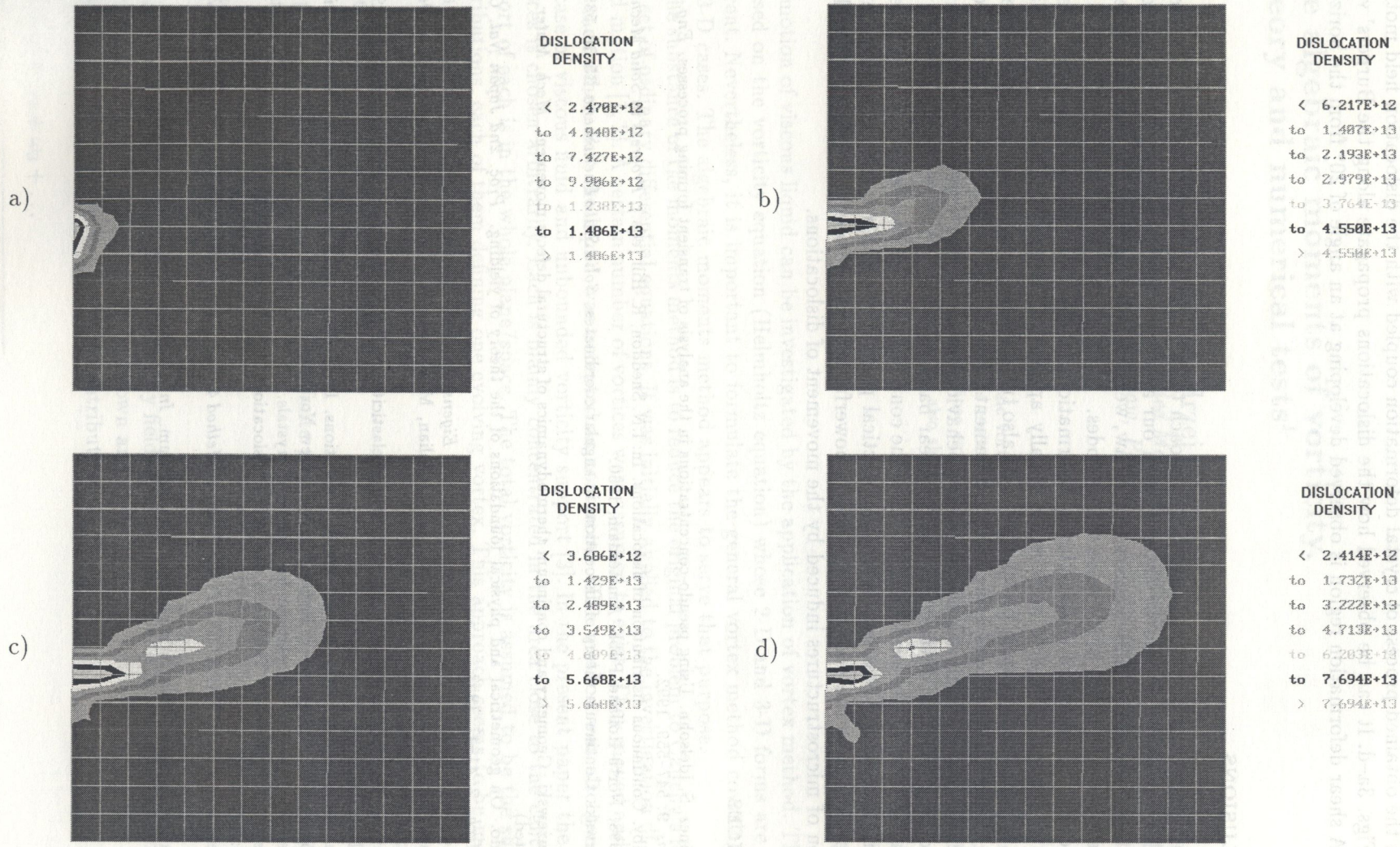


**Fig. 3.** Dislocation density distributions at a) $t = 1\,\mathrm{s}$, b) $t = 10\,\mathrm{s}$, c) $t = 20\,\mathrm{s}$, d) $t = 33\,\mathrm{s}$

been integrated using the backward Euler method with the time step $\Delta t = 1\,\mathrm{s}$. As a result of this calculation the obtained process of crystal deformation coupled with the dislocation field motion is shown in Figs. 3a–d. It can be observed how the dislocations propagate along the Burgers' vector direction. A shear deformation region is observed developing at an angle of 20° from the horizontal axis.

## 5. Conclusions

The present results can be treated as a first approach to the application of FEM to the continuum theory of dislocations. It should be noted that in our approach the fundamental role is played by the dislocation balance law (22). Thanks to this law, we were able to predict the dislocation density inside the elements in terms of its value in the nodes.

While solving problems of elastic-plastic deformations of solids the phenomenological theories based on the concept of a yield surface are usually applied. The presented computer simulation shows that the continuum theory of defects can be also treated as an alternative approach, moreover, this theory can be also employed using the finite element method. The results shown in the numerical example reflect many additional aspects of the behaviour of deforming crystals, e.g. the coupling of the defect flux with the development of the shear band regions.

These capabilities of the model indicate that the continuum theory of defects has large potential abilities for practical applications. From the practical point of view this means also that the considered approach gives the possibility to built a powerful tool for the analysis of the elastic-plastic deformation of microstructures induced by the movement of dislocations.

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