

A NOTE ON THE KINEMATICS OF DISLOCATIONS IN CRYSTALS.

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ABSTRACT. A part of the theory of dislocations in crystals is revised with the aim to fit it into the framework of the nonlinear theory of plasticity initially designed for amorphous glassy materials.

1. GEOMETRY OF DISLOCATIONS.

Dislocations provide a microscopic mechanism explaining the plasticity of crystals. The idea of dislocations suggested by Taylor and Orowan in 1934 is illustrated

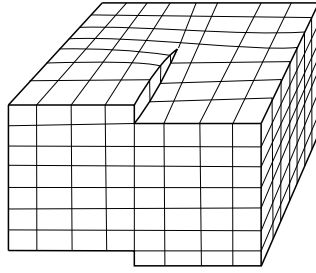


Fig. 1.1

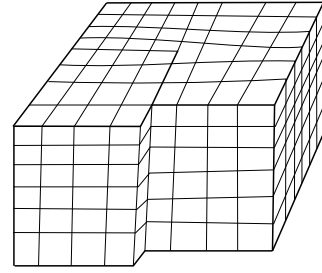


Fig. 1.2

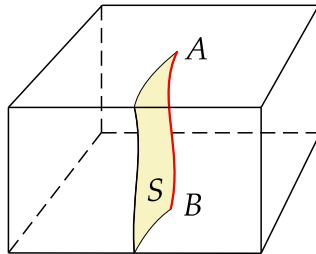


Fig. 1.3

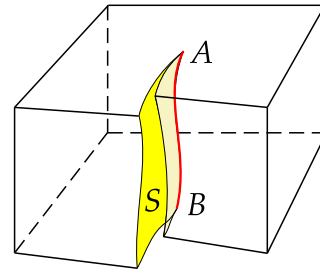


Fig. 1.4

on the first two figures. Fig. 1.1 and Fig. 1.2 show screw-type and edge-type dislo-

cations respectively. There are also mixed type dislocations combining the features of both screw and edge dislocations.

In the continuous limit, a single dislocation can be understood as shown on Fig. 1.3 and Fig. 1.4 above. Imagine a smooth curve AB within the continuous medium being the edge of some surface S . This fact is denoted as $AB = \partial S$. Imagine that the medium is cut along the surface S and then glued with some displacement (see Fig. 1.4). Upon gluing, all points of the surface S outside the dislocation line AB become regular points of the medium (as regular as all other points within the medium). Though a dislocation produces the stress and elastic deformation around itself, it doesn't produce the defects of crystalline grid outside the dislocation line AB . Therefore, if we cut out a sufficiently small spherical neighborhood G of some point $C \notin AB$ and then release it, we get some stress-free crystalline body with no defects of the crystalline grid (see Fig. 1.5 and Fig. 1.6). Mathematically this fact is expressed by a map from the spherical neighborhood G

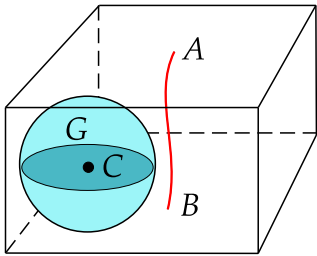


Fig. 1.5

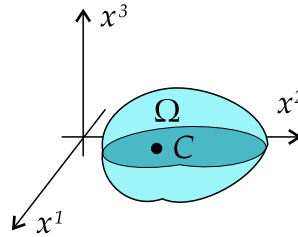


Fig. 1.6

of the point C to some domain Ω in \mathbb{R}^3 (see Fig. 1.6). This map can be given by three functions

$$\begin{cases} x^1 = x^1(y^1, y^2, y^3), \\ x^2 = x^2(y^1, y^2, y^3), \\ x^3 = x^3(y^1, y^2, y^3). \end{cases} \quad (1.1)$$

Here y^1, y^2, y^3 are some curvilinear coordinates within the real crystalline body, while x^1, x^2, x^3 are Cartesian coordinates in the three-dimensional space \mathbb{R}^3 which we used in our mental experiment where we cut out the ball G . The Jacobi matrix

$$\hat{T}_j^i = \frac{\partial x^i}{\partial y^j} \quad (1.2)$$

of the map (1.1) is non-degenerate since otherwise it would mean the infinite compressibility of the medium. The map $f : G \rightarrow \Omega$ is invertible and due to the non-degeneracy condition $\det \hat{\mathbf{T}} \neq 0$, the inverse map $f^{-1} : \Omega \rightarrow G$ is also given by three smooth functions similar to (1.1):

$$\begin{cases} y^1 = y^1(x^1, x^2, x^3), \\ y^2 = y^2(x^1, x^2, x^3), \\ y^3 = y^3(x^1, x^2, x^3). \end{cases} \quad (1.3)$$

By differentiating (1.3) we find the inverse Jacobi matrix $\hat{\mathbf{S}} = \hat{\mathbf{T}}^{-1}$:

$$\hat{S}_j^i = \frac{\partial y^i}{\partial x^j}. \quad (1.4)$$

Note that the map (1.1) can be extended to any connected and simply connected domain within the crystalline body that comprises the point C and does not comprise the points of dislocation, line AB . Such an extension is non-degenerate ($\det \hat{\mathbf{T}} \neq 0$), but in the general case it is not globally bijective. In such a case, the inverse map (1.3) is defined only locally. However, the components of the mutually inverse Jacobi matrices (1.2) and (1.4) can be treated as global functions

$$\hat{T}_j^i = \hat{T}_j^i(y^1, y^2, y^3), \quad \hat{S}_j^i = \hat{S}_j^i(y^1, y^2, y^3) \quad (1.5)$$

defined at all points of the crystal except for those lying on the dislocation line AB .

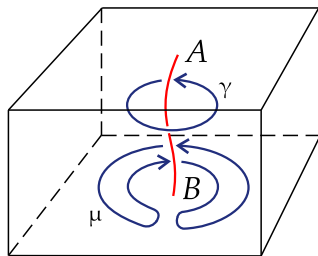


Fig. 1.7

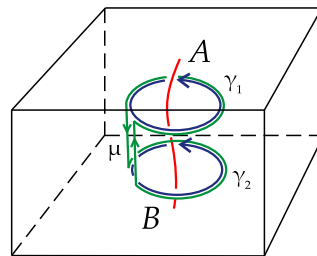


Fig. 1.8

Now let's consider a crystal with one dislocation line AB and define the following path integral along some closed path γ that encircles the dislocation line AB :

$$b^i = \oint_{\gamma} \sum_{j=1}^3 \hat{T}_j^i \tau^j ds \quad (1.6)$$

(see Fig. 1.7). Here τ^1, τ^2, τ^3 are the components of the tangent vector $\boldsymbol{\tau}$ of the path γ . For the path given parametrically by three functions

$$y^1 = y^1(s), \quad y^2 = y^2(s), \quad y^3 = y^3(s)$$

this tangent vector is defined by three derivatives

$$\tau^j = \frac{dy^j}{ds}, \quad j = 1, 2, 3.$$

Note that the path integral (1.6) along any path that does not encircle the dislocation line (see Fig. 1.7) is identically zero:

$$\oint_{\mu} \sum_{j=1}^3 \hat{T}_j^i \tau^j ds = 0. \quad (1.7)$$

Indeed, due to (1.2) the integral (1.7) is transformed into the path integral of the second kind applied to the total differential of the smooth function $x^i(y^1, y^2, y^3)$:

$$\oint_{\mu} \sum_{j=1}^3 \hat{T}_j^i \tau^j ds = \oint_{\mu} dx^i(y^1, y^2, y^3) = 0.$$

Theorem 1.1. *The value of the integral (1.6) is an invariant of the dislocation AB . It does not depend on a particular contour γ encircling the dislocation line.*

The proof of this theorem is obvious from Fig. 1.8. Indeed, for the pair of contours γ_1 and γ_2 on Fig. 1.8 we have

$$\oint_{\gamma_1} \sum_{j=1}^3 \hat{T}_j^i \tau^j ds - \oint_{\gamma_2} \sum_{j=1}^3 \hat{T}_j^i \tau^j ds = \oint_{\mu} \sum_{j=1}^3 \hat{T}_j^i \tau^j ds = 0.$$

Definition 1.1. Three constants b^1, b^2, b^3 determined by the integral (1.6) are the components of a vector \mathbf{b} characterizing the dislocation line. This vector is called the *Burgers vector* of a dislocation.

Note that the Burgers vector \mathbf{b} is not a vector in the space of real crystalline body. It is associated with the imaginary space of stress-free crystalline matter shown on Fig. 1.6. In what follows we shall call this space the *Burgers space*.

The concept of Burgers space is convenient for understanding the nature of matrices (1.5). Although they have upper and lower indices and depend on the coordinates of a point in the real crystalline body, they are not components of traditional tensor fields. They are *double space tensors*. The index j in \hat{T}_j^i is a covariant index associated with the space of real crystalline body, while i is a contravariant index associated with the Burgers space. As for the inverse matrix $\hat{\mathbf{S}} = \hat{\mathbf{T}}^{-1}$ in (1.5), its lower index j is associated with the Burgers space, while its upper index is related to the real crystalline body.

Usually each dislocation line is a closed path within crystalline body. Otherwise, if it is not closed, it should begin at some point on the boundary of the crystalline body and it should end at some other point which is on the boundary as well.

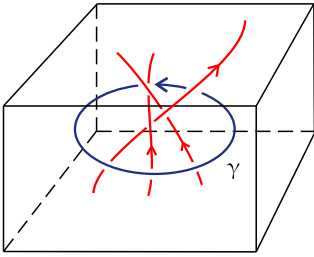


Fig. 1.9

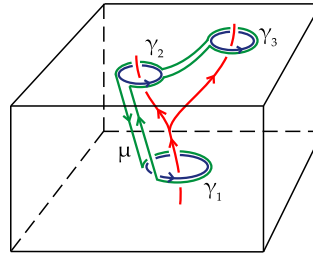


Fig. 1.10

Usually, each dislocation line is taken with some orientation assigned to it. One can change the orientation of a dislocation line, however, in this case its Burgers

vector \mathbf{b} is changed for the opposite one: $\mathbf{b} \rightarrow -\mathbf{b}$. If the closed contour γ encircles several dislocation lines (see Fig. 1.9), then

$$\oint_{\gamma} \sum_{j=1}^3 \hat{T}_j^i \tau^j ds = \pm b^i(1) \pm \dots \pm b^i(N). \quad (1.8)$$

The sign of each Burgers vector in right hand side of (1.8) is determined by the orientation of corresponding dislocation line.

In some cases dislocation lines have brunching points as shown on Fig. 1.10. For the Burgers vectors of dislocation lines in this case we have the equality

$$\mathbf{b}_1 = \mathbf{b}_2 + \mathbf{b}_3. \quad (1.9)$$

The equality (1.9) is an analog of Kirchhoff rule for currents in electromagnetism. Its proof is clear from Fig. 1.10.

2. CONTINUAL LIMIT FOR DISLOCATIONS.

In order to detect macroscopic phenomena associated with dislocations we should have a substantial amount of dislocations in each macroscopically essential volume of the medium. In this case, instead of considering individual dislocation lines, we consider the density of Burgers vectors for dislocations

$$\rho_j^i = \rho_j^i(y^1, y^2, y^3). \quad (2.1)$$

Like \mathbf{S} and \mathbf{T} in (1.5), the functions (2.1) are components of a double space tensorial field. The upper index i in (2.1) is associated with the Burgers space, while j is a traditional tensorial index associated with the space of real crystalline body.

Since dislocation lines cannot end in the interior of a crystal and since they obey the conservation law (1.9) at their brunching points, the amount of Burgers vectors flowing into some domain trough its boundary with dislocation lines is equal to the amount of this vector flowing out of this domain. This fact is written as the following integral equality for the density of Burgers vectors (2.1):

$$\int_{\partial\Omega} \sum_{j=1}^3 \rho_j^i n^j dS = 0. \quad (2.2)$$

Here n^1, n^2, n^3 are components of the unit vector \mathbf{n} of the external normal to the boundary $\partial\Omega$ of the domain Ω . The differential form of the equality (2.2) looks like

$$\sum_{j=1}^3 \sum_{k=1}^3 g^{kj} \nabla_k \rho_j^i = 0. \quad (2.3)$$

The covariant derivative $\nabla_k \rho_j^i$ in the formula (2.3) is calculated as follows:

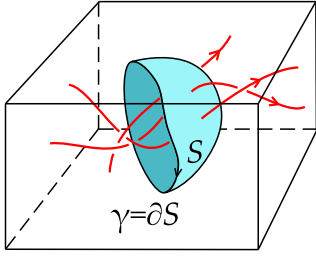
$$\nabla_k \rho_j^i = \frac{\partial \rho_j^i}{\partial y^k} - \sum_{q=1}^3 \Gamma_{kj}^q \rho_q^i. \quad (2.4)$$

Note that g^{kj} in (2.3) are components of the metric tensor and Γ_{kj}^q in (2.4) are components of the metric connection. They are determined by the choice of curvilinear coordinates y^1, y^2, y^3 (see [1]). Note also that in writing (2.4), we do not apply the standard rule of covariant differentiation to the upper index i . This is because it is associated with the Burgers space other than the space of real crystalline body. In short form the equality (2.3) is written as

$$\operatorname{div} \boldsymbol{\rho} = 0. \quad (2.5)$$

In this form (2.5) the equality (2.3) resembles the Maxwell equation $\operatorname{div} \mathbf{H} = 0$ in electromagnetism. However, one should remember the difference: \mathbf{H} is a vector, while $\boldsymbol{\rho}$ in (2.5) is a double space tensor.

Let S be some surface spanned onto the contour γ . Then $\gamma = \partial S$ (see Fig. 2.1). The total flow of Burgers vectors across the surface S is given by the following surface integral (compare with (2.2)):



$$b^i = \int_S \sum_{j=1}^3 \rho_j^i n^j dS. \quad (2.6)$$

The value of the integral (2.6) cannot change unless some dislocation lines move and cross the contour γ . For this reason the time derivative db^i/dt is given by some path integral along the contour γ :

$$\frac{db^i}{dt} = - \oint_{\gamma} \sum_{k=1}^3 j_k^i \tau^k ds. \quad (2.7)$$

Fig. 2.1

The double space tensorial quantity j_k^i in (2.7) is called the *current of Burgers vectors* produced by moving dislocations. Combining (2.6) and (2.7), we get

$$\int_S \sum_{j=1}^3 \frac{\partial \rho_j^i}{\partial t} n^j dS + \oint_{\partial S} \sum_{k=1}^3 j_k^i \tau^k ds = 0. \quad (2.8)$$

The integral equation (2.8) can be transformed to differential form by applying the Stokes formula. As a result we obtain the following equation:

$$\frac{\partial \rho_k^i}{\partial t} + \sum_{q=1}^3 \sum_{p=1}^3 \sum_{r=1}^3 \sum_{m=1}^3 \omega_{kqp} g^{qr} g^{pm} \nabla_r j_m^i = 0. \quad (2.9)$$

Here g^{qr} and g^{pm} are the components of metric tensor, and ω_{kqp} are the components of a completely skew-symmetric tensor. It is called the *volume tensor*. Its components are expressed through Levi-Civita symbol:

$$\omega_{kqp} = \sqrt{\det(g_{ij})} \varepsilon_{kqp}$$

(see more details in [1]). When applying the covariant derivative ∇_r to a double space tensor one should remember that the indices associated with the Burgers space are ignored. For the derivative $\nabla_r j_m^i$ in (2.9) we have

$$\nabla_r j_m^i = \frac{\partial j_m^i}{\partial y^r} - \sum_{s=1}^3 \Gamma_{rm}^s j_s^i \quad (2.10)$$

(compare (2.10) and (2.4)). Like the equation (2.5) above, the differential equation (2.9) can be written in a shorter form:

$$\frac{\partial \boldsymbol{\rho}}{\partial t} + \text{rot } \mathbf{j} = 0. \quad (2.11)$$

Like the equation (2.5), this equation (2.11) is an analog of corresponding Maxwell equation in electromagnetism (see [2]):

$$\frac{1}{c} \frac{\partial \mathbf{H}}{\partial t} + \text{rot } \mathbf{E} = 0.$$

Now let's return to the matrices (1.5). For a single dislocation they are determined by formulas (1.2) and (1.4). Usually they are singular functions at the points of dislocation line, just like Coulomb potential of a point charge. However, if charges are treated as continuously smeared in the space, the electric potential $\varphi(t, y^1, y^2, y^3)$ is a smooth function. Similarly, in continuous limit of dislocation theory $\hat{T}_j^i(t, y^1, y^2, y^3)$ and $\hat{S}_j^i(t, y^1, y^2, y^3)$ are smooth functions forming two matrices inverse to each other. In this case they are not determined by formulas (1.2) and (1.4) any more. Instead, we have the equality

$$\oint_{\partial S} \sum_{j=1}^3 \hat{T}_j^i \tau^j ds = \int_S \sum_{j=1}^3 \rho_j^i n^j dS \quad (2.12)$$

derived from (1.8). Applying the Stokes formula to (2.12), we get

$$\text{rot } \hat{\mathbf{T}} = \boldsymbol{\rho}. \quad (2.13)$$

In coordinate form the equation (2.13) is written as follows:

$$\sum_{q=1}^3 \sum_{p=1}^3 \sum_{r=1}^3 \sum_{m=1}^3 \omega_{kqp} g^{qr} g^{pm} \nabla_r \hat{T}_m^i = \rho_k^i.$$

Comparing (2.13) with $\mathbf{H} = \text{rot } \mathbf{A}$, we conclude that the double space tensor field $\hat{\mathbf{T}}$ with components $\hat{T}_j^i(t, y^1, y^2, y^3)$ here plays the same role as the vector-potential \mathbf{A} in electromagnetism.

3. DEFORMATION TENSORS.

Let's consider the motion of a crystalline medium in the presence of dislocations in it. Here we reproduce in part the content of [3] in order to have the same

notations. Suppose that a point of the medium with coordinates $\tilde{y}^1, \tilde{y}^2, \tilde{y}^3$ has moved to the point with coordinates y^1, y^2, y^3 . Then we have a map:

$$\begin{cases} y^1 = y^1(t, \tilde{y}^1, \tilde{y}^2, \tilde{y}^3), \\ y^2 = y^2(t, \tilde{y}^1, \tilde{y}^2, \tilde{y}^3), \\ y^3 = y^3(t, \tilde{y}^1, \tilde{y}^2, \tilde{y}^3). \end{cases} \quad (3.1)$$

This is the displacement map τ . The argument t in (3.1) is responsible for the time evolution of the displacement. The time derivatives of the functions (3.1) determine the components of the velocity vector \mathbf{v} :

$$v^i = \dot{y}^i = \frac{\partial y^i}{\partial t}, \quad i = 1, 2, 3. \quad (3.2)$$

As defined in (3.2), v^1, v^2, v^3 are the functions of $t, \tilde{y}^1, \tilde{y}^2, \tilde{y}^3$. However, in order to interpret them as the components of a vector field, they should depend on the coordinates of the current actual position of a point of the medium. To change the arguments of the derivatives (3.2) we use the inverse displacement map τ^{-1} :

$$\begin{cases} \tilde{y}^1 = \tilde{y}^1(t, y^1, y^2, y^3), \\ \tilde{y}^2 = \tilde{y}^2(t, y^1, y^2, y^3), \\ \tilde{y}^3 = \tilde{y}^3(t, y^1, y^2, y^3). \end{cases} \quad (3.3)$$

The time dependent maps (3.1) and (3.4) define two Jacobi matrices \tilde{S} and \tilde{T} :

$$\tilde{S}_j^i = \frac{\partial y^i}{\partial \tilde{y}^j}, \quad \tilde{T}_j^i = \frac{\partial \tilde{y}^i}{\partial y^j}. \quad (3.4)$$

The nonlinear deformation tensor \mathbf{G} then is defined as follows (see [3]):

$$G_{ij} = \sum_{r=1}^3 \sum_{s=1}^3 g_{rs}(\tilde{y}^1, \tilde{y}^2, \tilde{y}^3) \tilde{T}_i^r \tilde{T}_j^s. \quad (3.5)$$

Upon transforming all arguments in (3.5) into t, y^1, y^2, y^3 we get a tensor field \mathbf{G} with components $G_{ij} = G_{ij}(t, y^1, y^2, y^3)$. Differentiating (3.5), by direct calculations one can derive the following formula:

$$\frac{\partial G_{ij}}{\partial t} + \sum_{k=1}^3 v^k \nabla_k G_{ij} = - \sum_{k=1}^3 G_{kj} \nabla_i v^k - \sum_{k=1}^3 G_{ik} \nabla_j v^k. \quad (3.6)$$

In order to describe the plasticity of amorphous materials in [3] the following decomposition of the deformation tensor \mathbf{G} was suggested:

$$G_{ij} = \sum_{k=1}^3 \sum_{q=1}^3 \check{G}_i^k \hat{G}_{kq} \check{G}_j^q. \quad (3.7)$$

Here \hat{G}_{kq} are components of the elastic deformation tensor $\hat{\mathbf{G}}$, while \check{G}_i^k and \check{G}_j^q are components of the plastic deformation tensor $\check{\mathbf{G}}$. For these tensor fields $\hat{\mathbf{G}}$ and $\check{\mathbf{G}}$ in [3] the following evolution equations were suggested:

$$\begin{aligned} \frac{\partial \hat{G}_{kq}}{\partial t} + \sum_{r=1}^3 v^r \nabla_r \hat{G}_{kq} = & - \sum_{r=1}^3 \nabla_k v^r \hat{G}_{rq} - \sum_{r=1}^3 \hat{G}_{kr} \nabla_q v^r + \\ & + \sum_{r=1}^3 \theta_k^r \hat{G}_{rq} + \sum_{r=1}^3 \hat{G}_{kr} \theta_q^r. \end{aligned} \quad (3.8)$$

$$\frac{\partial \check{G}_i^k}{\partial t} + \sum_{r=1}^3 v^r \nabla_r \check{G}_i^k = \sum_{r=1}^3 (\check{G}_i^r \nabla_r v^k - \nabla_i v^r \check{G}_r^k) - \sum_{r=1}^3 \theta_r^k \check{G}_i^r. \quad (3.9)$$

The main goal of the present paper is to show that the decomposition (3.7) and the differential equations (3.8) and (3.9) can be consistently incorporated into the existing theory of plasticity in crystals in its nonlinear version.

4. KINEMATICS OF A DISLOCATED MEDIUM.

Let's begin with the equation (2.11) and substitute (2.13) into it. As a result we obtain the following differential equation:

$$\text{rot} \left(\frac{\partial \hat{\mathbf{T}}}{\partial t} + \mathbf{j} \right) = 0.$$

It is known that a vectorial field with zero curl is the gradient of some scalar field:

$$\frac{\partial \hat{\mathbf{T}}}{\partial t} + \mathbf{j} = -\text{grad } \mathbf{w}. \quad (4.1)$$

In our case all of the fields $\hat{\mathbf{T}}$, \mathbf{j} and \mathbf{w} in (4.1) are double space tensors; they have one upper index associated with the Burgers space. Therefore, (4.1) is written as

$$\frac{\partial \hat{T}_k^i}{\partial t} + j_k^i = -\frac{\partial w^i}{\partial y^k}. \quad (4.2)$$

The vector \mathbf{w} in (4.2) can be interpreted as the velocity vector (it easy to check that its components w^1, w^2, w^3 are measured in $cm \cdot sec^{-1}$). However, $\mathbf{w} \neq \mathbf{v}$. Indeed, the components of the velocity vector \mathbf{v} defined in (3.2) and then transformed into the arguments t, y^1, y^2, y^3 by means of the map (3.3) represent a traditional tensor field with one upper index, while \mathbf{w} is a double space tensor field. Below we shall understand \mathbf{w} as an independent parameter of a dislocated medium. The physical nature of this parameter is not yet clear to us, it will be studied in separate paper. However, there is a transparent analogy with electromagnetism:

$$\frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} + \mathbf{E} = -\text{grad } \varphi.$$

Comparing (4.1) with this equality, we find that \mathbf{w} is an analog of the scalar potential φ of electromagnetic field. Moreover, this equality supports our previous associations of $\hat{\mathbf{T}}$ with \mathbf{A} , \mathbf{j} with \mathbf{E} and $\boldsymbol{\rho}$ with \mathbf{H} .

Suppose that the initial state of our crystalline medium is free of dislocations. Below we assume that it is stress-free too. Then

$$\rho_k^i(0, \tilde{y}^1, \tilde{y}^2, \tilde{y}^3) = 0, \quad j_k^i(0, \tilde{y}^1, \tilde{y}^2, \tilde{y}^3) = 0. \quad (4.3)$$

Due to (4.3) we can arrange the bijective map from the space of the real crystalline body to the Burgers space. It is given by three functions

$$\begin{cases} x^1 = x^1(\tilde{y}^1, \tilde{y}^2, \tilde{y}^3), \\ x^2 = x^2(\tilde{y}^1, \tilde{y}^2, \tilde{y}^3), \\ x^3 = x^3(\tilde{y}^1, \tilde{y}^2, \tilde{y}^3). \end{cases} \quad (4.4)$$

The map (4.4) is an isometry because we assume that the initial state of the crystal has no deformation. The isometry condition is written as

$$g_{rs}(\tilde{y}^1, \tilde{y}^2, \tilde{y}^3) = \sum_{p=1}^3 \sum_{q=1}^3 \dot{g}_{pq} \overset{\star}{T}_r^p \overset{\star}{T}_s^q. \quad (4.5)$$

Here \dot{g}_{pq} are the components of metric tensor in the Burgers space, while $\overset{\star}{T}_r^p$ and $\overset{\star}{T}_s^q$ are the components of Jacobi matrix for the map (4.4):

$$\overset{\star}{T}_r^p = \frac{\partial x^p}{\partial \tilde{y}^r}.$$

Note that $\dot{g}_{pq} = \text{const}$ since we choose Cartesian coordinates in the Burgers space (see Fig. 1.6).

The next step is to add the time variable to the map (4.4). For this purpose let's use the inverse evolution map (3.3) and let's consider the composite map

$$\begin{cases} x^1 = x^1(\tilde{y}^1(t, y^1, y^2, y^3), \dots, \tilde{y}^3(t, y^1, y^2, y^3)), \\ x^2 = x^2(\tilde{y}^1(t, y^1, y^2, y^3), \dots, \tilde{y}^3(t, y^1, y^2, y^3)), \\ x^3 = x^3(\tilde{y}^1(t, y^1, y^2, y^3), \dots, \tilde{y}^3(t, y^1, y^2, y^3)). \end{cases} \quad (4.6)$$

Using the chain rule, for the Jacobi matrix of the map (4.6) we write

$$T_r^p = \frac{\partial x^p}{\partial y^i} = \sum_{r=1}^3 \overset{\star}{T}_r^p \tilde{T}_i^r. \quad (4.7)$$

From (3.5), (4.5), and (4.7) one easily derives

$$G_{ij} = \sum_{r=1}^3 \sum_{s=1}^3 \dot{g}_{pq} \overset{\star}{T}_i^p \overset{\star}{T}_j^q. \quad (4.8)$$

The equality (4.8) means that the deformation tensor \mathbf{G} can be defined through the composite map (4.6). As for the matrix (4.7), we interpret T_r^p as the components of a double space tensor \mathbf{T} . Both tensors \mathbf{T} and $\hat{\mathbf{T}}$ are called the *distorsion tensors* (see [4–7]): \mathbf{T} represents the *compatible distorsion* since it is given by partial derivatives in (4.7), while $\hat{\mathbf{T}}$ represents the *incompatible distorsion* since the equality (1.2) is not valid upon passing to the continuous limit (see (2.12) and (2.13), see also the comment above the formula (2.12)).

The compatible distorsion arises due to the macroscopic deformation of a crystal. In the elastic case, the macroscopic deformation is transferred to the microscopic level and produces the same distorsion of interatomic bonds (see Fig. 4.1 and Fig. 4.2). The plastic deformation is that very case, when some interatomic bonds

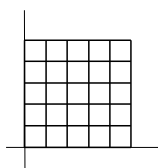


Fig. 4.1

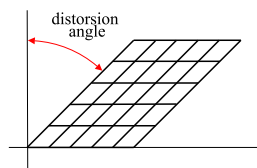


Fig. 4.2

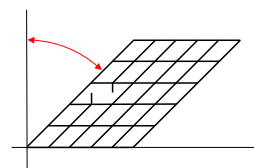


Fig. 4.3

get torn and then relinked in a different way. On Fig. 4.3 we see the birth of a pair of the edge dislocations with mutually opposite Burgers vectors. On Fig. 4.4, Fig. 4.5, and Fig. 4.6 one of them moves from the left to the right. Behind the mov-

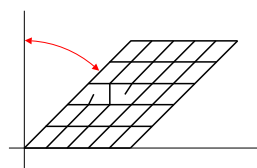


Fig. 4.4

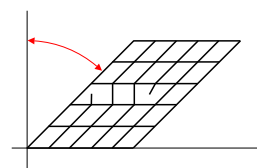


Fig. 4.5

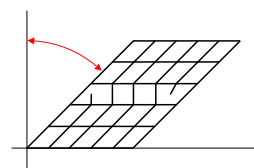


Fig. 4.6

ing dislocation the series of undistorted cells arises, while the total (macroscopic) distorsion angle remains unchanged. This fact explains why $\hat{\mathbf{T}} \neq \mathbf{T}$ for plastic deformations.

The elastic response of a body is determined by the elongation and/or contraction of interatomic bonds within it. For this reason let's define the elastic deformation tensor $\hat{\mathbf{G}}$ by analogy with (4.8), but using $\hat{\mathbf{T}}$ instead of \mathbf{T} :

$$\hat{G}_{ij} = \sum_{p=1}^3 \sum_{q=1}^3 \hat{g}_{pq} \hat{T}_i^p \hat{T}_j^q. \tag{4.9}$$

The components of the plastic deformation tensor $\check{\mathbf{G}}$ are defined as follows:

$$\check{G}_i^k = \sum_{p=1}^3 \hat{S}_p^k T_i^p. \tag{4.10}$$

Here \hat{S}_p^k are components of the inverse matrix $\hat{\mathbf{S}} = \hat{\mathbf{T}}^{-1}$. Though defined through the double space tensors, the deformation tensors $\hat{\mathbf{G}}$ and $\check{\mathbf{G}}$ are traditional tensor fields in the space of the real crystalline body. The indices p and q associated with the Burgers space in (4.9) and (4.10) both are summation indices. They disappear when the sums are evaluated.

Note that now the decomposition (3.7) follows immediately from the expressions (4.8), (4.9), and (4.10). Therefore, it is sufficient to derive the equation (3.9). The equation (3.8) then is derived from (3.9) and (3.6) due to the decomposition (3.7). As the first step in deriving the differential equation (3.9), we differentiate the equality (4.10) with respect to the time variable t :

$$\frac{\partial \check{G}_i^k}{\partial t} = \sum_{p=1}^3 \frac{\partial \hat{S}_p^k}{\partial t} T_i^p + \sum_{p=1}^3 \hat{S}_p^k \frac{\partial T_i^p}{\partial t}. \quad (4.11)$$

In order to differentiate the inverse matrix $\hat{\mathbf{S}} = \hat{\mathbf{T}}^{-1}$ in formula (4.11), we use the well-known standard formula $\hat{\mathbf{S}}' = -\hat{\mathbf{S}} \hat{\mathbf{T}}' \hat{\mathbf{S}}$:

$$\frac{\partial \hat{S}_p^k}{\partial t} = - \sum_{q=1}^3 \sum_{r=1}^3 \hat{S}_q^k \frac{\partial \hat{T}_r^q}{\partial t} \hat{S}_p^r. \quad (4.12)$$

Substituting (4.12) into (4.11) and applying the formula (4.2), now we derive

$$\frac{\partial \check{G}_i^k}{\partial t} = \sum_{q=1}^3 \sum_{r=1}^3 \hat{S}_q^k \left(j_r^q + \frac{\partial w^q}{\partial y^r} \right) \check{G}_i^r + \sum_{p=1}^3 \hat{S}_p^k \frac{\partial T_i^p}{\partial t}. \quad (4.13)$$

For the time derivative of T_i^p in formula (4.13) we have the following equality:

$$\frac{\partial T_i^p}{\partial t} = - \sum_{r=1}^3 \frac{\partial (v^r T_r^p)}{\partial y^i} \quad (4.14)$$

The equality (4.14) is derived in few steps by applying the chain rule to the mapping functions (4.6) and to their inverse mapping functions

$$\begin{cases} y^1 = y^1(t, \tilde{y}^1(x^1, x^2, x^3), \dots, \tilde{y}^3(x^1, x^2, x^3)), \\ y^2 = y^2(t, \tilde{y}^1(x^1, x^2, x^3), \dots, \tilde{y}^3(x^1, x^2, x^3)), \\ y^3 = y^3(t, \tilde{y}^1(x^1, x^2, x^3), \dots, \tilde{y}^3(x^1, x^2, x^3)). \end{cases}$$

Apart from (4.14) we need the identity

$$\frac{\partial T_r^p}{\partial y^i} = \frac{\partial T_i^p}{\partial y^r}, \quad (4.15)$$

which follows immediately from (4.7). Now, applying the formulas (4.14) and (4.15) to (4.13), we derive the following equality:

$$\begin{aligned} \frac{\partial \check{G}_i^k}{\partial t} &= \sum_{q=1}^3 \sum_{r=1}^3 \hat{S}_q^k \left(j_r^q + \frac{\partial w^q}{\partial y^r} \right) \check{G}_i^r - \sum_{r=1}^3 \frac{\partial v^r}{\partial y^i} \check{G}_r^k - \\ &\quad - \sum_{p=1}^3 \sum_{r=1}^3 \hat{S}_p^k v^r \frac{\partial T_i^p}{\partial y^r}. \end{aligned} \quad (4.16)$$

The last term in (4.16) can be transformed as follows:

$$\begin{aligned} \sum_{p=1}^3 \sum_{r=1}^3 \hat{S}_p^k v^r \frac{\partial T_i^p}{\partial y^r} &= \sum_{p=1}^3 \sum_{r=1}^3 v^r \frac{\partial(\hat{S}_p^k T_i^p)}{\partial y^r} - \sum_{p=1}^3 \sum_{r=1}^3 v^r \frac{\partial \hat{S}_p^k}{\partial y^r} T_i^p = \\ &= \sum_{r=1}^3 v^r \frac{\partial \check{G}_i^k}{\partial y^r} + \sum_{q=1}^3 \sum_{p=1}^3 \sum_{r=1}^3 S_q^k v^r \frac{\partial \hat{T}_p^q}{\partial y^r} \check{G}_i^p. \end{aligned}$$

Upon substituting this expression into (4.16) we derive

$$\begin{aligned} \frac{\partial \check{G}_i^k}{\partial t} + \sum_{r=1}^3 v^r \frac{\partial \check{G}_i^k}{\partial y^r} &= \sum_{r=1}^3 \left(\check{G}_i^r \frac{\partial v^k}{\partial y^r} - \frac{\partial v^r}{\partial y^i} \check{G}_r^k \right) - \\ &- \sum_{r=1}^3 \left(\frac{\partial v^k}{\partial y^r} + \sum_{q=1}^3 \hat{S}_q^k \left(-j_r^q - \frac{\partial w^q}{\partial y^r} + \sum_{p=1}^3 v^p \frac{\partial \hat{T}_r^q}{\partial y^p} \right) \right) \check{G}_i^r. \end{aligned} \quad (4.17)$$

Now let's introduce the following notations:

$$\theta_r^k = \frac{\partial v^k}{\partial y^r} + \sum_{q=1}^3 \hat{S}_q^k \left(-j_r^q - \frac{\partial w^q}{\partial y^r} + \sum_{p=1}^3 v^p \frac{\partial \hat{T}_r^q}{\partial y^p} \right). \quad (4.18)$$

Then the differential equation (4.17) for plastic deformation tensor is rewritten as

$$\frac{\partial \check{G}_i^k}{\partial t} + \sum_{r=1}^3 v^r \frac{\partial \check{G}_i^k}{\partial y^r} = \sum_{r=1}^3 \left(\check{G}_i^r \frac{\partial v^k}{\partial y^r} - \frac{\partial v^r}{\partial y^i} \check{G}_r^k \right) - \sum_{r=1}^3 \theta_r^k \check{G}_i^r. \quad (4.19)$$

By direct calculations one can verify that all of the partial derivatives in (4.19) can be replaced by covariant derivatives. As a result (4.19) takes the form of the equation (3.9), which was derived in [3] for amorphous materials.

The partial derivatives in formula (4.18) can also be replaced by covariant ones. As a result this formula is rewritten as

$$\theta_r^k = \nabla_r v^k - \sum_{q=1}^3 \hat{S}_q^k j_r^q - \sum_{q=1}^3 \hat{S}_q^k \nabla_r w^q + \sum_{q=1}^3 \sum_{p=1}^3 v^p \hat{S}_q^k \nabla_p \hat{T}_r^q. \quad (4.20)$$

Indeed, if we remember that

$$\nabla_r v^k = \frac{\partial v^k}{\partial y^r} + \sum_{p=1}^3 \Gamma_{rp}^k v^p, \quad \nabla_r w^q = \frac{\partial w^q}{\partial y^r}, \quad \nabla_p \hat{T}_r^q = \frac{\partial \hat{T}_r^q}{\partial y^p} - \sum_{m=1}^3 \Gamma_{rp}^m \hat{T}_m^q$$

(see (2.4) and (2.10) for comparison), we see that the Christoffel symbols Γ_{rp}^k do cancel each other when substituting the above expressions into (4.20).

The formula (4.20) written in terms of covariant derivatives reveals the tensorial nature of the quantities θ_r^k : they are the components of a traditional tensor field $\boldsymbol{\theta}$ (not a double space tensor unlike $\hat{\mathbf{T}}$, $\boldsymbol{\rho}$, and \mathbf{j}).

Theorem 4.1. *The nonlinear deformation tensor \mathbf{G} in the theory of crystalline dislocations admits the decomposition (3.7) into elastic and plastic parts $\hat{\mathbf{G}}$ and $\check{\mathbf{G}}$, both satisfying the same differential equations (3.8) and (3.9) as in the theory of plasticity for amorphous materials.*

5. CONCLUSIONS.

The theorem 4.1 proved by the above calculations is the main result of present paper. It is a purely kinematic (i. e. geometric) result. Among other results, one should mention the concept of the Burgers space. The interpretation of Burgers vectors as the vectors of a separate space (and, hence, the use of double space tensors) is our methodical achievement (in linear theory this feature is completely hidden, see [8]). The further development of this technique and the further comparison of amorphous and crystalline plasticity theories (including the dynamics and thermodynamics of media) will be done in separate papers.

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