

Interaction of defects with the elastic field

E. KOSSECKA (WARSZAWA)

THE ACTION functional, describing the interaction of defects with the external elastic field in the continuous medium, and its variations are considered. The force acting on a linear defect, dislocation and disclination, is proportional to the discontinuity vector of the displacement field representing a defect. The wedge disclination line can be fixed by the external stress field in the position of its rotation axis.

Rozpatruje się funkcjonal opisujący oddziaływanie defektu z polem sprężystym w ośrodku ciągłym i jego wariacje. Siła działająca na defekt liniowy — dyslokację lub dysklinację — jest proporcjonalna do wektora nieciągłości pola przemieszczeń opisującego defekt. Dysklinacja klinowa może być unieruchomiona przez pole naprężeń zewnętrznych w położeniu swej osi obrotu.

Рассматривается функционал описывающий взаимодействие дефекта с упругим полем в сплошной среде и его вариации. Сила действующая на линейный дефект — дислокацию или дисклинацию — пропорциональна вектору разрыва поля перемещений описывающего дефект. Клиновидная дисклинация может быть остановлена полем внешних напряжений в положении своей оси вращения.

1. Introduction

WE SHALL consider the action functional W_1 describing the interaction of defects with the external field of stresses and velocities in the infinite linearly-elastic medium. We calculate the variation of this functional with respect to the variation of position of a discrete defect. For the so-called linear defects, dislocations and disclinations, such a variation is an integral over the defect's line. The variational derivative of W_1 then means a force density acting on a unit length of a defect's line in the external field. The forces acting on a defect tend in general to move it in a definite direction, depending on the defect's parameters and the elastic field applied. It leads to the ejection of a defect to the medium surface. Some components of a stress field may have no effect on a defect. We can also deal with the case when a defect — disclination — is fixed in its primary position by the stress field; we discuss this problem in detail in Sect. 6.

2. Surface defects

In the frames of mechanics of continuous media, defects are considered as the forced deformations of a perfect medium. A discrete defect is defined as the discontinuity U of the displacement field u forced in the continuous medium over a certain surface S , called the defect's surface (see e.g. [1, 2, 3, 4]). The displacement field with a discontinuity does

not represent the state of the medium with a defect in a unique way. For the so-called linear defects, dislocations and disclinations, the elastic strain and velocity field depend only on the defect's line L which is the boundary of the surface S . The surface S resting on L may be chosen in an arbitrary way.

The state of the medium with a defect is represented by the so-called elastic strain \mathbf{e} and velocity \mathbf{v} for linear defects which are continuous outside the defect's line. The derivatives of the discontinuous displacement field \mathbf{u} differ from these quantities in the singular expressions of the type of a delta function concentrated over the surface S . They are called plastic strain $\mathring{\mathbf{e}}$ and plastic velocity $\mathring{\mathbf{v}}$ (see e.g. [2, 3, 4]). The notions of the elastic and plastic distortion β and $\mathring{\beta}$ corresponding to the gradient of the \mathbf{u} field are also in use although β is not always the state variable:

$$(2.1) \quad \begin{aligned} \beta_{ik} &= u_{i,k} - \mathring{\beta}_{ik}, \\ e_{ik} &= \beta_{\langle ik \rangle}, \\ v_i &= \dot{u}_i - \mathring{v}_i. \end{aligned}$$

For a discrete surface defect, the fields $\mathring{\beta}$ and \mathring{v} are of the form

$$(2.2) \quad \begin{aligned} \mathring{\beta}_{ik}(\mathbf{x}) &= \int_S ds_k U_i \delta_3(\mathbf{x} - \zeta), \\ \mathring{v}_i(\mathbf{x}) &= - \int_S ds_b \zeta_b U_i \delta_3(\mathbf{x} - \zeta), \quad \zeta \in S, \end{aligned}$$

where ζ is the radius vector of the surface S , $\dot{\zeta}$ the surface velocity.

To simplify the calculations we shall assume in what follows that U and $\dot{\zeta}$, and also the other functions given on the surface S , can be extended outside the surface and represented as the smooth functions of the vector ζ . Dislocations and disclinations are to be described in the following way. The constant discontinuity vector corresponding to a dislocation is

$$(2.3) \quad U = -\mathbf{b}, \quad \mathbf{b} = \text{const},$$

\mathbf{b} is to be called the Burgers vector. To a disclination corresponds the discontinuity vector representing the forced rotation Ω around the axis, to which belongs the vector $\dot{\zeta}$:

$$(2.4) \quad U_i = -\varepsilon_{ipq} \Omega_p (\dot{\zeta}_q - \dot{\zeta}_q^0), \quad \zeta \in S.$$

3. The action functional

Let us consider the action functional W_1 representing the interaction of the elastic fields \mathbf{e} and \mathbf{v} , due to a defect, and the elastic fields \mathbf{e}^* and \mathbf{v}^* , due to other sources, which will be called "external" fields. We neglect here the parts of the functional describing the so-called self-interactions. σ^* will denote the external stress, ρ the density of the medium

$$(3.1) \quad W_1 = \int dt \int d_3x [\rho v_i^* v_i - \sigma_{ik}^* e_{ik}].$$

We consider the infinite medium, so the integrations in the formula (3.1) are taken over all space and time.

Having once introduced the fields \mathbf{e} and \mathbf{v} , we shall then consider the action functional W_I constructed of them. Its particular terms then have a good physical interpretation of the kinetic and potential energy. But we might consider the action functional constructed of the derivatives of the field \mathbf{u} as well.

We shall calculate the variation of this functional with respect to the variation of the defect's field. The variations of the fields \mathbf{e} and \mathbf{v} can be represented, according to Eq. (2.1), as

$$(3.2) \quad \begin{aligned} \delta e_{ik} &= \delta \beta_{\langle ik \rangle}, \\ \delta \beta_{ik} &= \delta u_{i,k} - \delta \dot{\beta}_{ik}, \\ \delta v_i &= \delta \dot{u}_i - \delta \dot{v}_i. \end{aligned}$$

The discontinuity condition for the field \mathbf{u} does not restrict the variations δu_i . The variations of the fields $\dot{\beta}$ and \dot{v} are dependent on the variations $\delta \zeta$ of the position vector ζ . Calculating the variation δW_I , we thus obtain

$$(3.3) \quad \delta W_I = \int dt \int d_3x \{ [\rho v_i^* \delta \dot{u}_i - \sigma_{ik}^* \delta u_{i,k}] - [\rho v_i^* \delta \dot{v}_i - \sigma_{ik}^* \delta \dot{e}_{ik}] \},$$

and, after performing integration by parts,

$$(3.4) \quad \delta W_I = \int dt \int d_3x \left\{ - \left[\rho \frac{\partial v_i^*}{\partial t} - \sigma_{ik,k}^* \right] \delta u_i - [\rho v_i^* \delta \dot{v}_i - \sigma_{ik}^* \delta \dot{e}_{ik}] \right\}.$$

The "external" fields σ^* and v^* satisfy the homogeneous equations of motion (also in the case when σ^* and v^* are due to other defects, see [2, 3, 4]):

$$(3.5) \quad \rho \frac{\partial v_i^*}{\partial t} - \sigma_{ik,k}^* = 0.$$

The variation δW_I thus depends on the variations $\delta \dot{v}$ and $\delta \dot{e}$ which are to be calculated assuming the arbitrary variations $\delta \zeta$:

$$(3.6) \quad \delta W_I = - \int dt \int d_3x [\rho v_i^* \delta \dot{v}_i - \sigma_{ik}^* \delta \dot{e}_{ik}].$$

4. Variations of the plastic fields

We shall now calculate the variations of the plastic fields. It will be convenient to calculate first the variation of the plastic distortion $\dot{\beta}$. From the formula (2.2),

$$(4.1) \quad \delta \dot{\beta}_{ik} = \int_S \delta ds_k U_i \delta_3(\mathbf{x} - \zeta) + \int_S ds_k \frac{\partial U_i}{\partial \zeta_r} \delta \zeta_r \delta_3(\mathbf{x} - \zeta) + \int_S ds_k U_i \left[\frac{\partial}{\partial \zeta_r} \delta_3(\mathbf{x} - \zeta) \right] \delta \zeta_r.$$

The variations of the surface element (given as the function of the vector ζ) is equal (see [2]):

$$(4.2) \quad \delta ds_k = ds_k \frac{\partial \delta \zeta_r}{\partial \zeta_r} - ds_r \frac{\partial \delta \zeta_r}{\partial \zeta_k}.$$

Hence:

$$(4.3) \quad \delta \hat{\beta}_{ik} = \int_S \left[ds_k \frac{\partial}{\partial \zeta_r} - ds_r \frac{\partial}{\partial \zeta_k} \right] U_i \delta_3(\mathbf{x} - \zeta) \delta \zeta_r + \int_S ds_r \frac{\partial U_i}{\partial \zeta_k} \delta_3(\mathbf{x} - \zeta) \delta \zeta_r + \int_S ds_r U_i \left[\frac{\partial}{\partial \zeta_k} \delta_3(\mathbf{x} - \zeta) \right] \delta \zeta_r.$$

By Stokes' theorem we replace the first surface integral in the formula (4.3) by the line integral over the boundary L of the surface S . The expression $\mathbf{ds} \times \frac{\partial}{\partial \zeta}$ is to be replaced then by the line element $d\zeta$:

$$(4.4) \quad \varepsilon_{abc} ds_b \frac{\partial}{\partial \zeta_c} \Rightarrow d\zeta_a, \\ ds_k \frac{\partial}{\partial \zeta_r} - ds_r \frac{\partial}{\partial \zeta_k} \Rightarrow \varepsilon_{akr} d\zeta_a.$$

Hence:

$$(4.5) \quad \delta \hat{\beta}_{ik} = \varepsilon_{kra} \oint_L d\zeta_a U_i \delta_3(\mathbf{x} - \zeta) \delta \zeta_r + \int_S ds_r U_{i,k} \delta_3(\mathbf{x} - \zeta) \delta \zeta_r - \nabla_k \int_S ds_r U_i \delta_3(\mathbf{x} - \zeta) \delta \zeta_r, \\ \nabla_k \equiv \frac{\partial}{\partial x_k}.$$

We introduce the notation

$$(4.6) \quad - \int_S ds_r U_i \delta_3(\mathbf{x} - \zeta) \delta \zeta_r = \delta \psi_i.$$

The field ψ is equal to zero if we make the restriction that the variations $\delta \zeta$ are tangent to the surface S , or if only the boundary of S undergoes variations. So we rewrite Eq. (4.5) in the form

$$(4.7) \quad \delta \hat{\beta}_{ik} = \varepsilon_{kra} \oint_L d\zeta_a U_i \delta_3(\mathbf{x} - \zeta) \delta \zeta_r + \int_S ds_r U_{i,k} \delta_3(\mathbf{x} - \zeta) \delta \zeta_r + \delta \psi_{i,k}, \\ \delta \hat{\varrho}_{ik} = \varepsilon_{kra} \oint_L d\zeta_a U_i \delta_3(\mathbf{x} - \zeta) \delta \zeta_r + \int_S ds_r U_{\langle i,k \rangle} \delta_3(\mathbf{x} - \zeta) \delta \zeta_r + \delta \psi_{\langle i,k \rangle},$$

$U_{i,k}$ denotes here $\partial U_i / \partial \zeta_k$.

In the same way we calculate the variation of the field $\hat{\mathbf{v}}$:

$$(4.8) \quad \delta \hat{v}_i = - \int_S \delta ds_b \dot{\zeta}_b U_i \delta_3(\mathbf{x} - \zeta) - \int_S ds_b \delta \dot{\zeta}_b U_i \delta_3(\mathbf{x} - \zeta) \\ - \int_S ds_b \dot{\zeta}_b \frac{\partial U_i}{\partial \zeta_r} \delta_3(\mathbf{x} - \zeta) \delta \zeta_r - \int_S ds_b \dot{\zeta}_b U_i \left[\frac{\partial}{\partial \zeta_r} \delta_3(\mathbf{x} - \zeta) \right] \delta \zeta_r.$$

Taking into account the formula for the time derivative of the surface element

$$(4.9) \quad \frac{d}{dt} ds_k = d\dot{s}_k = ds_k \frac{\partial \dot{\zeta}_b}{\partial \zeta_b} - ds_b \frac{\partial \dot{\zeta}_b}{\partial \zeta_k},$$

we transform Eq. (4.8) as follows:

$$\begin{aligned}
 (4.10) \quad \delta \dot{v}_i = & - \int_S \left[ds_b \frac{\partial}{\partial \zeta_r} - ds_r \frac{\partial}{\partial \zeta_b} \right] \dot{\zeta}_b U_i \delta_3(\mathbf{x} - \zeta) \delta \zeta_r \\
 & - \int_S ds_r \dot{U}_i \delta_3(\mathbf{x} - \zeta) \delta \zeta_r - \int_S ds_r \dot{\zeta}_b \frac{\partial U_i}{\partial \zeta_b} \delta_3(\mathbf{x} - \zeta) \delta \zeta_r \\
 & - \int_S ds_r \dot{\zeta}_b U_i \left[\frac{\partial}{\partial \zeta_b} \delta_3(\mathbf{x} - \zeta) \right] \delta \zeta_r - \int_S ds_b \delta \dot{\zeta}_b U_i \delta_3(\mathbf{x} - \zeta) \\
 & - \int_S ds_r \frac{\partial U_i}{\partial t} \delta_3(\mathbf{x} - \zeta) \delta \zeta_r + \int_S ds_r \frac{\partial U_i}{\partial t} \delta_3(\mathbf{x} - \zeta) \delta \zeta_r.
 \end{aligned}$$

The first term of the above formula can be converted to a line integral, the next five collected together constitute the total derivative with respect to the time of the above defined expression $\delta \psi_i$; for this purpose the term with $\frac{\partial U_i}{\partial t} = \dot{U}_i$ was added and subtracted. Consequently,

$$(4.11) \quad \delta \dot{v}_i = -\varepsilon_{kra} \oint_L d\zeta_a \dot{\zeta}_k U_i \delta_3(\mathbf{x} - \zeta) \delta \zeta_r + \delta \dot{\psi}_i + \int_S ds_r \dot{U}_i \delta_3(\mathbf{x} - \zeta) \delta \zeta_r.$$

5. Force acting on a defect

When the field equation (3.5) is satisfied, the terms containing $\delta \psi_{i,k}$ and $\delta \dot{\psi}_i$ do not contribute to the variation (3.6). In the case when the following conditions are satisfied,

$$\begin{aligned}
 (5.1) \quad U_{\langle l,k \rangle} &= 0, \\
 \dot{U}_i &= 0,
 \end{aligned}$$

the expression (3.6) is reduced to a line integral:

$$(5.2) \quad \delta W_1 = \int dt \oint_L d\zeta_a \varepsilon_{kra} U_i [\rho v_i^* \dot{\zeta}_k + \sigma_{ik}^*] \delta \zeta_r.$$

The conditions (5.1) are satisfied naturally for a dislocation having the constant discontinuity vector $\mathbf{U} = -\mathbf{b} = \text{const}$. For a disclination (see (2.4)),

$$\begin{aligned}
 (5.3) \quad U_{i,k} &= \varepsilon_{ikp} \Omega_p, \\
 U_{\langle l,k \rangle} &= 0, \\
 \dot{U}_i &= 0 \quad \text{for} \quad \dot{\zeta} = 0.
 \end{aligned}$$

We thus conclude that a disclination interacts with the external field as a linear defect, if it constitutes a defect described by the formula (2.4), with the rotation axis fixed in time, $\dot{\zeta} = 0$. It can be proved also that the deformation field due to the mobile disclination is really a field of a linear defect if the position of the rotation axis is represented by the constant vector ζ (see [6, 7]).

Introducing the vector τ tangent to the line L ,

$$(5.4) \quad d\zeta_a = \tau_a dl$$

we rewrite the formula (5.2) in the form

$$(5.5) \quad \delta W_1 = \int dt \oint_L dl \varepsilon_{rak} \tau_a U_i [\rho v_i^* \dot{\zeta}_k + \sigma_{ik}^*] \delta \zeta_r.$$

The expression

$$(5.6) \quad f_r = \varepsilon_{rak} \tau_a U_i [\rho v_i^* \dot{\zeta}_k + \sigma_{ik}^*]$$

means the force density per unit length of a defect line due to the external stress field σ^* and external velocity field v^* . For the static case

$$(5.7) \quad f_r = \varepsilon_{rak} \tau_a U_i \sigma_{ik}^*.$$

For a dislocation, Eq. (5.7) is the well-known Peach-Koehler formula. For a disclination it was discussed for example in [8]. The vector $U_i = -\varepsilon_{ipq} \Omega_p (\zeta_q - \dot{\zeta}_q)$, $\zeta \in L$, can be called the intensity vector of a disclination line at the point ζ .

6. Force acting on the wedge disclination

When we have to do with dislocations, from Eq. (5.7) with $U_i = -b_i$ it follows that, screw dislocations ($\tau \parallel \mathbf{b}$) interact only with the shear stress, whether the edge dislocations ($\tau \perp \mathbf{b}$) interact both with the shear stress and normal stresses. Nevertheless, if only a given component of the stress does have effect on a dislocation, it tries to move it. This leads to the emerging of a dislocation on the medium surface if it is not stopped by internal obstacles.

The situation is different when we consider wedge disclination. Wedge disclination is easy to visualize: it is of the form of an infinite wedge inserted or removed from the material. Its angle of opening in a real crystal depends on the symmetry of the crystal structure but in the continuous medium it is arbitrary. The disclination line is parallel to its rotation axis; it may, at the same time, coincide with the rotation axis or not. In the first case we deal with the "pure wedge", in the second with the wedge plus the edge dislocation. From Eq. (5.7) we obtain the formula for the force on the unit length of the disclination line L :

$$(6.1) \quad f_r = \tau_a \varepsilon_{rka} \varepsilon_{lpq} \Omega_p (\zeta_q - \dot{\zeta}_q) \sigma_{ik}^*, \quad \zeta \in L.$$

We note that the force is equal to zero for the disclination line coinciding with the rotation axis:

$$(6.2) \quad \Omega \times (\zeta - \dot{\zeta}) = 0, \quad \zeta \in L.$$

It remains only to examine whether in the given stress field such a position is a position of stable or unstable equilibrium.

Let us consider the wedge disclination line with the rotation vector Ω parallel to the z axis and the rotation axis coinciding with the z axis:

$$(6.3) \quad \begin{aligned} \Omega &= [0, 0, \Omega], \\ \zeta &= [0, 0, 0], \\ \tau &= [0, 0, 1]. \end{aligned}$$

If the disclination line itself coincides with the z axis at the moment, the external stress σ^* has no effect on the disclination. We now examine the forces which will act when the line moves from the point $(0, 0)$ to the point (ζ_1, ζ_2) in the plane (x, y) . From Eq. (6.1) it follows that in this case only the stresses acting in the plane (x, y) can give contribution to the force f . Taking into account the axial symmetry of such a defect as the wedge disclination line coinciding with its axis, we may continue our considerations in the coordinate system where the two-dimensional tensor σ^* takes a diagonal form. We then obtain:

$$(6.4) \quad \begin{aligned} f_1 &= \Omega \zeta_1 \sigma_{22}^*, \\ f_2 &= \Omega \zeta_2 \sigma_{11}^*. \end{aligned}$$

Let us assume that the disclination considered is negative, $\Omega < 0$. To such a disclination corresponds the "inserted wedge". If we go back to the displacement description and the formula (2.4) for the discontinuity U , we realize that for a disclination described by Eqs. (6.3) with the surface S being the semi-plane $y = 0, x \geq 0$: $U = [0, -\Omega x, 0]$. Consequently, the negative Ω corresponds to the forced positive discontinuity of the displacement U , that is to the "inclusion wedge". On the contrary, the "positive" disclination with $\Omega > 0$ corresponds to the "removed wedge" of the material. Let one of the stresses, e.g. σ_{11}^* , be different from zero. For a negative disclination with $\Omega < 0$ and for $\sigma_{11}^* > 0$, what means extension, we have:

$$(6.5) \quad \begin{aligned} f_2 &> 0 \quad \text{for} \quad \zeta_2 < 0, \\ f_2 &< 0 \quad \text{for} \quad \zeta_2 > 0. \end{aligned}$$

The forces try to shift the disclination to the origin. On the other hand for $\sigma_{11}^* < 0$, what means compression, the forces have opposite directions:

$$(6.6) \quad \begin{aligned} f_2 &> 0 \quad \text{for} \quad \zeta_2 > 0 \\ f_2 &< 0 \quad \text{for} \quad \zeta_2 < 0. \end{aligned}$$

A disclination which was displaced from its zero position is acted by the force which has the direction of the displacement and is proportional to it. Both cases are visualized in Fig. 1a, b. The disclinations with $\Omega < 0$ are denoted there by white triangles and disclin-

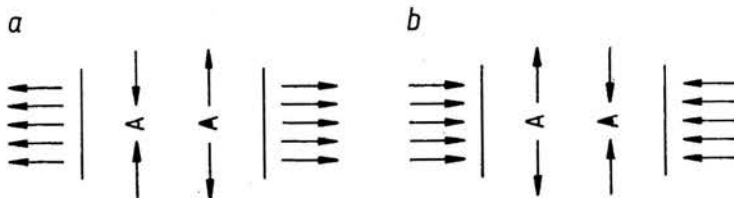


FIG. 1.

ations with $\Omega > 0$ by black triangles. So the "inclusion wedge" is in the field of compressive stress in the unstable equilibrium position; the medium tends to get rid of it.

For a positive disclination with $\Omega > 0$, what denotes the "lack of the wedge", we have the reversed situation. In the compressive stress field it is in the position of stable equilibrium, whereas in the tensile stress field it is in the position of the unstable equilibrium. If it moves by a small distance from the equilibrium position in a direction perpendicular to the direction of extension, the internal forces will try to push it out of the medium. On the other hand the forces exerted by the field of compression will push the disclination, which has moved out of the origin, again to this point.

However, one should notice that the motion of a "pure wedge disclination" line with respect to its rotation axis is nonconservative, that is it requires the influx of point defects (vacancies or inclusions) to the disclination line. The condition that the volume gap opened up from the movement of the disclination be zero is of the form (see [8, 4])

$$(6.7) \quad 0 = \dot{\zeta}_m \varepsilon_{mak} \tau_a \varepsilon_{kpq} \Omega_p (\zeta_q - \dot{\zeta}_q),$$

what means that the defect line does not move in the plane perpendicular to the vector U , as this would be in the case examined above. For the wedge disclination line the condition (6.7) takes the form

$$(6.8) \quad \dot{\zeta}_i (\zeta_i - \dot{\zeta}_i) = 0$$

what means that a disclination line can only rotate around its rotation axis. However, the condition (6.7) does not restrict infinitesimal motions of disclination coinciding with its rotation axis, as in the case $\zeta - \dot{\zeta} = 0$.

It follows, therefore, that pure wedge disclination, the motion of which with respect to the rotation axis is restricted, can be additionally fixed in its equilibrium position by the internal forces due to the externally applied stress field, considering the reduced possibilities of the material influx or outflux in the environment of a defect.

7. Conclusions

For a linear defect, the variation of the action functional describing its interaction with an external stress field is reduced to the integral over the defect's line. The mobile disclination interacts with an external stress field as a linear defect if its rotation axis is fixed in time.

The force acting on the linear defect, in external stress field, is proportional to its intensity vector.

If the rectilinear wedge disclination coincides with its rotation axis, it does not interact with the external stress field. However, if it is a negative disclination, in the compressive stress field it is in the position of unstable equilibrium, whereas in the tensile stress field it is in the position of stable equilibrium. For a positive wedge disclination the situation is reversed. In the compressive stress field it is in the position of stable equilibrium, whereas in the tensile stress field it is in the position of unstable equilibrium.

References

1. H. ZORSKI, *Theory of discrete defects*, Arch. Mech., **18**, 3, 301, 1966.
2. E. KOSSECKA, *Theory of dislocation lines in a continuous medium*, Arch. Mech., **21**, 2, 167-190, 1969.
3. E. KOSSECKA, *Defects as initial deformations*, Arch. Mech., **25**, 1, 3-11, 1973.
4. E. KOSSECKA, *Mathematical theory of defects, Part I, Statics; Part II, Dynamics*, Arch. Mech., **26**, 6, 995-1010, 1974; **27**, 1, 79-92, 1975.
5. R. DE WIT, in: *Fundamental aspects of dislocation theory*, ed. by J. A. SIMMONS, R. DE WIT and R. BULLOUGH, U.S. Government Printing Office, p. 651, Washington 1970.
6. E. KOSSECKA, R. DE WIT, *Disclination kinematics*, Arch. Mech., **29**, 5, 633-651, 1977.
7. E. KOSSECKA, R. DE WIT, *Disclination dynamics*, Arch. Mech., **29**, 6, 749-767, 1977.
8. E. S. P. DAS, M. J. MARCINKOWSKI, R. W. ARMSTRONG, *The movement of Volterra disclinations and the associated mechanical forces*, Phil. Mag., **27**, 2, 369-391, 1973.

POLISH ACADEMY OF SCIENCES
INSTITUTE OF FUNDAMENTAL TECHNOLOGICAL RESEARCH.

Received October, 27, 1978.