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ISSN 0250 3638

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PREPRINT SERIES IN MATHEMATICS
No.54/1981

BUCURESTI

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June 1981

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NON-LINEAR ELASTIC MODELS OF SINGLE DISLOCATIONS

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C.TEODOSIU* and E.SOÓS**

The present paper deals with the formulation of the non-linear boundary-value problem associated with the determination of the elastic state produced by single dislocations in the vicinity of their cores. Both Eulerian and Lagrangian formulations are given to this problem for dislocation loops and straight dislocations. It is shown that the Lagrangian form is much more intricate than the Eulerian one and requires a very careful kinematic analysis.

1. INTRODUCTION

There was a renewed interest in the last few years for the determination of the non-linear elastic field of single dislocations, ever since analytical solutions for anisotropic elastic media have become available [1 - 3] and combined atomistic and continuum calculations have shown that non-linear effects play an important role in the determination of the core configuration and the estimation of the overall dilatation produced by dislocations [4-6].

However, only straight dislocations have been considered so far. In addition, only particular choices for the cuts

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used to define single-valued deformations have been investigated [7 - 9]. As shown in the present paper, the general case of arbitrary dislocation loops and cuts requires a careful analysis of the kinematic fields and of the conditions to be imposed on the cuts in order to preserve the continuity of the dislocated crystal.

Sects.2 and 3 are devoted to the Eulerian and Lagrangian formulation of the boundary-value problem associated with the determination of the elastic state produced by dislocation loops in the neighbourhood of their cores. The Eulerian formulation uses as reference configuration the dislocated crystal, while the Lagrangian one employs the perfect lattice as reference configuration. It is argued that the Lagrangian formulation leads generally to a more sophisticated boundary-value problem.

Sect.4 concerns the discussion of the concept of local Burgers vector and of its connection with the true Burgers vector.

Finally, the case of straight dislocations is considered in Sect.5. A special attention is given to the particular situation where the cut surface is a plane passing through the dislocation line and parallel to the Burgers vector. In the latter case, both Eulerian and Lagrangian formulations are shown to be of comparable complexity.

2. EULERIAN DESCRIPTION

Consider an elastic body $\mathcal{B}$ free of body forces and surface tractions, occupying a simply-connected region v bounded by a surface s, and containing a single dislocation loop of line L. Denote by (k) this configuration of $\mathcal{B}$, and by $\underset{\sim}{x}$ the position vector of a current particle X of $\mathcal{B}$ in (k).

It is known that the dislocation produces a state of self-stress of the body and that there exists no global stress-free configuration of the dislocated body. Let N(X) denote a material neighbourhood of X. We assume that there exists a local stress-free configuration $\varkappa(X)$ of N(X), which may be obtained, at least in principle, by cutting out of the body this neighbourhood and allowing it to relax.

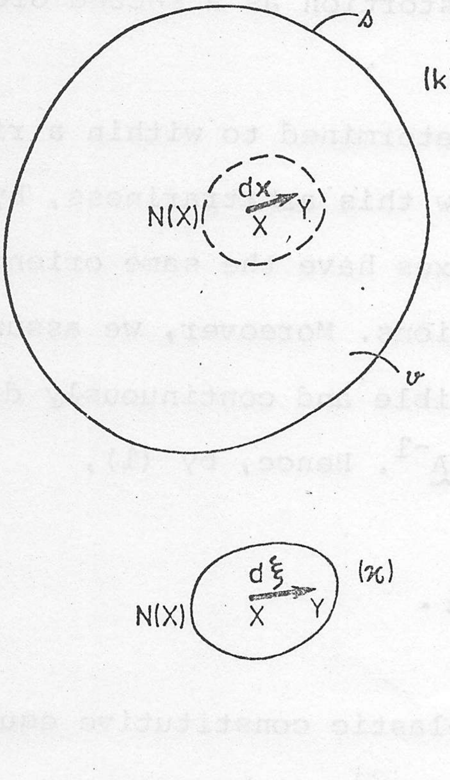

Fig.1.

Let Y be another particle of N(X) and denote by $d\underset{\sim}{x}$ and $d\underset{\sim}{\xi}$ the position vectors of Y with respect to X in the configurations (k) and $\varkappa(X)$, respectively (Fig.1). The tensor $\underset{\sim}{A}$ defined by

$$d\underset{\sim}{x} = \underset{\sim}{A}\, d\underset{\sim}{\xi} \qquad (1)$$

is called after Kröner the <u>elastic distortion.</u> We assume that, when N(X) is sufficiently small, $\underset{\sim}{A}$ depends only on X and $\varkappa(X)$, being independent of the choice of $Y \in N(X)$.

Suppose that the above cut-and-relax procedure is repeated for all particles $X \in \mathcal{B}$ outside a thin tube τ_0 of boundary σ_0 having the dislocation line as axis and with circular cross section of radius r_o. Then, denoting by v_o the region $v \setminus \tau_o$, Eq. (1) defines the elastic distortion as a second-order tensor field on v_o.

Clearly, $\varkappa(X)$ is determined to within a rigid-body displacement. We restrict now this arbitrariness, by requiring that the crystallographic axes have the same orientation in all local stress-free configurations. Moreover, we assume that the distortion field $\underset{\sim}{A}$ is invertible and continuously differentiable together with its inverse $\underset{\sim}{A}^{-1}$. Hence, by (1),

$$d\underset{\sim}{\xi} = \underset{\sim}{A}^{-1} d\underset{\sim}{x}\,. \qquad (2)$$

The (non-linear) elastic constitutive equation will be given by

$$\underset{\sim}{T} = j\underset{\sim}{A}\, \frac{\partial W(\underset{\sim}{D})}{\partial \underset{\sim}{D}}\, \underset{\sim}{A}^{T}, \qquad (3)$$

where $\underset{\sim}{T}$ is the Cauchy stress tensor, $j = \det \underset{\sim}{A}^{-1} > 0$, W is the strain-energy density per unit volume in the relaxed configuration $\varkappa(X)$, and

$$\underset{\sim}{D} = \frac{1}{2}(\underset{\sim}{A}^T\underset{\sim}{A}-\underset{\sim}{1}) \tag{4}$$

is the strain tensor.

The change in volume of the body $\mathcal{B}$ produced by the dislocation is given by

$$\Delta V=\Delta V_o + \int_{\mathcal{V}_o} (1-j)\,dv, \tag{5}$$

where ΔV_o denotes the change in volume of the material inside $\mathcal{T}_o$.

Arbitrarily choose a positive sense on L. By analogy with single crystal dislocations, we require that

$$\int_c d\underset{\sim}{\xi}(\underset{\sim}{x})= \int_c \underset{\sim}{A}^{-1}(\underset{\sim}{x})\,d\underset{\sim}{x}=\underset{\sim}{b}, \tag{6}$$

where $\underset{\sim}{b}$ is the true Burgers vector of the dislocation[1], and c denotes any smooth curve which encircles once $\mathcal{T}_o$ in the right-handed sense with respect to the positive sense on L.

It is easily seen from (6) that

$$\int_c \underset{\sim}{A}^{-1}(\underset{\sim}{x})\,d\underset{\sim}{x}=\underset{\sim}{0}, \tag{7}$$

where c is any closed circuit in $\mathcal{V}_o$ not encircling $\mathcal{T}_o$. Consequently, by a known theorem of integral calculus, we deduce that

$$\underset{\sim}{A}^{-1}=\text{grad}\,\underset{\sim}{\chi}^*, \tag{8}$$

---

[1] We use throughout the SF/RH sign convention for the true Burgers vector.

where χ^* is a class C^2 vector field in $\mathcal{V}_0$ defined by

$$\chi^*(x)=\chi^*_0 + \int_{x_0}^{x} A^{-1}(x)dx. \qquad (9)$$

The line integral in (9) is to be calculated on any smooth curve in $\mathcal{V}_0$, x_0 is any fixed point in $\mathcal{V}_0$, while χ^*_0 is an arbitrary constant vector. Generally, by (6), χ^* is a multiple-valued function having b as cyclic period.

In order to obtain a single-valued function χ^* satisfying (8), we may introduce a two-sided barrier s bounded by L and rendering $\mathcal{V}_0$ simply-connected (Fig.2). Let s_0 be the part of s outside τ_0, and n the unit normal to s_0 directed in the right-handed sense with respect to the positive sense on L. Denote by s_0^+ the face of s_0 into which points n and by s_0^- the opposite face of s_0. Then, from (6) and (9) it follows that the vector field $\chi^*(x)$ is of class C^2 in $\mathcal{V}_0 \setminus s_0$ and satisfies the jump relation

$$\chi^*(x^+)-\chi^*(x^-)=-b \quad \text{for } x\in s_0. \qquad (10)$$

Here and in the following, the superscripts + and - are used to distinguish between the limiting values on the positive and negative faces of the barrier, respectively.

Clearly, the single-valued function χ^* depends on the barrier s. Thus, by choosing another barrier, say $\hat{s}$, non-intersecting with s in $\mathcal{V}_0$, we obtain from (9) another single-valued vector field, say $\hat{\chi}^*$, of class C^2 in $\mathcal{V}_0 \setminus \hat{s}_0$ and satisfying the jump relation

$$\hat{\chi}^*(x^+)-\hat{\chi}^*(x^-)=-b \quad \text{for } x\in \hat{s}_0. \qquad (11)$$

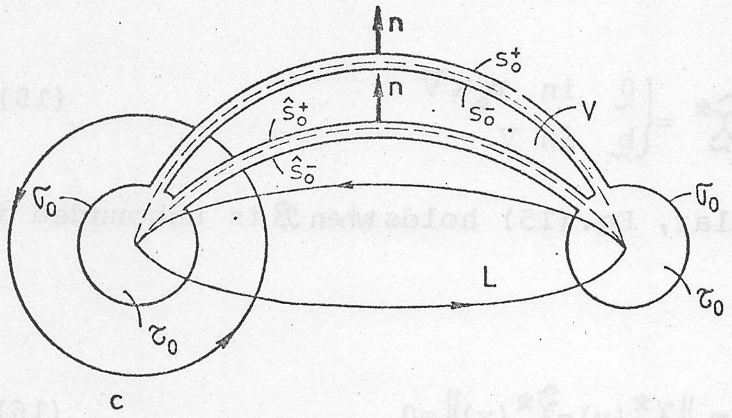

Fig.2

Next, let us denote by V the region bounded by the two barriers and σ_o. Since

$$\operatorname{grad} \underset{\sim}{\chi}^* = \operatorname{grad} \hat{\underset{\sim}{\chi}}^* \qquad \text{in } v_o \setminus (s_o \cup \hat{s}_o),$$

the vector fields $\underset{\sim}{\chi}^*$ and $\hat{\underset{\sim}{\chi}}^*$ must differ by a constant vector in either of the regions $v_o \setminus \overline{V}$ and V, where $\overline{V}$ is the closure of V. Let

$$\underset{\sim}{\chi}^* - \hat{\underset{\sim}{\chi}}^* = \begin{cases} \underset{\sim}{a} & \text{in } \quad v_o \setminus \overline{V} \\ \hat{\underset{\sim}{a}} & \text{in V.} \end{cases} \tag{12}$$

On the other hand, since $\underset{\sim}{\chi}^*$ is continuous across s_o, we have

$$\underset{\sim}{\chi}^*(\underset{\sim}{x}^+) - \underset{\sim}{\chi}^*(\underset{\sim}{x}^-) = \underset{\sim}{0} \quad \text{for } \underset{\sim}{x} \in \hat{s}_o. \tag{13}$$

Hence, by subtracting (13) from (11) and taking into account

(12) we conclude that

$$\hat{\underset{\sim}{a}} - \underset{\sim}{a} = \underset{\sim}{b}. \tag{14}$$

Moreover, if we require that $\underset{\sim}{\chi}^* = \hat{\underset{\sim}{\chi}}^*$ in $\mathcal{V}_o \setminus \overline{V}$, we obtain $\underset{\sim}{a} = \underset{\sim}{0}$, $\hat{\underset{\sim}{a}} = \underset{\sim}{b}$, and

$$\underset{\sim}{\chi}^* - \hat{\underset{\sim}{\chi}}^* = \begin{cases} \underset{\sim}{0} & \text{in } \mathcal{V}_o \setminus \overline{V} \\ \underset{\sim}{b} & \text{in } V. \end{cases} \tag{15}$$

In particular, Eq. (15) holds when $\mathcal{B}$ is unbounded if we require that

$$\lim_{\|\underset{\sim}{x}\| \to \infty} \|\underset{\sim}{\chi}^*(\underset{\sim}{x}) - \hat{\underset{\sim}{\chi}}^*(\underset{\sim}{x})\| = 0. \tag{16}$$

In the case of single dislocations we may be interested to obtain a relaxed configuration of the body by using a minimum number of cuts. Let us first choose as cut surface the barrier s and denote

$$\underset{\sim}{X} = \underset{\sim}{\chi}^*(\underset{\sim}{x}) \quad \text{for } \underset{\sim}{x} \in \mathcal{V}_o \setminus s_o. \tag{17}$$

This equation defines a mapping of $\mathcal{V}_o \setminus s_o$ in the Euclidean space $\mathcal{E}$. Let (K) denote the configuration assumed by the crystal through this mapping. We denote by capital letters and a superposed tilde the position of the material volumes and surfaces in (K).

By virtue of (10), we infer that $\tilde{S}_o^-$ is translated with respect to $\tilde{S}_o^+$ by the true Burgers vector $\underset{\sim}{b}$ (Fig.3), i.e.

$$\underset{\sim}{\chi}^*(\underset{\sim}{x}^-) = \underset{\sim}{\chi}^*(\underset{\sim}{x}^+) + \underset{\sim}{b} \qquad \text{for } \underset{\sim}{x} \in s_o. \tag{18}$$

Inspection of Fig.3 shows that the relaxation of the cut body

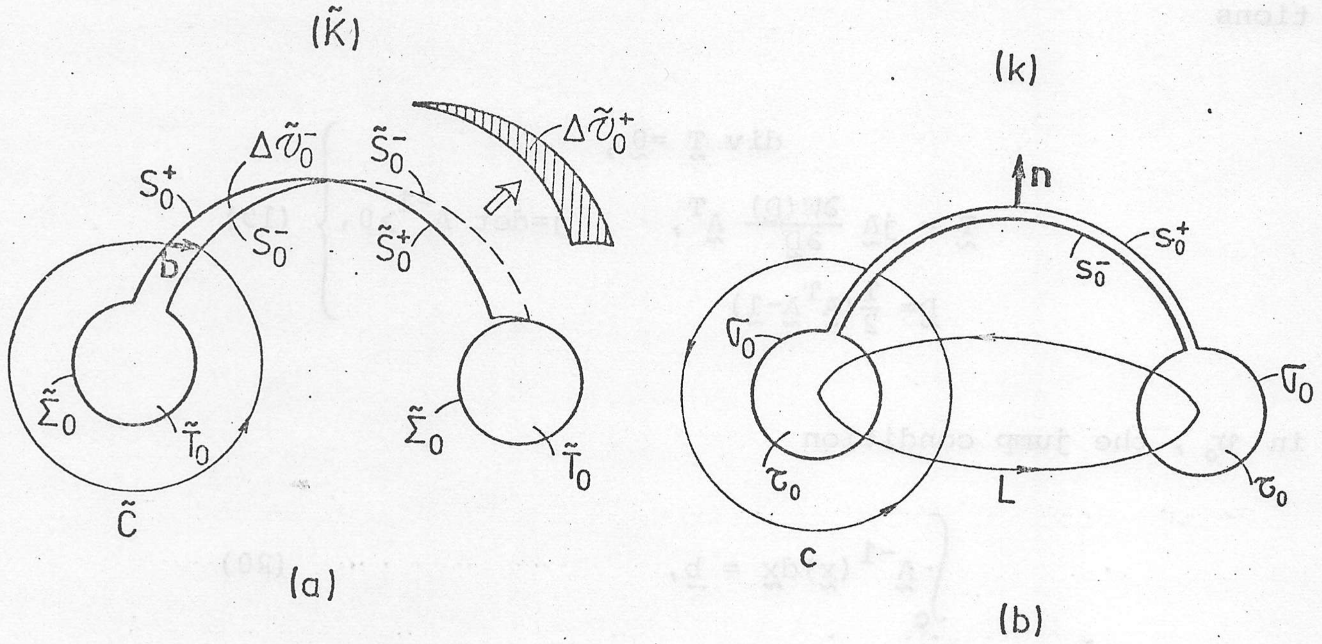

Fig. 3

leads eventually to the occurrence of a gap $\Delta\tilde{\mathcal{V}}_o^-$ and of a region of overlapping $\Delta\tilde{\mathcal{V}}_o^+$. Consequently, a complete relaxation requires to introduce a second cut along the part of S_o^+ bounding $\Delta\tilde{\mathcal{V}}_o^+$. From the mathematical point of view this corresponds to restricting $\underset{\sim}{\chi}^*$ (which generally is not injective) to a one-to-one mapping.

When L is a dislocation line ending at the external surface of the body, a part of the boundary of the cut surface s will be situated on the external surface $\mathcal{S}$; however, the whole reasoning above still holds.

On physical grounds we should require the continuity of the stress vector $\underset{\sim}{t} = \underset{\sim}{T}\,\underset{\sim}{n}$ through the barriers s_o. In our case, however, this condition is merely a consequence of the assumed continuity of $\mathbf{A}$ through s_0 and of the constitutive equation (3).

We are now in position to give the Eulerian formulation of the boundary-value problem. Find an invertible second-order tensor field $\mathbf{A}=\mathbf{A}(\mathbf{x})$ of class C^1 in $\mathcal{V}_0$ that satisfies the field equations

$$\left.\begin{aligned} &\operatorname{div} \mathbf{T} = \mathbf{0}, \\ &\mathbf{T} = j\mathbf{A}\, \frac{\partial W(\mathbf{D})}{\partial \mathbf{D}}\, \mathbf{A}^T, \qquad j = \det \mathbf{A}^{-1} > 0, \\ &\mathbf{D} = \tfrac{1}{2}(\mathbf{A}^T\mathbf{A} - \mathbf{1}) \end{aligned}\right\} \tag{19}$$

in $\mathcal{V}_0$, the jump condition

$$\int_c \mathbf{A}^{-1}(\mathbf{x})\,d\mathbf{x} = \mathbf{b}, \tag{20}$$

and the boundary conditions[1]

$$\mathbf{T}\mathbf{n} = \begin{cases} \mathbf{0} & \text{on } \mathcal{S} \\ \hat{\mathbf{t}} & \text{on } \sigma_0, \end{cases} \tag{21}$$

where $\hat{\mathbf{t}}$ is the traction on σ_0, and $\mathbf{n}$ is the outward unit normal to $\mathcal{S} \cup \sigma_0$. After solving this boundary-value problem, $\boldsymbol{\chi}^*(\mathbf{x})$ may be found as a multiple-valued function in $\mathcal{V}_0$ by making use of (9) and arbitrarily prescribing the value $\boldsymbol{\chi}_0^*$ at an arbitrary point $\mathbf{x}_0 \in \mathcal{V}_0$.

Alternatively, we may formulate the above boundary-value problem in terms of $\boldsymbol{\chi}^*$ as follows. Find a (single-valued) vector field $\boldsymbol{\chi}^*=\boldsymbol{\chi}^*(\mathbf{x})$ of class C^2 in $\mathcal{V}_0 \setminus s_0$ that satisfies the jump

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[1] The values of $\hat{\mathbf{t}}$ on σ_0 may be determined only by combining the elastic model with the atomistic model of the dislocation core, i.e. by using a semidiscrete method. Anyhow, the resultant force of the tractions $\hat{\mathbf{t}}$ on σ_0 must be zero for stationary dislocations.

condition

$$\chi^*(x^+)-\chi^*(x^-)=-b \quad \text{for } x\in s_o \tag{22}$$

and whose gradient

$$A^{-1}(x)=\text{grad}\,\chi^*(x) \tag{23}$$

together with its inverse A satisfy the field equations (19) and the boundary condition (21).

Finally, χ^* may be replaced in the latter formulation by the displacement field defined by

$$u^*(x)=x-\chi^*(x). \tag{24}$$

Then (22) and (23) become, respectively,

$$u^*(x^+)-u^*(x^-)=b \quad \text{for } x\in s_o, \tag{25}$$
$$A^{-1}(x)=1 - \text{grad}\,u^*(x). \tag{26}$$

2. LAGRANGIAN DESCRIPTION

The state of self-strain of a dislocated crystal may be also simulated by starting from the perfect lattice and using a Lagrangian description. To this end we consider an imaginary line L in a perfect crystal that occupies a region $\mathcal{V}$ of boundary $\mathcal{S}$ in a configuration (K). Cut out a thin tube T_o of boundary Σ_o, having L as axis and with circular cross section of radius R_o. Let $\mathcal{V}_o$ be the region $\mathcal{V}\setminus T_o$, S a smooth and two-sided cut surface passing through L and rendering $\mathcal{V}_o$ simply-connected, and S_o the part of S outside T_o. Arbitrarily choose a positive sense on L and denote by $\underset{\sim}{N}$ the unit normal to S_o in the right-handed sense with respect to the positive sense on L, by S_o^+ the face of S_o into which points $\underset{\sim}{N}$, and by S_o^- the opposite face of S_o (Fig.4a).

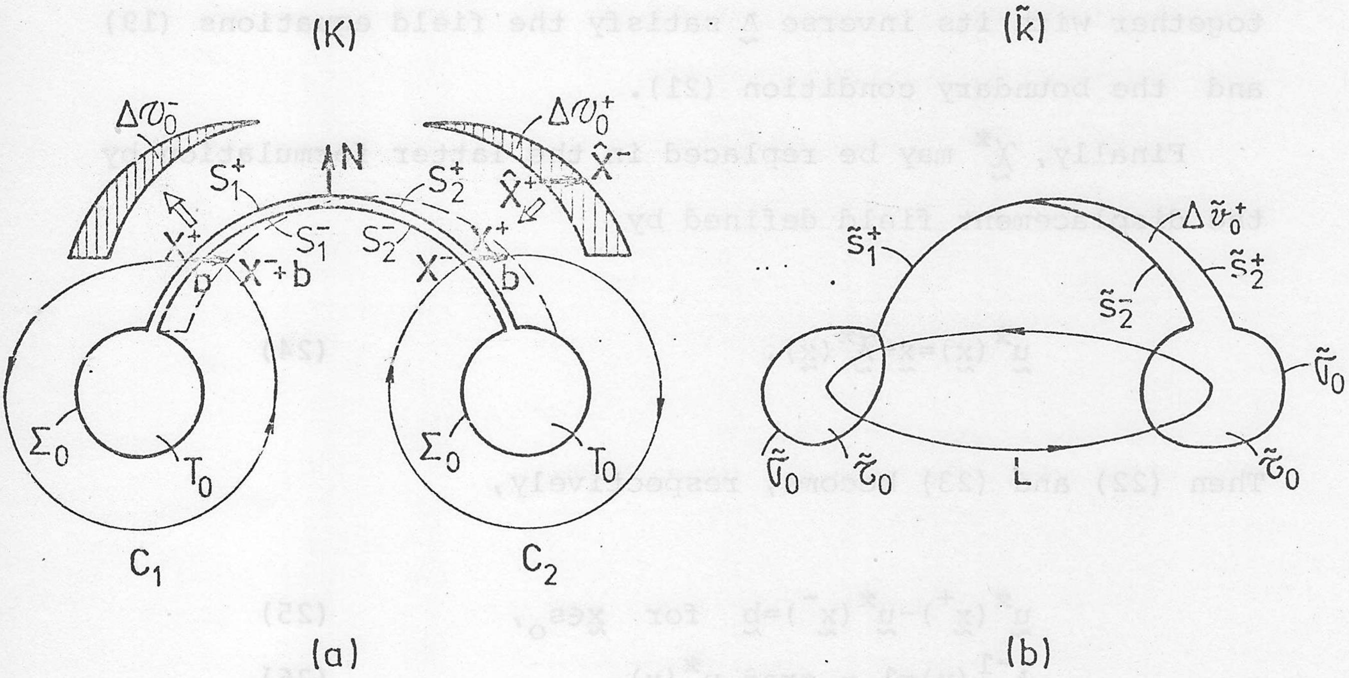

Fig.4

Assume now that S_o^+ is translated with respect to S_o^- by the true Burgers vector $\underset{\sim}{b}$. Clearly, this operation requires removing the material volume $\Delta\mathcal{V}_o^-$, whereas the continuity of the deformed lattice requires the introduction of the material volume $\Delta\mathcal{V}_o^+$, as shown in Fig.4. Suppose that the continuity of the body is reestablished and the forces used to deform it are removed, such that the crystal attains a new equilibrium configuration $(\tilde{k})$

(Fig.4b). We denote by small letters and a superposed tilde the positions of the material volumes and surfaces in $(\tilde{k})$.

Let us designate by $\underset{\sim}{\chi}$ the mapping from $(\mathcal{V}_o \setminus \Delta\mathcal{V}_o^- \setminus S_o) \cup \Delta\mathcal{V}_o^+$ to $\mathcal{E}$ defined by

$$\underset{\sim}{x} = \underset{\sim}{\chi}(\underset{\sim}{X}), \tag{27}$$

where $\underset{\sim}{X}$ and $\underset{\sim}{x}$ denote the position vectors of the same material particle in the configurations (K) and $(\tilde{k})$, respectively.

Clearly, we may identify $(\tilde{k})$ with (k) and assume that the crystallographic axes in $\mathcal{V}_o \setminus \Delta\mathcal{V}_o^-$ and $\Delta\mathcal{V}_o^+$ have the common orientation adopted for the local stress-free configurations in the Eulerian description. Then, the deformation gradient of $\underset{\sim}{\chi}$ will coincide with the distortion field $\underset{\sim}{A}$, i.e.

$$\underset{\sim}{A} = \text{Grad}\, \underset{\sim}{\chi}(\underset{\sim}{X}) \tag{28}$$

for any $\underset{\sim}{X}$ in $(\mathcal{V}_o \setminus \Delta\mathcal{V}_o^-) \cup \Delta\mathcal{V}_o^+$, except the points of S_o situated on the boundary of $\Delta\mathcal{V}_o^-$. Moreover, $d\underset{\sim}{X} = d\underset{\sim}{\xi}$ and we may write

$$d\underset{\sim}{x} = \underset{\sim}{A}\, d\underset{\sim}{X}, \tag{29}$$

where $d\underset{\sim}{X}$ and $d\underset{\sim}{x}$ denote the position vectors of the particle $\underset{\sim}{X} + d\underset{\sim}{X}$ with respect to $\underset{\sim}{X}$ in the configurations (K) and $(\tilde{k})$, respectively.

Let us denote $S_1 = S_o \cap \Delta\mathcal{V}_o^-$ and $S_2 = S_o \setminus S_1$. Examination of Fig.4 shows that a current particle $\underset{\sim}{X}^+$ situated on S_1^+ in (K) is connected with the particle $\underset{\sim}{X}^- + \underset{\sim}{b}$, and hence their positions in $(\tilde{k})$ will coincide. Consequently, we require that

$$\underset{\sim}{\chi}(\underset{\sim}{X}^+) = \underset{\sim}{\chi}(\underset{\sim}{X}^- + \underset{\sim}{b}), \quad \underset{\sim}{A}(\underset{\sim}{X}^+) = \underset{\sim}{A}(\underset{\sim}{X}^- + \underset{\sim}{b}) \quad \text{for } \underset{\sim}{X} \in S_1. \tag{30}$$

By (28), the first of these conditions is equivalent to

$$\int_{\underset{\sim}{X}^+}^{\underset{\sim}{X}^-+\underset{\sim}{b}} \underset{\sim}{A}(\underset{\sim}{Y})d\underset{\sim}{Y}=\underset{\sim}{0} \qquad \text{for } \underset{\sim}{X}\in S_1, \tag{31}$$

where the line integral may be taken on any curve C_1 in $\mathcal{V}_0 \setminus \Delta\mathcal{V}_0^-$ connecting the points $\underset{\sim}{X}^+$ and $\underset{\sim}{X}^- + \underset{\sim}{b}$ (Fig.4).

The jump conditions on S_2 require a more intricate analysis. Let us denote by $\hat{\underset{\sim}{X}}^+$ and $\hat{\underset{\sim}{X}}^-$ the particles on the boundary of $\Delta\mathcal{V}_0^+$ that are brought in coincidence with the particles $\underset{\sim}{X}^-\in S_2^-$ and $\underset{\sim}{X}^+\in S_2^+$, respectively. Clearly, according to our convention on the orientation of $\Delta\mathcal{V}_0^+$, we may write

$$\hat{\underset{\sim}{X}}^+=\underset{\sim}{X}^++\underset{\sim}{w}, \qquad \hat{\underset{\sim}{X}}^-=\underset{\sim}{X}^-+\underset{\sim}{b}+\underset{\sim}{w}, \tag{32}$$

where the constant vector $\underset{\sim}{w}$ defines some suitably chosen translation. It is easily seen now that the continuity of the dislocated crystal requires that

$$\underset{\sim}{\chi}(\underset{\sim}{X}^-)=\underset{\sim}{\chi}(\hat{\underset{\sim}{X}}^+), \qquad \underset{\sim}{\chi}(\underset{\sim}{X}^+)=\underset{\sim}{\chi}(\hat{\underset{\sim}{X}}^-), \tag{33}$$

$$\underset{\sim}{A}(\underset{\sim}{X}^-)=\underset{\sim}{A}(\hat{\underset{\sim}{X}}^+), \qquad \underset{\sim}{A}(\underset{\sim}{X}^+)=\underset{\sim}{A}(\hat{\underset{\sim}{X}}^-) \tag{34}$$

for any $\underset{\sim}{X}\in S_2$. By (28), conditions (33) imply that

$$\int_{\hat{\underset{\sim}{X}}^-}^{\hat{\underset{\sim}{X}}^+} \underset{\sim}{A}(\underset{\sim}{Y})d\underset{\sim}{Y} = \int_{\underset{\sim}{X}^+}^{\underset{\sim}{X}^-} \underset{\sim}{A}(\underset{\sim}{Y})d\underset{\sim}{Y} \qquad \text{for } \underset{\sim}{X}\in S_2, \tag{35}$$

where the line integral in the left-hand side is taken on any smooth curve $\hat{C}$ connecting $\hat{\underset{\sim}{X}}^+$ with $\hat{\underset{\sim}{X}}^-$ in $\Delta\mathcal{V}_0^+$, while the line integral in the right-hand side is taken on any smooth curve C_2 connecting $\underset{\sim}{X}^+$ with $\underset{\sim}{X}^-$ in $\mathcal{V}_0 \setminus \Delta\mathcal{V}_0^-$ (Fig.4). Clearly, the conditions (30), (33), and (34), together with the constitutive equation (3), assure the continuity of the stress vector in $(\tilde{k})$.

In order to formulate the traction boundary-value problem we shall use instead of the Cauchy stress tensor $\underset{\sim}{T}$ the first Piola-Kirchoff stress tensor $\underset{\sim}{S}$ defined by

$$\underset{\sim}{T} = j\underset{\sim}{S}\underset{\sim}{A}^T.$$

It may shown that the constitutive equation (3) and the traction boundary conditions (21) become in terms of $\underset{\sim}{S}$:

$$\underset{\sim}{S} = \underset{\sim}{A}\frac{\partial W(\underset{\sim}{D})}{\partial \underset{\sim}{D}},$$
$$\underset{\sim}{S}\underset{\sim}{N} = \begin{cases} \underset{\sim}{0} & \text{on } \mathcal{S} \\ \hat{\underset{\sim}{s}} & \text{on } \Sigma_o, \end{cases}$$

where $\underset{\sim}{N}$ is the unit outward normal to $\mathcal{S} \cup \Sigma_o$, while $\hat{\underset{\sim}{s}}$ denotes the traction on $\tilde{\sigma}_o$ in the deformed configuration $(\tilde{k})$, measured per unit underformed area. Finally, the equilibrium equation $(19)_1$ becomes

$$\text{Div}\, \underset{\sim}{S} = \underset{\sim}{0},$$

where Div is the divergence calculated with respect to $\underset{\sim}{X}$.

We may give now the Lagrangian formulation of the boundary-value problem: Find an invertible second-order tensor field $\underset{\sim}{A} = \underset{\sim}{A}(\underset{\sim}{X})$ of class C^1 in $(\mathcal{V}_o \setminus \Delta\mathcal{V}_o^- \setminus S_o) \cup \Delta\mathcal{V}_o^+$ that satisfies the field equations

$$\text{Div}\, \underset{\sim}{S} = \underset{\sim}{0},$$
$$\underset{\sim}{S} = \underset{\sim}{A}\frac{\partial W(\underset{\sim}{D})}{\partial \underset{\sim}{D}}, \qquad \underset{\sim}{D} = \frac{1}{2}(\underset{\sim}{A}^T\underset{\sim}{A} - \underset{\sim}{1}), \tag{36}$$

the jump conditions

$$\underset{\sim}{A}(\underset{\sim}{X}^{+})=\underset{\sim}{A}(\underset{\sim}{X}^{-}+\underset{\sim}{b}), \quad \int_{\underset{\sim}{X}^{+}}^{\underset{\sim}{X}^{-}+\underset{\sim}{b}} \underset{\sim}{A}(\underset{\sim}{Y})d\underset{\sim}{Y}=\underset{\sim}{0} \quad \text{for } \underset{\sim}{X}\in S_1, \tag{37}$$

$$\left.\begin{aligned} &\underset{\sim}{A}(\underset{\sim}{X}^{-})=\underset{\sim}{A}(\hat{\underset{\sim}{X}}^{+}), \quad \underset{\sim}{A}(\underset{\sim}{X}^{+})=\underset{\sim}{A}(\hat{\underset{\sim}{X}}^{-}), \\ &\int_{\hat{\underset{\sim}{X}}^{-}}^{\hat{\underset{\sim}{X}}^{+}} \underset{\sim}{A}(\underset{\sim}{Y})d\underset{\sim}{Y} = \int_{\underset{\sim}{X}^{+}}^{\underset{\sim}{X}^{-}} \underset{\sim}{A}(\underset{\sim}{Y})d\underset{\sim}{Y} \quad \text{for } \underset{\sim}{X}\in S_2, \end{aligned}\right\} \tag{38}$$

and the boundary conditions

$$\underset{\sim}{S}\underset{\sim}{N} = \begin{cases} \underset{\sim}{0} & \text{on } \mathcal{S} \\ \hat{\underset{\sim}{s}} & \text{on } \Sigma_0. \end{cases} \tag{39}$$

After solving this boundary-value problem, $\underset{\sim}{\chi}(\underset{\sim}{X})$ may be found as single-valued vector field by the formulae

$$\underset{\sim}{\chi}(\underset{\sim}{X})=\underset{\sim}{\chi}_0 + \int_{\underset{\sim}{X}_0}^{\underset{\sim}{X}} \underset{\sim}{A}(\underset{\sim}{Y})d\underset{\sim}{Y} \quad \text{for } \underset{\sim}{X}\in \mathcal{V}_0 \setminus \Delta\mathcal{V}_0^{-}, \tag{40}$$

$$\underset{\sim}{\chi}(\underset{\sim}{X})=\hat{\underset{\sim}{\chi}}_0 + \int_{\hat{\underset{\sim}{X}}_0}^{\underset{\sim}{X}} \underset{\sim}{A}(\underset{\sim}{Y})d\underset{\sim}{Y} \quad \text{for } \underset{\sim}{X}\in \Delta\mathcal{V}_0^{+}. \tag{41}$$

The line integral in (40) is taken on any smooth curve in $\mathcal{V}_0 \setminus \Delta\mathcal{V}_0^{-}$, that in (41) on any smooth curve in $\Delta\mathcal{V}_0^{+}$, $\underset{\sim}{X}_0$ and $\hat{\underset{\sim}{X}}_0$ are any fixed points in $\mathcal{V}_0 \setminus \Delta\mathcal{V}_0^{-}$ and $\Delta\mathcal{V}_0^{+}$, respectively, while $\underset{\sim}{\chi}_0$, $\hat{\underset{\sim}{\chi}}_0$ are arbitrary constant vectors satisfying the consistency relations

$$\underset{\sim}{\chi}_0 + \int_{\underset{\sim}{X}_0}^{\underset{\sim}{X}^{-}} \underset{\sim}{A}(\underset{\sim}{Y})d\underset{\sim}{Y} = \hat{\underset{\sim}{\chi}}_0 + \int_{\hat{\underset{\sim}{X}}_0}^{\hat{\underset{\sim}{X}}^{+}} \underset{\sim}{A}(\underset{\sim}{Y})d\underset{\sim}{Y}, \tag{42}$$

$$\underset{\sim}{\chi}_0 + \int_{\underset{\sim}{X}_0}^{\underset{\sim}{X}^{+}} \underset{\sim}{A}(\underset{\sim}{Y})d\underset{\sim}{Y} = \hat{\underset{\sim}{\chi}}_0 + \int_{\hat{\underset{\sim}{X}}_0}^{\hat{\underset{\sim}{X}}^{-}} \underset{\sim}{A}(\underset{\sim}{Y})d\underset{\sim}{Y}. \tag{43}$$

These conditions are implied by (33) and are mutually compatible by $(38)_2$.

Alternatively, the above boundary-value problem may be formulated in terms of $\underset{\sim}{\chi}$ as follows. Find a (single-valued) vector field $\underset{\sim}{\chi}=\underset{\sim}{\chi}(\underset{\sim}{X})$ of class C^2 in $(\mathcal{V}_0 \setminus \Delta\mathcal{V}_0^{-} \setminus S_0) \cup \Delta\mathcal{V}_0^{+}$ that satisfies the jump conditions $(30)_1$, (33), and whose gradient (28) satisfies the field equations $(36)_1$, the jump conditions (37), (38), and the boundary conditions (39).

Finally, $\underset{\sim}{\chi}$ may be replaced in this formulation by the displacement field defined by

$$\underset{\sim}{u}(\underset{\sim}{X})=\underset{\sim}{\chi}(\underset{\sim}{X})-\underset{\sim}{X}. \tag{44}$$

Then $(30)_1$, (33), and (28) become, respectively,

$$\underset{\sim}{u}(\underset{\sim}{X}^+)=\underset{\sim}{u}(\underset{\sim}{X}^-+\underset{\sim}{b})+\underset{\sim}{b} \quad \text{for } \underset{\sim}{X}\in S_1, \tag{45}$$

$$\underset{\sim}{u}(\underset{\sim}{X}^-)=\underset{\sim}{u}(\hat{\underset{\sim}{X}}^+)+\underset{\sim}{w}, \quad \underset{\sim}{u}(\underset{\sim}{X}^+)=\underset{\sim}{u}(\hat{\underset{\sim}{X}}^-)+\underset{\sim}{b}+\underset{\sim}{w} \quad \text{for } \underset{\sim}{X}\in S_2, \tag{46}$$

$$\underset{\sim}{A}(\underset{\sim}{X})=\underset{\sim}{1} + \operatorname{Grad}\underset{\sim}{u}(\underset{\sim}{X}). \tag{47}$$

A comparison between the Eulerian and the Lagrangian formulation of the boundary-value problem shows that the latter is much more complicated in the general case of an arbitrary dislocation loop. The main difficulty arises from the fact that the solution is defined on the union of two disjoint regions, so that the conditions required in order to assure the continuity of the dislocated crystal are much more sophisticated. In addition, the first Piola-Kirchoff stress tensor is asymmetric and this leads to supplementary complications when using stress functions [2]. These difficulties disapper, of course, in the linearized theory, when terms of the order $0(b^2)$ and higher are neglected, and both Eulerian and Lagrangian formulations lead to essentially the same boundary-value problem.

3. THE LOCAL BURGERS VECTOR

In order to define the local Burgers vector we ought to sum the infinitesimal vectors corresponding to the vectors $d\underset{\sim}{X}$ taken along a circuit around T_o and closed in (K). Consequently, by

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analogy with crystal dislocations, we extend $\mathbf{A}$ to the field $\mathbf{A}_E$ defined on $(\mathcal{V}_o \setminus S_o) \cup \Delta\mathcal{V}_o^+$ by

$$\mathbf{A}_E(\mathbf{X}) = \begin{cases} \mathbf{A}(\mathbf{X}) & \text{for } \mathbf{X} \in (\mathcal{V}_o \setminus \Delta\mathcal{V}_o^- \setminus S_o) \cup \Delta\mathcal{V}_o^+ \\ \mathbf{A}(\mathbf{X}-\mathbf{b}) & \text{for } \mathbf{X} \in \Delta\mathcal{V}_o^- . \end{cases} \qquad (48)$$

Unlike $\mathbf{A}$, the field $\mathbf{A}_E$ is generally not injective.

Consider now, a smooth circuit C closed in $\mathcal{V}_o$ which encircles once T_o in the right-handed sense with respect to the positive sense on L. We define the local Burgers vector $\mathbf{b}^*$ by

$$\mathbf{b}^* = -\int_C d\mathbf{x}(\mathbf{X}) = -\int_C \mathbf{A}_E(\mathbf{X})\,d\mathbf{X}. \qquad (49)$$

Fig.5b shows the local Burgers vectors corresponding to two different choices of the circuit, which intersect the parts S_1 and S_2 of S_o and are denoted by C_1 and C_2, respectively. It is easily seen that, unlike the true Burgers vector $\mathbf{b}$, the local Burgers vector $\mathbf{b}^*$ does depend on the local deformation of the lattice in the neighbourhood of the intersection of the circuits with the cut surface S_o.

We can give this assertion a quantitative form by establishing the connection between $\mathbf{b}$ and $\mathbf{b}^*$. Let us first consider the circuit C_1. With the notation in Fig.5 we have

$$\mathbf{b}^*(\mathbf{X}) = -\int_{M_1N_1P_1Q_1} \mathbf{A}_E(\mathbf{Y})\,d\mathbf{Y} \quad \text{for } \mathbf{X} \in S_1 .$$

On the other hand,

$$\int_{M_1N_1P_1} \mathbf{A}_E(\mathbf{Y})\,d\mathbf{Y} = \int_{\tilde{M}\tilde{N}\tilde{P}} d\mathbf{y} = \mathbf{0},$$

since M_1 coincides with P_1. By adding the last two relations, we obtain

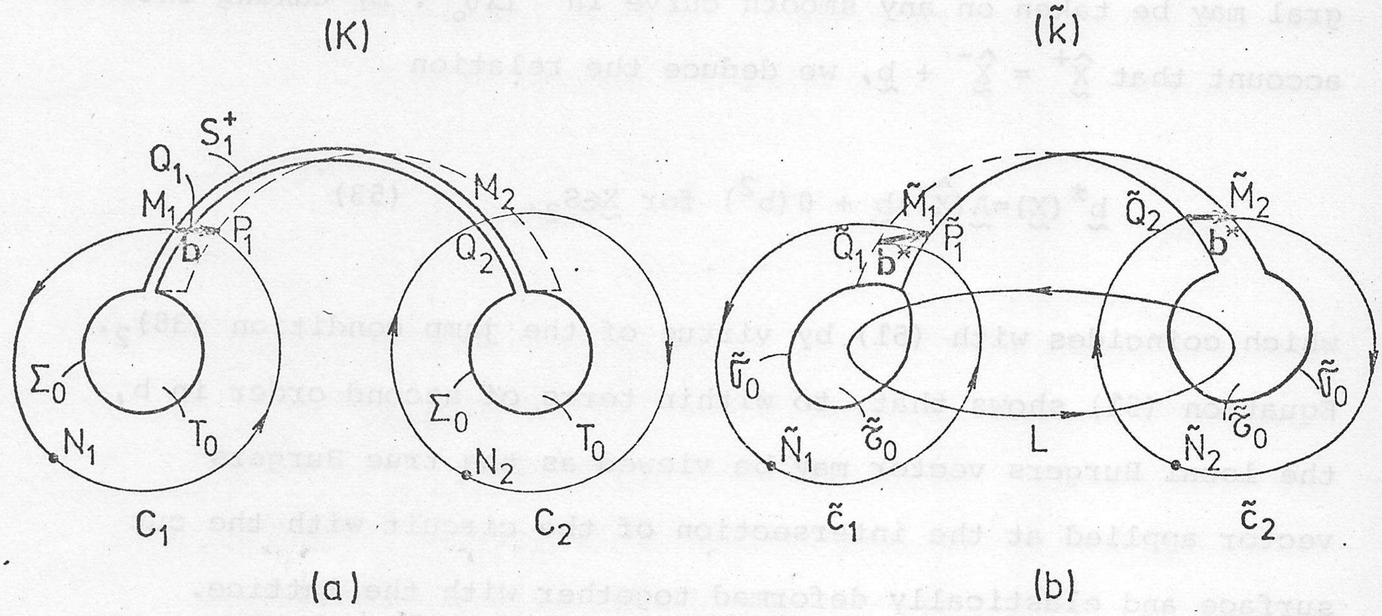

Fig.5

$$\mathbf{b}^*(\mathbf{X}) = \int_{\mathbf{X}^-}^{\mathbf{X}^+ + \mathbf{b}} \mathbf{A}_E(\mathbf{Y})d\mathbf{Y} \quad \text{for } \mathbf{X}\in S_1$$

and, considering (48), we infer

$$\mathbf{b}^*(\mathbf{X}) = \int_{\mathbf{X}^-}^{\mathbf{X}^+ + \mathbf{b}} \mathbf{A}(\mathbf{Y}-\mathbf{b})d\mathbf{Y} \quad \text{for } \mathbf{X}\in S_1. \qquad (50)$$

Now, the mean theorem of integral calculus yields

$$\mathbf{b}^*(\mathbf{X}) = \mathbf{A}(\mathbf{X}^+)\mathbf{b} + 0(b^2) \quad \text{for } \mathbf{X}\in S_1, \qquad (51)$$

where b is the magnitude of the true Burgers vector.

Analogously, we have for the circuit C_2

$$\mathbf{b}^*(\mathbf{X}) = -\int_{M_2N_2Q_2} \mathbf{A}(\mathbf{Y})d\mathbf{Y},$$

and hence, considering also $(38)_3$,

$$\underset{\sim}{b}^{*}(\underset{\sim}{X}) = -\int_{\underset{\sim}{X}^{+}}^{\underset{\sim}{X}^{-}} \underset{\sim}{A}(\underset{\sim}{Y})d\underset{\sim}{Y} = -\int_{\hat{\underset{\sim}{X}}^{-}}^{\hat{\underset{\sim}{X}}^{+}} \underset{\sim}{A}(\underset{\sim}{Y})d\underset{\sim}{Y} \quad \text{for } \underset{\sim}{X}\in S_2, \quad (52)$$

where the first integral is taken on C_2, while the second integral may be taken on any smooth curve in $\Delta\mathcal{V}_o^+$. By taking into account that $\hat{\underset{\sim}{X}}^{+} = \hat{\underset{\sim}{X}}^{-} + \underset{\sim}{b}$, we deduce the relation

$$\underset{\sim}{b}^{*}(\underset{\sim}{X}) = \underset{\sim}{A}(\hat{\underset{\sim}{X}}^{-})\underset{\sim}{b} + 0(b^2) \quad \text{for } \underset{\sim}{X}\in S_2, \qquad (53)$$

which coincides with (51) by virtue of the jump condition $(38)_2$. Equation (51) shows that, to within terms of second order in b, the local Burgers vector may be viewed as the true Burgers vector applied at the intersection of the circuit with the cut surface and elastically deformed together with the lattice. Consequently, although the Lagrangian formulation could be simplified by using the local Burgers vector, this cannot be considered as a datum of the problem.

Finally, from (28), (50), and $(52)_1$ it follows that

$$\underset{\sim}{b}^{*}(\underset{\sim}{X}) = \underset{\sim}{\chi}(\underset{\sim}{X}^{+}) - \underset{\sim}{\chi}(\underset{\sim}{X}^{-} - \underset{\sim}{b}) \quad \text{for } \underset{\sim}{X}\in S_1, \qquad (54)$$
$$\underset{\sim}{b}^{*}(\underset{\sim}{X}) = \underset{\sim}{\chi}(\underset{\sim}{X}^{+}) - \underset{\sim}{\chi}(\underset{\sim}{X}^{-}) \quad \text{for } \underset{\sim}{X}\in S_2. \qquad (55)$$

4. STRAIGHT DISLOCATIONS

The most frequently treated situation is that of an infinite straight dislocation in the axis of a circular elastic cylinder. Let us choose as tube T_o isolating the dislocation line a coaxial circular cylinder of radius R_o and boundary Σ_o and denote as before by $\mathcal{V}_o$ the region between Σ_o and the external boundary $\mathcal{S}$.

Clearly, we may use as cut any surface connecting Σ_o with $\mathcal{S}$ and rendering $\mathcal{V}_o$ simply-connected. Generally, any choice of the cut leads to a particular case of the general model presented in Sect.2. A special situation, however, occurs when using a plane cut passing through the dislocation line and parallel to the true Burgers vector.

To be more specific, let us consider an edge dislocation and choose a right Cartesian system of co-ordinates (X_1, X_2, X_3) with the X_3-axis directed in the positive sense of the dislocation line, and the X_1 - axis in the sense of $\underset{\sim}{b}$ (Fig.6).

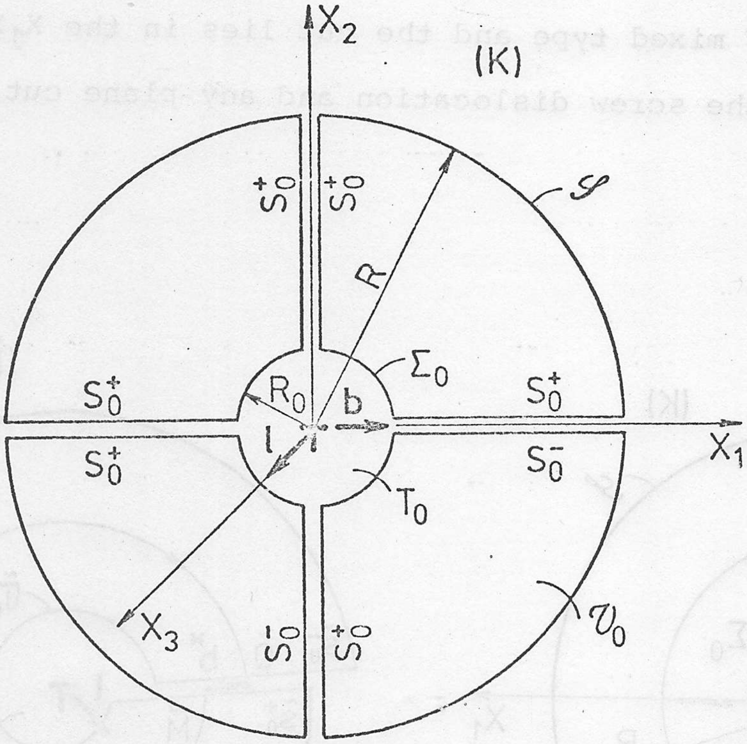

Fig.6

We consider alternatively four typical cuts shown in Fig.6. The positive and negative faces of the cuts are defined by extending L to the whole boundary of the cut. It is easily seen that the cuts perpendicular to the X_1X_3 - plane lead to particular cases of the general model. Namely, we have $\Delta v_0^- \neq \phi$, $\Delta v_0^+ = \phi$, $S_1=S_0$, $S_2=\phi$ for the cut $X_1=0$, $R_0 \leqslant X_2 \leqslant R$, and $\Delta v_0^- = \phi$, $\Delta v_0^+ \neq \phi$, $S_1=\phi$, $S_2=S_0$ for the cut $X_1=0$, $-R \leqslant X_2 \leqslant -R_0$, where R is the radius of the external boundary $\mathcal{S}$.

On the other hand, the cuts situated in the X_1X_3-plane require a special treatment, since $\Delta v_0^- = \phi$, $\Delta v_0^+ = \phi$, and hence the cut surfaces remain in contact when passing to the deformed configuration $(\tilde{k})$. The same special situation occurs when the dislocation is of mixed type and the cut lies in the X_1X_3-plane, and also for the screw dislocation and any plane cut passing through L.

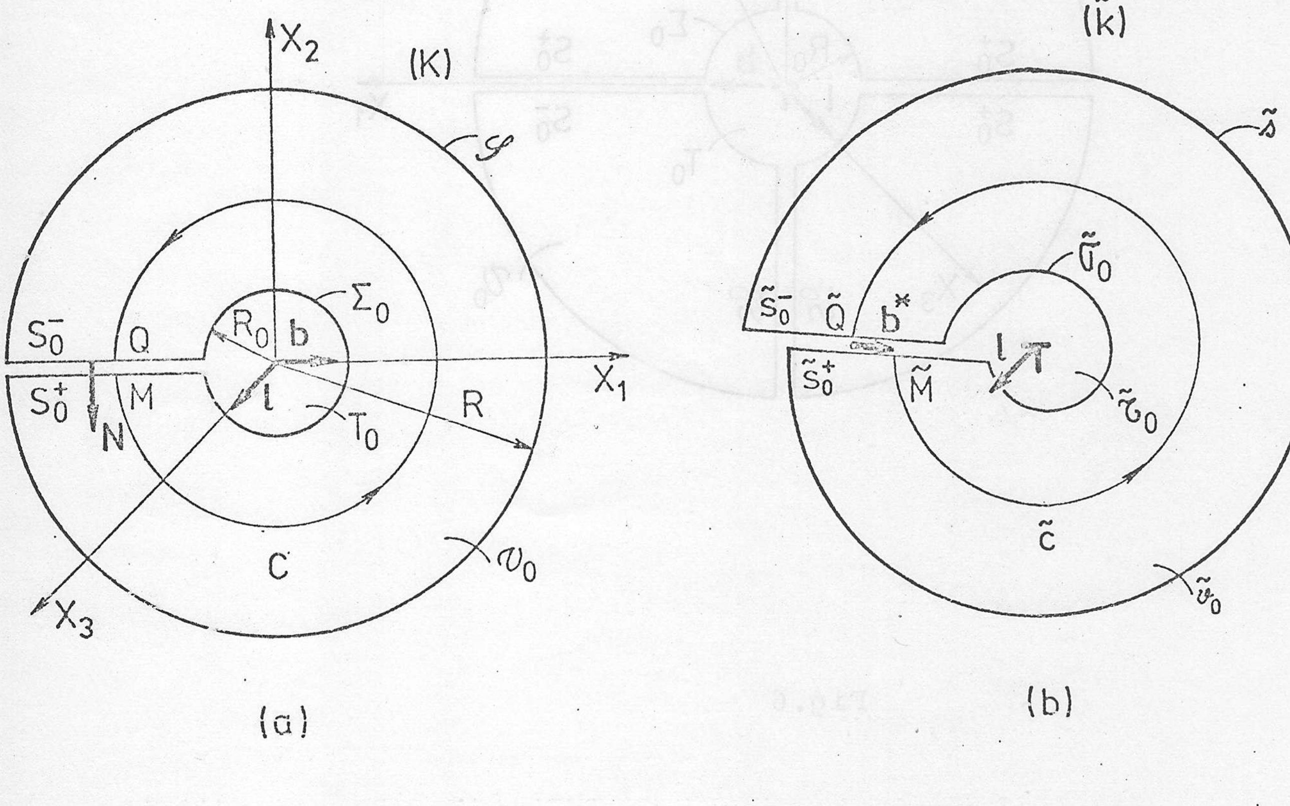

Fig.7

Let us consider for example an edge dislocation lying along the X_3-axis and the cut $X_2=0$, $-R\leqslant X_1\leqslant -R_o$. Inspection of Fig.7 shows that the jump conditions (30), (33), (34) must be simply replaced by

$$\underset{\sim}{\chi}(\underset{\sim}{X}^+)=\underset{\sim}{\chi}(\underset{\sim}{X}^-+\underset{\sim}{b}),\quad \underset{\sim}{A}(\underset{\sim}{X}^+)=\underset{\sim}{A}(\underset{\sim}{X}^-+\underset{\sim}{b})\quad \text{for } \underset{\sim}{X}\in S_o, \qquad (56)$$

the relations (40), (41) by

$$\underset{\sim}{\chi}(\underset{\sim}{X})=\underset{\sim}{\chi}_o+\int_{\underset{\sim}{X}_o}^{\underset{\sim}{X}}\underset{\sim}{A}(\underset{\sim}{Y})\,d\underset{\sim}{Y}\quad \text{for } \underset{\sim}{X}\in \mathcal{V}_o, \qquad (57)$$

and the jump conditions (45), (46) by

$$\underset{\sim}{\mu}(\underset{\sim}{X}^+)-\underset{\sim}{\mu}(\underset{\sim}{X}^-+\underset{\sim}{b})=\underset{\sim}{b}\quad \text{for } \underset{\sim}{X}\in S_o. \qquad (58)$$

Finally, relations (50), (52) are to replaced by

$$\int_{\underset{\sim}{X}^+}^{\underset{\sim}{X}^-+\underset{\sim}{b}}\underset{\sim}{A}(\underset{\sim}{Y})\,d\underset{\sim}{Y}=\underset{\sim}{b}^*(\underset{\sim}{X})\quad \text{for } \underset{\sim}{X}\in S_o \qquad (59)$$

and any smooth circuit C connecting $\underset{\sim}{X}^+$ with $\underset{\sim}{X}^- + \underset{\sim}{b}$ in $\mathcal{V}_o$, while (54) and (55) become

$$\underset{\sim}{\chi}(\underset{\sim}{X}^+)-\underset{\sim}{\chi}(\underset{\sim}{X}^-)=\underset{\sim}{b}^*(\underset{\sim}{X})\quad \text{for } \underset{\sim}{X}\in S_o, \qquad (60)$$

or

$$\underset{\sim}{\mu}(\underset{\sim}{X}^+)-\underset{\sim}{\mu}(\underset{\sim}{X}^-)=\underset{\sim}{b}^*(\underset{\sim}{X})\quad \text{for } \underset{\sim}{X}\in S_o. \qquad (61)$$

For the sake of completeness we consider also the Eulerian formulation corresponding to this special case. We choose as tube τ_o in the configuration (k) of the dislocated crystal a coaxial circular cylinder of radius r_o and boundary σ_o and denote as before by $\mathcal{V}_o$ the region between σ_o and the external boundary $\mathcal{S}$.

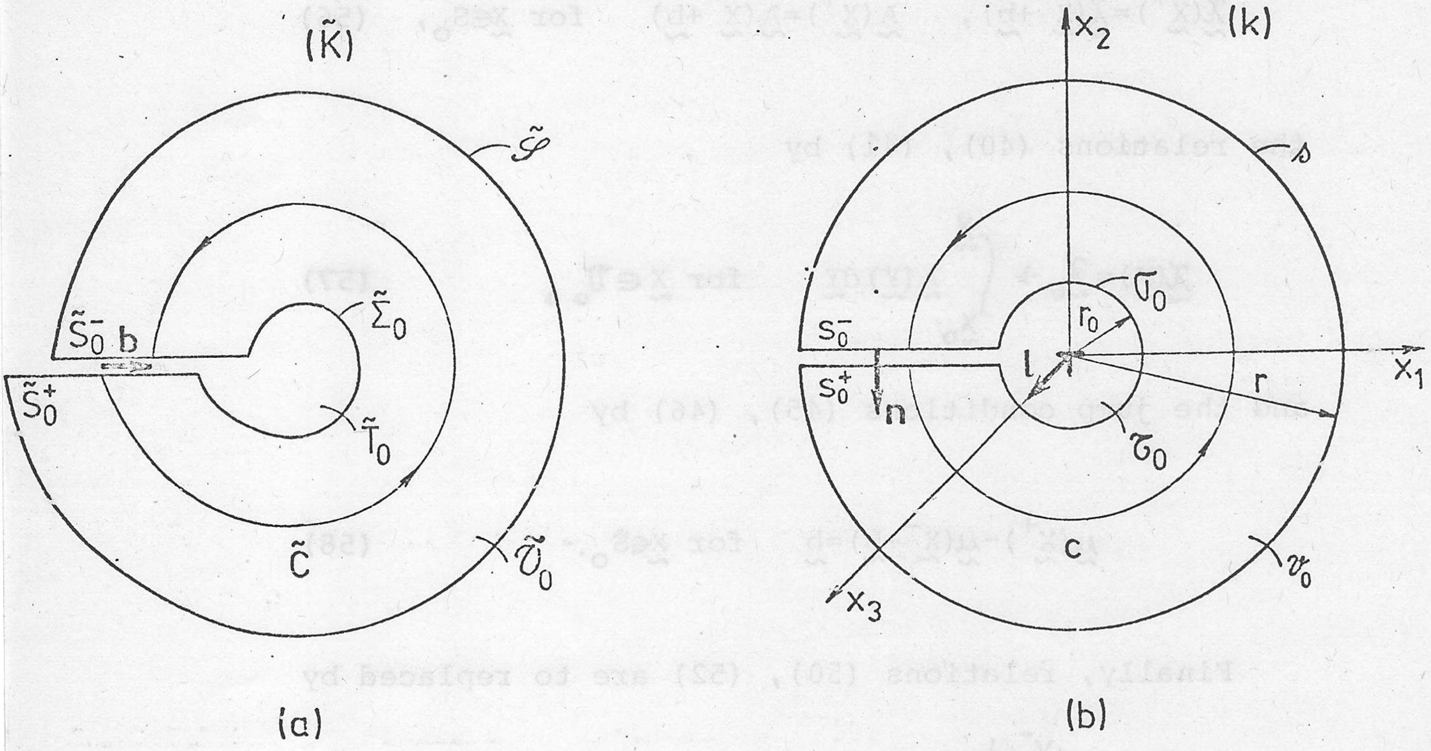

Fig.8

Let (x_1, x_2, x_3) be a right system of Cartesian co-ordinates oriented as shown in Fig.8. We choose as cut the plane surface $x_2=0$, $-r\leq x_1\leq -r_o$, where r is the radius of $\mathcal{S}$. Inspection of Fig.8 shows that cut surfaces $\tilde{S}_o^+$ and $\tilde{S}_o^-$ remain in contact and the continuity conditions (22) and (25) remain unchanged.

Finally, the considerations in this paper show that the Eulerian formulation has one more advantage in comparison with the Lagrangian one, namely its form invariance with respect to the cut, for both dislocation loops and straight dislocations.

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