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On the Connection Between the Discrete Dislocation Slip Model And the Orowan Equation.

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1. INTRODUCTION

The concept of "internal variables" plays a very important role in the theory of plasticity, relating a macroscopic inelastic response of a material element to structural rearrangements (e.g. of dislocations) within it (see, e.g., [1,2]). Traditionally these internal variables are divided into two classes: "specific structural variables" [1] and "internal variables of the averaging type" [1,2]. In the first case the general formalism is developed in terms of a finite number of discrete scalar internal variables ξ_i *(j=1,...,n)*, with each variable characterizing the extent of some local microstructural rearrangement taking place at one of *n* different sites within a given sample of material. When the number of sites increases in proportion to the size of the sample, so also does the number of structural variables[1] [1]. The main utility of structural variables is the remarkable *normality structure* of constitutive laws of plasticity, which arises in the case when the rate of structural (e.g. dislocation) rearrangements depends only on the associated thermodynamic force [1]. This normality structure implies that in the case of rate- independent flow theory the

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[1] Consequently, any function depending on such structural variables, will be *homogeneous degree one* (HD1) and will satisfy the following fundamental property [3]: $F(\lambda \mathbf{x}) = \lambda F(\mathbf{x})$

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increment of plastic strain must be normal to the yield surface, while for rate-dependent case the existence of the flow potential can be proven.

However, in practice it is more convenient to operate with a few "internal variables of the averaging type" which are related to specific structural variables in exactly the same way as extensive and intensive functions in equilibrium thermodynamics and do not depend on the size of the system under consideration. Thus plastic deformation is considered simultaneously on microstructural scale (specific structural-variables) and macroscopic scale (averaging variables), and it is important to understand how the connection between the two is established.

In the present work we demonstrate that the well-known Orowan equation relating the density of gliding dislocations N_g ("internal-variable of the averaging type"), their Burgers vector **b** and their velocity $\mathbf{v}_g$ to plastic strain rate, under certain assumptions can be related to Rice's thermodynamic approach with specific internal-variables. The Orowan equation plays a remarkable role in dislocation density-related constitutive modeling of plasticity, and it can be written as follows [4]:

$$\dot{\varepsilon}_{pl} = N_g v_g b \qquad (1)$$

here v_g and b are the lengths of the vectors $\mathbf{v}_g$ and **b**, respectively.

The Orowan equation (1) serves as a constitutive law relating the stress-strain response of a material element to the underlying dislocation dynamics[2]. For this reason it is important to

[2] The so-called "machine equation" used to describe deformation of a sample in a testing machine gives an example of such usage. This equation incorporates deformation of both the sample, based on its constitutive model, and the machine, based on the properties ascribed to it. In the case of homogeneous yielding the machine equation

understand the microscopic assumptions, with specific structural variables, which lead to this constitutive equation. To clarify this connection was the goal of the present note.

2. SPECIFIC STRUCTURAL VARIABLES AND THE OROWAN EQUATION

The complete discussion of the discrete dislocation slip-model in terms of finite deformations was given in [1]. Within the framework of this model deformation is viewed as a sequence of constrained equilibrium states. The change of the internal energy of a crystal between such neighboring states can be expressed:

$$V^0\mathbf{S}:\delta\mathbf{E} - \int_L q\,ds\,dL + \theta\delta\left(V^0\eta\right) = \delta\left(V^0 u\right) \qquad (2)$$

Here q denotes a force per unit length of dislocation line and the integral is understood to be taken over all dislocation lines in the material sample, Differential dL is a themoelastically invariant measure of arc length along dislocations, and δs is an invariant measure of perpendicular advance of dislocation lines along their slip planes. A complete description of conceptual operations which result in the introduction of these measures can be found in Rice's original work [1][3].

Consider now q as a function of **S**, θ and various thermoelastically invariant features of the

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can be written as follows: $\dot{\sigma} = k\left[\dot{\varepsilon}_{tot} - \dot{\varepsilon}_{pl}\right]$. Where $\dot{\sigma}$ is the stress rate, $\dot{\varepsilon}_{tot}$ is the complete (i.e., elastic+plastic) strain rate and k is the generalized stiffness of the sample+machine system

[3] "These measures are defined by the following conceptual operations: For dL, we scribe a line in the slip plane at a fixed small perpendicular distance ε from the dislocation line, cut out a small surrounding tube about this line (of radius smaller than ε) such that the material of the tube is stress-free, reduce the temperature to θ_0 and take dL as the corresponding arc length along the scribe line when $\varepsilon \to 0$" [1]. A similar operation can be performed for δs.

slipped state γ. Then the inelastic portion of a general strain increment can be written as:

$$(\delta \mathbf{E})^{p} = \frac{1}{V^{0}} \int_{L} \frac{\partial q(\mathbf{S},\theta,\gamma)}{\partial \mathbf{S}} \delta s \, dL \tag{3}$$

or in the rate form:

$$\left(\delta \dot{\mathbf{E}}\right)^{p} = \frac{1}{V^{0}} \int_{L} \frac{\partial q(\mathbf{S},\theta,\gamma)}{\partial \mathbf{S}} \frac{\delta s}{\delta t} dL = \frac{1}{V^{0}} \int_{L} \frac{\partial q(\mathbf{S},\theta,\gamma)}{\partial \mathbf{S}} v \, dL \tag{4}$$

where $v \equiv {\delta s}/{\delta t}$ denotes the invariant lattice velocity. Assuming further that for a given set of dislocations the invariant lattice velocity $v \equiv {\delta s}/{\delta t}$ depends on stress only through the associated force per unit length at that point, one can demonstrate the existence of a flow potential which is related to the plastic portion of strain rate through the following equation:

$$\left(\dot{\mathbf{E}}\right)^{p} = \partial \Omega / \partial \mathbf{S} \tag{5}$$

where the flow potential is:

$$\Omega(\mathbf{S},\theta,\gamma) = \frac{1}{V^{0}} \int_{L} \left\{ \int_{0}^{q(\mathbf{S},\theta,\gamma)} v(\mathbf{S},\theta,\gamma) dq \right\} dL \tag{6}$$

Assume now that the invariant lattice velocity is constant for all glissile dislocations in the material sample together with $\frac{\partial q(\mathbf{S},\theta,\gamma)}{\partial \mathbf{S}}$ (i.e., we assume that the function under the integral in (4) is independent of arc length). With this assumption the expression (4) can be rewritten in the as follows:

$$\left(\dot{\mathbf{E}}\right)^{p} = \frac{1}{V^{0}} \int_{L} dL \frac{\partial q(\mathbf{S},\theta,\gamma)}{\partial \mathbf{S}} v = \frac{L}{V^{0}} \frac{\partial q(\mathbf{S},\theta,\gamma)}{\partial \mathbf{S}} v = N_{g} \frac{\partial q(\mathbf{S},\theta,\gamma)}{\partial \mathbf{S}} v \tag{7}$$

where N_{g} denotes the density of glissile dislocations.

In order to evaluate expression (7) it is necessary to consider a force exerted by an external stress on a dislocation loop[4]. As the loop is created, the stress does the work[5]:

$$W = \int_A -\mathbf{b} \cdot (\mathbf{S} \cdot d\mathbf{A}) \tag{8}$$

where **b** denotes the Burger's vector of the loop, A is the area covered by the loop and $d\mathbf{A} = \mathbf{n}dA$, with **n** being the positive normal of $d\mathbf{A}$. Then, if every line element $d\mathbf{l} = \mathbf{m}dl$ (where **m** is a unit tangential vector in the counter-clockwise direction) is displaced by some distance $\delta\mathbf{r}$, the stress **S** does additional work which can be evaluated as follows:

$$\delta W = -\oint_C \mathbf{b} \cdot \left[\mathbf{S} \cdot (\delta\mathbf{r} \times d\mathbf{l})\right] \tag{9}$$

or, using the definition $d\mathbf{l} = \mathbf{m}dl$ and rewriting:

$$\delta W = -\oint_C \mathbf{b} \cdot \left[\mathbf{S} \cdot (\delta\mathbf{r} \times \mathbf{m})\right] dl \tag{10}$$

Defining $\delta\mathbf{r} \times \mathbf{m} = \mathbf{k}\delta s$ with **k** being some unit vector, we get:

$$\delta W = -\oint_C \mathbf{b} \cdot \mathbf{S} \cdot \mathbf{k}\delta s dl \tag{11}$$

The only difference between equation (11) and the integral ($-\int_L qdsdL$) appearing in (2) is that the latter integral is understood to be taken over all dislocation lines in the material sample, while (11) is written for a particular dislocation loop. This means, that in our case q must be defined as follows:

$$q = \mathbf{b} \cdot \mathbf{S} \cdot \mathbf{k} \tag{12}$$

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[4] Hirth and Lothe. *Theory of Dislocations*, second edition, Krieger Publishing Company, Malabar, Florida, 1992, Chapter 4, *The Theory of Curved Dislocations, pp. 96-111* [3].

[5] Hirth and Lothe, formula (4-42), p. 109. [3].

Assuming now that stress **S** is homogeneous everywhere in the sample, that all the loops have the same Burger's vector **b** and that dislocation loops are deformed in such a way that for all of them both the direction **k** and the distance δs are the same[6], i.e. the conditions for (7) are satisfied, we can substitute (12) into (7) which gives the following result:

$$\left(\dot{\mathbf{E}}\right)^{P} = N_{g}\frac{\partial q(\mathbf{S},\theta,\gamma)}{\partial \mathbf{S}}v = N_{g}v(\mathbf{bk}+\mathbf{kb}) \quad (13)$$

Due to the symmetry of both strain and stress tensors only the symmetric part of the dyadic product of the Burger's vector **b** and **k** is retained. This is the final expression that seems to be quite general, although we have had to make several plausible approximations and assumptions. It should be considered a generalization of the Orowan equation described in the beginning of the paper, equation (1). In the most general case the relation between the vectors **b** and $\mathbf{k} = \frac{\delta\mathbf{r}\times\mathbf{m}}{\|\delta\mathbf{r}\times\mathbf{m}\|}$ can be rather complex. For example, if **b** and **k** are perpendicular, the dislocation can move conservatively, by pure slip on the cylindrical surface containing the dislocation contour C and its Burger's vector **b** [4]. Note that this conservative motion is in an agreement with the volume conservation assumption used in continuum plasticity. In this simple case expression (13) is reduced to a simple component form

$$\left(\dot{\mathbf{E}}\right)_{ij}^{P} = N_{g}vb \quad (14)$$

where $\left(\dot{\mathbf{E}}\right)_{ij}^{P}$ denotes the shear component of the deformation rate corresponding to the dyad $\mathbf{bk}/b$. Some other assumptions about **b** and **k** can reduce (13) to the scalar Orowan equation (1)

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[6] The simplest assumption, for instance, would be that $\delta\mathbf{r}$ is perpendicular to $\mathbf{m}$.

in some more complicated forms involving different components and/or invariants of the plastic strain rate.

3. CONCLUSIONS

Within the framework of thermodynamic theory of plasticity and specific structural-variables (associated with individual dislocations) [1] a transition has been made to an expression containing one internal variable of the averaging type - the density of glissile dislocations, N_g. This expression should be considered a tensorial generalization of the well-known Orowan's equation and relates it directly to the simplest possible case of normal flow in metallic materials. Since most metals display deviations from normality in the flow rule[7] [4] it also clearly indicates that more rigorous assessment of the relation between plastic strain rate and dislocation populations is required, especially for materials displaying plastic instabilities in the form of dislocation patterning, strain-softening and strain-rate softening phenomena. The obtained result could be a useful starting point in establishing such rigorous macroscopic relations from microscopic considerations associated with individual dislocations and to find useful applications in dislocation density-related constitutive modeling of plastic deformation [7].

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[7] Such deviations seem to be quite universal, although might be caused by different reasons. For example, in the case of bcc-crystals nonplanar spreading of the dislocation cores on the primary slip system results in tension-compression asymmetry of the flow stress and also on its pressure dependence, while for fcc aluminum the underlying reason might be related to thee interaction of transient dilatation of the lattice associated with mobile dislocations, with external pressure [6].

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LITERATURE

1. J.Rice, Inelastic Constitutive Relations for Solids: An Internal- Variable Theory and Its Applications to Metal *Plasticity,J.Mech.Phys.Solids,* vol.19, p.433 (1971).
2. 2. O.Richmond, Microstructure-Based Modeling of Deformation Processes, *J. of Metals,* No.4, p16 (1986).
3. 3. J.W.Cahn and W.C.Carter, Crystal Shapes and Phase Equilibria: A Common Mathematical Basis, *Metallurgical and Materials Transactions* , v. 27A, p.1431 (1996).
4. 4. J.P .Hirth and J.Lothe, *Theory of Dislocations,* 2nd edition, Krieger Publishing Company, Malabar, Florida (1992).
5. 5. W .A.Spitzig and O.Richmond, The Effect of Pressure on the Flow Stress of Metals, *Acta Metall.,* v.32, p.457 (1984
6. V.V.Bulatov , O.Richmond and M. V .Glazov , On the Atomistic Dislocation Mechanism of Non-Normal Plastic Flow in Pure Aluminum, submitted *to Acta Mater.* (1998).
7. Yu.Estrin, Dislocation Density- Related Constitutive Modeling, In: Unified Constitutive Laws of Plastic Deformation, p.69 (1996)