# Plastic deformation of F.C.C. polycrystals in the microstrain region

# J. LAMBERMONT (LIEGE)

THE behaviour of pure polycrystalline materials in the early deformation range has received considerable attention. The plastic tensile strain in this region has experimentally been found to be related quadratically to the tensile stress and linearly to the grain volume. It is the purpose of this paper to show that the general thermodynamic theory of plasticity developed by the author leads to this result. The prevailing equations are also derived along the lines employed by metallurgists. This example provides a bridge to the gap which exists between the mathematical and physical theories of plasticity.

Dużo uwagi poświęcono zachowaniu się czystych materiałów polikrystalicznych we wczesnym zakresie odkształcenia. Stwierdzono doświadczalnie, że rozciągające odkształcenia plastyczne w tym obszarze są związane kwadratowo z naprężzniem rozciągającym i liniowo z wielkością ziaren. Celem tej pracy jest wykazanie, że ogólna termodynamiczna teoria plastyczności rozwijana przez autora prowadzi do tego rezultatu. Większość równań wyprowadzono również w sposób stosowany przez metalurgów. Fakt ten stanowi pomost nad luką, jaka istnieje między matematyczną i fizyczną teorią plastyczności.

Много внимания посвещено поведении чистых поликристаллических материалов в ранней стадии деформации. Экспериментально обнаружено, что растягивающие пластические деформации связаны, в этой области, квадратично с растягивающим напряжением и линейно с величиной зерен. Целью этой работы является доказательство, что общая термодинамическая теория пластичности, развиваемая автором, приводит к этому результату. Болышинство уравнений выведено тоже способом применяемым металлургами. Этот факт составляе тпомост над пробелом, какой существует между математической и физической теориями пластичности.

#### 1. Introduction

UNDER slow deformations of a pure annealed polycrystalline material composed of fairly elastically isotropic crystallites, the Frank-Read sources of the most favourable slip system will be activated first in emitting dislocation loops. These expand freely to sizes equal to the cross-sectional area of the grain where they pile up and are probably locked in place by the formation of dislocation locks as Lomer-Cottrell locks. Under increasing deformation the resolved shear stress on less favourable slip systems will reach the critical shear stress necessary for the activation of their sources. Thus under increasing stress more and more slip systems participate in the process. Due to the random distribution of the grains in a polycrystalline solid, the activated primary slip systems lie, in a sufficient early deformation stage, in grains remote from each other.

The stress field of an unrelaxed piled-up loop of *n* dislocations with mean diameter *D* falls off as  $n \frac{D}{r^2}$  for distances *r* larger than a few *D*, while the back stress on their source is proportional to n/D. Therefore, in the very early deformation region the stress

fields of dislocations lying in different grains may be assumed not to influence each other.

It has been found experimentally that under a simple tensile stress the microstrain region ends at a plastic strain of about  $10^{-4}$ .

The plastic tensile strain  $\varepsilon''$  in the microstrain range of pure polycrystalline metals has experimentally been found [3, 4, 5, 6] to be related parabolically to the tensile stress and linearly to the grain volume

(1.1) 
$$\varepsilon'' = BD^3(\sigma - \sigma^*)^2,$$

where D is the grain diameter and  $\sigma^*$  a reference stress.

The constants  $\sigma^*$  and B are nearly the same for a variety of metals such as copper and iron.

In their analyses of the microstrain region BROWN and LUKENS [5] and FRIEDEL [6] assumed that there is a linear relationship between the back stress on a source and the number of piled-up dislocations. However, we shall show that under this assumption, when the correct distribution function for the slip systems in a F.C.C. polycrystal is introduced, the relation (1.1) does not follow.

In order to obtain the correct tensile stress-strain relation one must introduce the constitutive assumption that the resolved shear back stress on the primary sources which have emitted on the average n dislocation loops in a grain with diameter D is proportional to  $\sqrt{n/mD}$ , where m is the Schmid orientation number of the primary slip system with respect to the tensile axis. In effect this means that the long range stresses of the primary piled-up dislocations are modified by slip on secondary slip systems<sup>(1)</sup>. Since the resolved shear stress acting on the sources in secondary slip systems depends not only on the primary dislocations induced stress but also on the macroscopic stress, one expects the relaxation of the primary pile-ups to depend on the orientation of the primary slip system. MITCHELL [7] and BASINSKI [8] calculated that the piled-up groups of dislocations in the primary system in F.C.C. crystals are capable of producing slip on many secondary systems over distances of the order of the pile-up length. The resulting Burgers vector of the pile-up group is thereby reduced, giving rise to a lower back stress. It has also been verified that the density of secondary dislocations is, in order of magnitude, equal to that of the primary dislocations, however, the slip distance is much smaller. The plastic strain due to the secondary dislocations is estimated to be about 2% of that of the primary dislocations and therefore we shall neglect its contribution.

The purpose of this paper is twofold. The calculation of the micro-strain tensile relation will be made by applying the general constitutive equations derived on thermodynamic grounds by the author [1, 2]. In Sect. 4 these relations will be derived directly along the lines used by metallurgists. Thereby, we shall show the equivalence of the thermodynamic and metallurgical approach to plasticity.

<sup>(1)</sup> By definition, the resolved shear stress due to the macroscopic applied stress exceeds, on a primary slip system, the critical stress necessary to activate the sources, while on a secondary or latent slip system the macroscopic resolved shear stress is smaller than the critical value.

### 2. Formulation of the problem

Figure 1 shows a Frank-Read source which has emitted several dislocation loops. To define the dislocation state we recall [1, 2] the following convention.

Consider first that the source when it is straight is a pure edge dislocation, i.e. consists of atoms inserted into the lattice on one side of the slip plane. The source can bow out



by conservative motion only in one slip plane. The Burgers vector of the source is parallel with this plane. We introduced [1] a unit normal  $\mathbf{n}$  to the slip plane by the convention that it points in the opposite direction of the extra atomic half plane making up the edge dislocation, see Fig. 1. A unit vector  $\mathbf{m}$  parallel to the Burgers vector of the source specifies the slip direction. Once  $\mathbf{n}$  and  $\mathbf{m}$  are selected they remain fixed. When the source is of mixed character its Burgers vector can be decomposed into a normal and tangential part. The normal component determines again an edge dislocation, having a strength less than the Burgers vector. The extra atomic half plane associated with it determines the unit normal  $\mathbf{n}$  as described above.

Lower and upper atom planes, adjacent to a slip plane, have been defined by the convention that n is directed from the lower to upper plane.

Under an applied resolved shear stress a source bows out by glide and becomes eventually unstable whereafter it emits dislocation loops. Often it is assumed that a source bows out in its stable region as a circle arc and becomes unstable when it bows out more than semi-circularly. MITCHELL and SMIALEK [9] have shown that at the critical stress the configuration corresponds more to an ellipse.

The distance between the nodes of a source is denoted by  $I_0$ . The state of a source in its stable region is specified when the glide direction is known as well as the are a enclosed between the straight and bowed out position. Thereto a scalar quantity A has been introduced, see Fig. 1, whose absolute value is equal to the enclosed area and is positive or negative when the source is bowed out in the direction of  $\mathbf{m}$  or  $-\mathbf{m}$ , respectively(<sup>2</sup>). Moreover, a quantity  $\lambda = \operatorname{sign} A$  was introduced.

<sup>(&</sup>lt;sup>2</sup>) More generally, one may select **n** as **m** arbitrarily and A by the convention that it is respectively positive or negative when the lower material is displaced relatively to the upper material in the direction of **m** or  $-\mathbf{m}$ , to bow out the source from the straight to the momentary position. Hewever, some of equations presented here must be modified accordingly.

To define the state of the dislocation loops which emanated during plastic flow from a source, a displacement vector  $\mathbf{g}$  was introduced; this vector specifies the relative displacement which the atoms below the slip plane have undergone relative to the atoms above the slip plane.

In small deformation theory the unit vectors n and m are, and remain constant over a slip plane. The relative displacement caused by the created loops can therefore be specified by a scalar quantity g defined by

 $\mathbf{g} = g\mathbf{m}$ .

When n loops have been milled out by a source, the absolute value of g is nb, where b is the magnitude of the Burgers vector.

The dislocation loops which are generated by a Frank-Read source expand unstably until they are stopped by obstacles or dislocation reactions. In the description of the dislocation state we jump over the unstable positions of an expanding loop (running dislocation). Thus only the change in state of the stabilized loops is considered. In a macroscopic description it is mandatory to adopt this view because a theory which attempts to describe the state of the unstable positions of a running dislocation necessarily becomes a macroscopically unstable theory.

In addition to g the distribution of the shapes or swept out areas of the loops emitted by a source must be specified. We adopt the continuous dislocation description as is often used in the calculation of a pile-up group of dislocations. Hence the discrete Burgers vector nature is smoothed out by a continuous distribution of dislocation loops of infinitesimal strength. During an infinitesimal loading increment a plastically activated (i.e., more than critically bowed out) source is thus thought to throw off a dislocation loop of infinitesimal strength dg which expands instantaneously to the position it takes when stabilized. The information about the swept out area of this loop is contained in the stoichiometric law introduced in [1].

Sources on the slip system which have milled out about the same number of loops with about the same mean area can be grouped together in a macroscopic description. We denote by  $A^p$  the average bowed out area of the sources of the  $p^{th}$  slip system defined by  $\mathbf{n}^p$  and  $\mathbf{m}^p$ . When during a loading increment the sources of this  $p^{th}$  group are plastically activated they throw off loops with a mean infinitesimal strength  $dg^p$ . The stabilized mean area swept out by them is denoted by  $\mathcal{A}^p$ .

In the dislocation state description the micro dislocation behaviour is smoothed out by jumping over the instabilities and by averaging many similar source-loops systems.

In the microstrain region the strain due to the secondary dislocations is small and may be neglected. Their only effect is the modification (relaxation) of the back stress acting at the primary Frank-Read sources. The stress fields set up by the modified piled-up dislocations do not influence each other in the early deformation region. In a pure metal the dislocations may be assumed to pile-up closely against the grain boundaries, i.e., the modified pile-up length is small compared to the grain size diameter.

This greatly simplifies the analysis at two points. Firstly, the piled-up dislocation loop diameters are closely equal to the grain diameter, so that the stoichiometric law  $(2.2^{1})(^{3})$  introduced in the general theory, which expresses how the swept out areas change with deformation, is superfluous.

However, under certain loading conditions, as cyclic loading, this assumption is bound to break down. Primary dislocations participate continuously in dislocation reactions with secondary ones whereby locks are formed. Therefore, when under reversed loading a source emits dislocation loops of opposite character, these will generally not annihilate, at least not completely, the previously emitted loops. Hence the swept out area becomes generally smaller and smaller and the fault introduced by assuming it to be equal to the grain area larger and larger. We recall [1, 2] that the dislocation state is determined not only by the values of the g's of the (primary) slip systems but also by the distribution of the dislocation loop areas. Therefore it is generally impossible, even if by a certain plastic loading path all g's could be made zero, to come back to the initial state. Non-conservative dislocation motion, as occurs during annealing, would be necessary to achieve this. We restrict the general theory to plasticity only where conservative dislocation motion is the controlling mode.

Secondly, in the yield function associated with the  $i^{\text{th}}$  primary slip system or grain, of all dislocation stress fields, only, the modified resolved shear back stress appears which the loops belonging to the slip system exert on the primary sources which have created these loops. It is to say that the conditions expressed by the relations (2.27<sup>2</sup>) are fulfilled and, consequently, Koiter's generalization (2.30<sup>2</sup>) of Drucker's relation is valid.

For isothermal quasi-static deformations we derived the Koiter relation

(2.1) 
$$d\varepsilon_{ij}^{\prime\prime} = \sum_{p} h^{p} \frac{\partial \phi^{p}}{\partial \sigma_{ij}} \bigg|_{T,g} \frac{\partial \phi^{p}}{\partial \sigma_{kl}} \bigg|_{T,g} d\sigma_{kl},$$

where  $\varepsilon_{ij}^{"}$  is the plastic strain tensor<sup>(4)</sup> and  $\sigma_{ij}$  the stress tensor.

The summation convention over repeated subscripts (but not superscripts) is valid. The incremental relation (2.1) has been derived [1, 2] from general thermodynamic considerations. Thereby, the history dependence of the yield functions  $\phi^i$  and hardening functions  $h^i$  has been eliminated by introducing the dislocation state. The hardening functions can be obtained from the yield functions by (2.31)<sub>2</sub>

(2.2) 
$$h^{p} = \left\{ \frac{bl_{0} + \mathscr{A}}{bl_{0} \frac{\partial \phi}{\partial g}} \right|_{T,\sigma} \right\}^{p} > 0,$$

where  $\mathscr{A}^p$  is the free mean area which the running dislocations of the slip system p sweep out before they are stopped by the grain boundaries. We assume, for reasons of simplicity, that the grains are cubes with sides  $D^p$  and that the grain boundary area is related to the size parameter by  $\mathscr{A}^p = (D^p)^2$ .

Plastic stability demands that the stress field of the emanated dislocation loops have the tendency to inhibit the sources from further dislocation production. This condition is reflected in the inequality sign of (2.2).

<sup>(3)</sup> A superscript 1 or 2 refers to an equation presented in reference [1] and [2], respectively.

<sup>(4)</sup> This does not include the strain caused by elastic bow out of dislocation segments which is small compared to the strain. For its calculation the reader is referred to [1, 2].

The summation in (2.1) goes over all primary slip systems which are activated during a process increment. The condition that a primary slip system is to be included in this set is given by the isothermal loading conditions  $(3.2^2)$  and  $(3.4^2)$ 

$$(2.3) \qquad \qquad \phi^p = \phi^p(\sigma_{kl}, T, g^p) = 0$$

and

(2.4) 
$$\lambda^{p} \frac{\partial \phi^{p}}{\partial \sigma_{ij}}\Big|_{g,T} d\sigma_{ij} < 0.$$

The change in dislocation state is given by  $(2.9^2)$ 

(2.5) 
$$dg^{p} = - \frac{\frac{\partial \phi^{p}}{\partial \sigma_{kl}}\Big|_{T,g}}{\frac{\partial \phi^{p}}{\partial g^{p}}\Big|_{T,\sigma}} d\sigma_{kl}.$$

This relation follows from differentiating the plastic equilibrium condition  $\phi^p = 0$ . The relation  $d\phi^p = 0$  expresses the fact that a quasi-static process consists of a succession of *macroscopically* infinitesimal nearby equilibrium states. Obviously, such a process is only possible if the material is stable.

Physically, the yield function  $\phi^p$  stands for the average resolved Peach-Koehler force acting at the critically bowed-out sources of the  $p^{th}$  primary slip group.

Disregarding elastic anisotropy of the crystallites,  $\phi^p$  is for the problem at hand, where the interaction stress due to the dislocations of the various primary slip systems can be neglected, given by (A.13<sup>1</sup>), *viz*.

(2.6) 
$$\phi^{p} = (\psi \mathcal{N} l_{0} b)^{p} \left\{ \left( \lambda C \frac{Gb}{l_{0}} \right)^{p} + \sigma_{ij} \alpha_{ij}^{p} + \tilde{\tau}_{back}^{p} (g^{p}) \right\},$$

where  $\mathcal{N}^p$  stands for the number of sources of the slip system p per unit grain volume and  $\psi^p = \frac{(D^3)^p}{V}$  is the volume fraction of the  $p^{\text{th}}$  grain. By definition,  $\lambda^p = \text{sign } A^p$ , i.e.,  $\lambda^p$  is respectively -1, +1 when the sources of the  $p^{\text{th}}$  slip system are bowed out in the direction of  $\mathbf{m}^p$ ,  $-\mathbf{m}^p$ .

The first term in brackets in (2.6) denotes the effect of the line tension which tends to straighten the critically bowed-out sources. The modulus of rigidity is G, while C is a numerical factor which MITCHELL and SMIALEK [9] showed to have a value ranging from 0.3 to 2 for a material having Poisson's ratio of 0.33.

This term does not include the effect resulting from the periodic nature of the crystal lattice which gives rise to a Peierls or friction stress. One can formally replace the term  $\lambda C \frac{Gb}{I_0}$  by  $\tau_0$  to include the effect due to an extended dislocation source. It is interesting to observe that ROSENFIELD and AVERBACH [4] showed that the explanation for the variation of the yield stress corresponding with a plastic strain of  $2 \times 10^{-6}$  cannot be completely found in the variation of G with temperature in copper and also not from current theories on friction forces or forest intersecting dislocations. To explain the temperature dependence of  $\tau_0$  they proposed that for dislocation motion to start an amount of ther-

mally activated stacking fault, differing from the equilibrium one, must be formed. Experimentally it is found that the variation of  $\tau_0$  with temperature has the form  $\tau_0 = \lambda A \exp B/T$ , while for copper this relation may be replaced by a linear one.

The symmetric tensor

(2.7) 
$$\alpha_{ij}^p = \frac{1}{2} (n_i m_j + n_j m_i)^p, \quad \alpha_{ii}^p = 0, \quad \alpha_{ij}^p \alpha_{ij}^p = \frac{1}{2}$$

associated with the p<sup>th</sup> slip system has constant components during the deformation.

The resolved shear stress acting at the sources of the slip system p due to the macroscopic stress vector T is

(2.8) 
$$T_i m_i^p = \sigma_{ij} n_j^p m_i^p = \sigma_{ij} \alpha_{ij}^p$$

The last term in (2.6)

(2.9)  $\tilde{\tau}_{\text{back}}^p = \tilde{p}_i^p m_i^p$ 

denotes the average resolved shear stress which the (modified) dislocation loops of the  $p^{th}$  primary slip system exert on their own sources. The microstress vector set up by the modified pile-up loops is  $p^{p}$ .

When  $\tilde{\tau}_{back}^{p}$  is specified as a function of  $g^{p}$ , the plastic potentials  $\phi^{p}$  can be calculated with (2.6). The knowledge of those is sufficient to calculate the plastic strains and dislocation state for the arbitrary quasi-static isothermal loading path, as follows from the relations (2.1) to (2.5).

The polycrystalline solid may have a texture, in which case the distribution of the  $\alpha_{ij}$ 's differs from that of an random oriented polycrystal while the grain diameters and other parameters as the  $l_0$ 's of the various slip groups may differ.

The present state of knowledge of  $\tilde{\tau}_{back}^{e}$  is rather poor, even for the microstrain region. We only know its form for uni-axial deformation and, strictly speaking, even then only for monotonically increasing or decreasing stress.

#### 3. The tensile stress-strain relation

Under an applied tensile stress  $\sigma_{11} = \sigma$  the plastic tensile strain  $\varepsilon_{11}' = \varepsilon''$  follows from (2.1) as

(3.1) 
$$d\varepsilon'' = \sum_{p} h^{p} \left\{ \frac{\partial \phi^{p}}{\partial \sigma} \Big|_{T,g} \right\}^{2} d\sigma,$$

while (2.6) reduces for the case when all crystallites have the same grain size  $\psi$  and dislocation source density  $\mathcal{N}$  with the same distance between the nodes  $l_0$  to

(3.2) 
$$\phi^{p} = \psi \mathcal{N} l_{0} b \left\{ \lambda^{p} C \frac{G b}{l_{0}} + \sigma \alpha^{p} + \tilde{\imath}^{p}_{back}(g^{p}) \right\},$$

where

$$(3.3) \qquad \qquad \alpha^p \equiv \alpha_{11}^p = (n_1 m_1)^p$$

as follows from (2.7). Here,  $n_1^p$  is the direction cosine between the tensile axis and the normal to the  $p^{\text{th}}$  slip plane, while  $m_1^p$  is the cosine between the tensile axis and the slip direction. We shall agree to select the directions of the unit vector  $\mathbf{m}^p$  such that  $0 \le \alpha^p \le \le 0.5$ . Then  $1/\alpha^p$  is the Schmid orientation number of the  $p^{\text{th}}$  slip system.

BROWN and LUKENS [5] and FRIEDEL [6] assumed that the piled-up dislocations are not plastically relaxed, while the various slip systems act independently. The resolved shear back stress at a source located near the middle of the slip plane resulting from piled-up loops of n dislocations with diameter D, equal to the grain diameter, is then given by

(3.4)<sub>1</sub> 
$$\tilde{\tau}^{p}_{back} = -\frac{G}{2KD} g^{p}, \quad K \approx 1,$$

where G is the modulus of rigidity. The average strength of the piled-up loops is  $|\mathbf{g}_p| = n^p b$ . This result is well known from the dislocation theory. A little reflection shows (see Fig. 1) that the sign of the back stress, which in a stable material must tend to bow the sources into a less than critical configuration, is correctly expressed by  $(3.4)_1$ .

In the introduction we have explained that  $(3.4)_1$  does not lead to the correct result. Therefore, the modified back stress on the primary sources of the slip system p must, for tensile deformation, be taken as

(3.4)<sub>2</sub> 
$$\tilde{\tau}_{back}^{p} = BG \operatorname{sign}(g^{p}) \sqrt{\frac{\alpha^{p}|g^{p}|}{D}}, \quad g^{p} = |g^{p}|\operatorname{sign}(g^{p}),$$

where B is a constant. The absolute value of  $g^p$  divided by the magnitude of the Burgers vector is equal to the average number of loops milled out by the primary sources of the  $p^{\text{th}}$  slip system.

From now on, a result obtained by using  $(3.4)_1$  will always carry an "1" in the equation number and similarly a "2" will be reserved for relations obtained from  $(3.4)_2$ .

Substitution of  $(3.4)_1$  and  $(3.4)_2$  into (3.2) leads to the following forms of constitutive relations:

(3.5)<sub>1</sub> 
$$\phi^{p} = \psi \mathcal{N} l_{0} b \left( \frac{\lambda^{p} C G b}{l_{0}} + \sigma \alpha^{p} + \frac{G}{2D} g^{p} \right),$$

(3.5)<sub>2</sub> 
$$\phi^{p} = \psi \mathcal{N} l_{0} b \left( \frac{\lambda^{p} CGb}{l_{0}} + \sigma \alpha^{p} + BG \operatorname{sign}(g^{p}) \sqrt{\frac{\alpha^{p} |g^{p}|}{D}} \right).$$

If we calculate with (3.5) the hardening parameters, we obtain

(3.6)<sub>1</sub> 
$$h^{p} = \frac{2D(D^{2} + bl_{0})}{(bl_{0})^{2}\psi \mathcal{N}G} > 0, \quad \mathcal{A} = D^{2}$$

for the Brown and Lukens assumption, whereas for the modified back stress we get

(3.6)<sub>2</sub> 
$$h^{p} = \frac{2(D^{2} + bl_{0})}{(bl_{0})^{2} \psi \mathcal{N} BG} \sqrt{\frac{D|g^{p}|}{\alpha^{p}}} > 0.$$

Both functions are positive as is required by the stability condition.

From (3.1), (3.5) and (3.6) the incremental tensile stress strain relation follows as

(3.7)<sub>1</sub> 
$$d\varepsilon'' = \frac{2D^3 \mathcal{N} \psi}{G} d\sigma \sum_{p} (\alpha^p)^2,$$

(3.7)<sub>2</sub> 
$$d\varepsilon'' = \frac{2D^2 \mathcal{N} \psi}{BG} \, d\sigma \sum_p \sqrt{\frac{D|g^p|}{\alpha^p}} \, (\alpha^p)^2,$$

where we have made use of the approximation  $bl_0 \ll D^2$ . The quantity  $|g^p|$  appearing in (3.7)<sub>2</sub> can be eliminated with the plastic equilibrium condition  $\phi^p = 0$ . Using (3.5)<sub>2</sub> gives

(3.7)<sub>3</sub> 
$$d\varepsilon'' = \frac{2D^3\psi\mathcal{N}}{B^2G^2} d\sigma \sum_p \left(\sigma\alpha^p - \frac{\sigma_0}{2}\right)\alpha^p,$$

where we have put

$$\frac{\sigma_0}{2} = -\frac{\lambda^p CGb}{l_0}$$

The summation in (3.7) goes over all grains which are plastically activated under the tensile stress increment  $d\sigma$ , i.e., for which

(3.9)<sub>1</sub> 
$$\frac{\lambda^p CGb}{l_0} + \sigma \alpha^p + \frac{G}{2D}g^p = 0, \quad \lambda^p \alpha^p d\sigma < 0,$$

(3.9)<sub>2</sub> 
$$\frac{\lambda^{p}CGb}{l_{0}} + \sigma\alpha^{p} + BG \operatorname{sign}(g^{p}) \sqrt{\frac{\alpha^{p}|g^{p}|}{D}} = 0, \quad \lambda^{p}\alpha^{p}d\sigma < 0$$

as follows from (2.3), (2.4) and (3.5).

The change in the dislocation state of the  $p^{\text{th}}$  primary slip system follows from (3.5) and (2.5) as

$$(3.10)_1 dg^p = -\frac{2D\alpha^p}{G}d\sigma,$$

$$(3.10)_2 dg^p = -\frac{2}{BG}\sqrt{D|g^p|\alpha^p}d\sigma = -\frac{2D}{B^2G^2}\left(\sigma\alpha - \frac{\sigma_0}{2}\right)d\sigma,$$

where, in Eq.  $(3.10)_2$  the plastic equilibrium condition  $\phi^p = 0$  has been used.

There are some interesting conclusions which can be drawn from the above equations and substantiate the general theory presented earlier.

Observe that the equilibrium condition  $\phi^p = 0$  not only determines which sources are critically bowed out but also the sign of  $\lambda^p$ , i.e., in which direction those sources are critically bowed out.

In practice, in order to determine whether the condition  $\phi^p = 0$  is met for the slip system defined by  $\alpha^p$ , one calculates for each incremental loading step the value of  $\phi^p$ which may be positive or negative. At the moment  $\phi^p$  becomes zero or changes sign, thereby necessarily passing through zero, the sources of the  $p^{th}$  slip system are critically bowed out.

It is also clear from (3.9) that, as long as the emitted dislocation loops are locked in place (D = const), the Bauschinger effect is manifested. This follows because the macroscopic resolved shear stress  $\sigma \alpha$  which must be applied to the sources of a particular slip system to bow them out from a critical position to the opposite critical position, corresponding to a change in the sign of  $\lambda$ , is twice the stress which must be applied to bring the sources from the straight to the critical position.

It follows from (3.5) that the sources of a particuler slip system will, for the first time  $(g^p = 0)$  be critically bowed out when

(3.11) 
$$\sigma \alpha^p = \frac{\sigma_0}{2} \equiv \tau_0.$$

 $\tau_0$  is the resolved shear stress which must be applied to bow the sources out from the straight to the critical position opposing its line tension. It is seen that  $|\sigma_0|$  defined by (3.8) is the tensile yield stress of a random F.C.C. polycrystal; this is the stress necessary to activate the Frank-Read sources of the most favourable slip system oriented at  $\alpha = 0.5$ .

For  $0 \le \alpha^p \le 0.5$  and  $\sigma$ ,  $d\sigma > 0$ , i.e., tensile loading, it follows from (3.9) that  $\lambda^p$  must be negative, and thus  $\tau_0$  and  $\sigma_0$  positive as follows from (3.8). This is easily verified because a positive value of  $\sigma \alpha^p$  means that the macroscopic shear stress acting at the lower side of the slip plane (that is the side of the slip plane on which **n** stands, see Fig. 1) points in the direction of  $\mathbf{m}^p$ . Under such shear stress a source clearly bows out in the opposite direction of  $\mathbf{m}^p$ , which corresponds with  $\lambda^p = -1$ . A little reflection shows (see Fig. 1) that a source which is bowed out critically in the opposite direction of  $\mathbf{m}^p(\lambda^p = -1)$  can only throw off loops in such a way that the lower side will be displaced in the opposite direction of  $\mathbf{m}^p$ , i.e., for which  $dg^p$  is negative. This also follows directly from (3.10) for tensile loading.

Once a particular slip system is triggered into emitting dislocation loops it will continue to do so under monotonically increasing tensile stress. This follows because with  $\lambda^p = -1$  and  $d\sigma > 0$ , the second loading condition (3.9) is satisfied, whereas calculating  $d\phi^p$  with (3.5) shows that this quantity is zero when (3.10) is substituted. Hence,  $\phi^p$  remains zero as is required by the first loading condition (3.9). This relation expresses the fact that, at equilibrium, the macroscopic resolved shear stress acting at the critically bowed-out sources is balanced by the line tension of the sources plus the back stress which the dislocation loops exert on them. The relation (3.10) expresses the fact that during a quasi-static process the increase of resolved macroscopic shear stress is balanced by the increased back stress which the emitted dislocation loops exert on the sources.

Under monotonically increasing tensile stress the number of activated grains or slip systems increases because the resolved macroscopic shear stress on less favourable oriented slip systems increases with tensile stress.

It is clear from (3.7) that the plastic tensile strain in the microstrain region results from non-coupled contributions of strains due to the individual grains.

For monotonically increasing tensile stress the relations (3.7) can be integrated when the initial condition (3.11) is used. The result is

(3.12) 
$$\varepsilon'' = \sum_{p} e''^{p}$$

wherein the contribution of the  $p^{th}$  grain is given by

$$(3.12)_1 e^{\prime\prime p} = \frac{2D^3 \,\mathcal{N}\psi}{G} \left(\sigma \alpha^p - \frac{\sigma_0}{2}\right) \alpha^p,$$

$$(3.12)_2 \qquad e^{\prime\prime p} = \frac{D^3 \,\mathcal{N} \psi}{B^2 G^2} \left( \sigma \alpha^p - \frac{\sigma_0}{2} \right)^2.$$

In Sect. 5 we shall introduce the distribution function for the slip system orientations whereby the summation in (3.12) can be replaced by an integral.

The summation in (3.12) goes over all grains with orientations such that

$$(3.13) \qquad \qquad \alpha^p \geqslant \frac{\sigma_0}{2\sigma}$$

because, in the case of monotonically increasing tensile stress, it follows from (3.10) that  $g^p$  is negative. Making use hereof in (3.9) leads to (3.13).

The equality sign can be included in (3.13) because we can see from  $(3.12)_{1,2}$  that this does not give a contribution to the plastic strain.

#### 4. Calculation of the tensile stress-strain relation directly from dislocation theory

To show the equivalence of the metallurgical approach to plasticity and the general theory we shall derive the relation  $(3.12)_1$  directly from the dislocation theory. We follow [5] and [6] but correct some errors made by them.

Therefore, we assume that the resolved shear back stress acting at the Frank-Read sources is proportional to the number of piled-up dislocations as expressed by  $(3.4)_1$ .

An important point must be clarified in order to understand the following equations. In the metallurgical approach to plasticity, researchers (FRIEDEL, HIRSCH, KUHLMANN-WILSDORF, SEEGER, MCCLINTOCK, etc.) jump over, in the description of the dislocation state, the unstable positions of the expanding loops which emanate from the sources.

It is quite natural to adopt this point of view because one intends to connect microscopic plasticity, which is the result of a succession of unstable dislocation jumps, with stable macroscopic plasticity. The same starting point was adopted by the author in the development of the thermodynamic theory. With this in mind it is easy to calculate the contribution of the  $p^{\text{th}}$  grain to the tensile strain. The macroscopic resolved plastic shear strain due to the  $p^{\text{th}}$  grain containing  $\mathcal{N}$  sources per unit grain volume which have emitted on the average each n square dislocation loops is

(4.1) 
$$e_r^{\prime\prime p} = \psi \mathcal{N} D^2 |g^p|, \quad |g^p| = b n^p,$$

where  $\psi$  is the volume fraction of the  $p^{\text{th}}$  grain and  $D^2$  the slip plane area.

The contribution to the plastic tensile strain due to the  $p^{th}$  grain follows from (4.1) as(<sup>5</sup>)

(4.2) 
$$e^{\prime\prime p} = \alpha^{p} \psi \mathcal{N} D^{2} |g^{p}|,$$

where  $1/\alpha^p$  is the Schmid factor.

(5) FRIEDEL [6] wrote  $e''^p = e''^p / \alpha^p$ , while BROWN and LUKENS [5] omitted  $\alpha^p$  altogether in (4.2). Actually, there is another contribution to the plastic strain due to the movement of the source itself.

<sup>15</sup> Arch. Mech. Stos. nr 3/76

To relate  $|g^p|$  appearing in (4.2) to the tensile stress the Peach-Koehler force equilibrium acting at a critically bowed out source is considered. The positive resolved macroscopic shear stress acting at a source of slip system p is  $\sigma \alpha^p$ , where  $\sigma$  is the tensile yield stress. This stress must, during a quasi-static process which consists of a succession of nearly equilibrium states, be balanced by the positive resolved shear stress due to the line tension of the source  $\tau_0$ , plus the positive resolved back shear stress which the loops in the  $p^{\text{th}}$  grain exert on their sources.

Hence(<sup>6</sup>)

(4.3) 
$$\sigma \alpha^{p} = \tau_{0} + \frac{G}{2D} |g^{p}|.$$

This relation is seen to follow from the equilibrium condition  $\phi^p = 0$  when  $(3.5)_1$  is used and tensile loading is considered. Combining (4.2) and (4.3) leads to  $(3.12)_1$ .

Analogically  $(3.12)_2$  may be derived when the back stress is specified by  $(3.4)_2$ .

## 5. Integration of the tensile relation

The number of grains in a representative element in a fine grained polycrystalline solid is very large. The discrete summation in (3.12) can therefore be replaced by an integral when the distribution function  $P(\alpha)$  is introduced such that the fraction of grains or primary slip systems which lay in the interval  $\alpha$ ,  $\alpha + d\alpha$  is  $P(\alpha)d\alpha$ .

Denote the contribution to the tensile plastic strain by the small group of slip systems lying in this interval by e''. Passing to a continuous distribution of primary slip systems the explicit expression herefore is given by  $(3.12)_1$  or  $(3.12)_2$ .

For monotonically increasing tensile stress, the Brown and Lukens back stress assumption leads to

(5.1)<sub>1</sub> 
$$\varepsilon'' = \frac{1}{\psi} \int_{\sigma_0/2\sigma}^{0.5} e'' P(\alpha) d\alpha = \frac{2D^3 \mathcal{N}}{G} \int_{\sigma_0/2\sigma}^{0.5} \left(\sigma \alpha - \frac{\sigma_0}{2}\right) \alpha P(\alpha) d\alpha.$$

Instead, for the modified back stress, we get from  $(3.12)_2$ 

(5.1)<sub>2</sub> 
$$\varepsilon'' = \frac{D^3 \mathcal{N}}{B^2 G^2} \int_{\sigma_0/2\sigma}^{0.5} \left(\sigma \alpha - \frac{\sigma_0}{2}\right)^2 P(\alpha) d\alpha.$$

The integration interval extends over all grains which contribute to the plastic strain, from the momentary activated one which has the value  $\alpha = \tau_0/\sigma = \sigma_0/2\sigma$  as follows from (3.11), to the first activated slip system with  $\alpha = 0.5$ .

When a source has thrown off *n* dislocations with Burgers vector **b**, the line between the nodes with distance  $l_0$  has moved forward the distance *nb*, and thus swept out the area  $l_0 bn = l_0|g|$ . This causes an additional plastic resolved strain of  $l_0 b|g|$ . Therefore, to  $D^2$  in (4.2) we should add  $l_0 b$ . However, this value is negligible as compared to  $D^2$ . In the general theory we had to carry this small contribution along (see Eq. (4.2) in [1]), otherwise, a contradiction would be apparent in the Maxwell equations.

<sup>(6)</sup> BROWN and LUKENS [5] also omitted the  $\alpha^p$  in (4.3).

To obtain the relation (1.1) one must take in  $(5.1)_1$ 

$$(5.3) P(\alpha) = \frac{C}{\alpha^4},$$

where C is a normalization constant. The result is $(^{7})$ 

(5.4) 
$$\varepsilon'' = \frac{2D^3C}{G\sigma_0} (\sigma - \sigma_0)^2.$$

Recently, ZAOUI [10] has derived the  $\alpha$  distribution function for an random oriented F.C.C. polycrystal under the assumption that not more than one primary slip system, the most favourable one, is activated in a grain. This function is shown in Fig. 2. Al-



though a short analysis shows that there are grain orientations in the interval  $\frac{2}{3\sqrt{6}} \leq$ 

 $\leq \alpha \leq 0.5$ , where more primary slip systems in one grain are activated, it is clear that Zaoui's distribution must be applicable for sufficiently small tensile stress. There seems to be some experimental observations [6, p. 270] indicating that the first activated primary slip plane continues to dominate the plastic behaviour. This may also support the validity of his distribution for larger stresses.

We shall proceed to show that Zaoui's distribution function leads to the correct stress-strain relation when the expression for the modified back stress  $(3.4)_2$  is used.

The tensile stress-strain slope follows from  $(5.1)_2$ , by Leibnitz's rule, as

(5.5) 
$$\frac{d\varepsilon''}{d\sigma} = \frac{2D^3\mathcal{N}}{B^2G^2} \int_{\sigma_0/2\sigma}^{0.5} \left(\sigma\alpha - \frac{\sigma_0}{2}\right) \alpha P(\alpha) d\alpha$$

15\*

 $<sup>(^{7})</sup>$  To obtain this result Brown and Lukens and Friedel had to assume a different distribution function differing from (5.3).

Fig. 3 shows a plot of the function

(5.6) 
$$I\left(\frac{\sigma}{\sigma_0}\right) = \frac{2}{\sigma_0} \int_{\sigma_0/2\sigma}^{0.5} \left(\sigma\alpha - \frac{\sigma_0}{2}\right) \alpha P(\alpha) d\alpha$$

obtained by numerical integration of Fig. 2 (Hereto Zaoui's [10] plots of the functions

$$\int_{\alpha}^{0.5} \alpha P d\alpha \quad \text{and} \quad \int_{\alpha}^{0.5} \alpha^2 P d\alpha$$

were used).



From Fig. 3 it can be seen that I varies linearly from  $\sigma/\sigma_0$  except for values of  $\sigma/\sigma_0$  close to 1:

(5.7) 
$$I = \frac{0.41}{\sigma_0} (\sigma - 1.09\sigma_0) \quad \text{for} \quad \frac{\sigma}{\sigma_0} \ge 1.15.$$

Substitution of (5.7) into (5.5) results in

(5.8) 
$$\frac{d\varepsilon''}{d\sigma} = 0.41 \frac{D^3 \mathcal{N}}{B^2 G^2} (\sigma - 1.09 \sigma_0) \quad \text{for} \quad \frac{\sigma}{\sigma_0} \ge 1.15.$$

Integration gives

(5.9) 
$$\varepsilon'' = 0.205 \frac{D^3 \mathcal{N}}{B^2 G^2} (\sigma - 1.09 \sigma_0)^2 \quad \text{for} \quad \frac{\sigma}{\sigma_0} \ge 1.15.$$

Thus, the microstrain should vary parabolically with stress for stresses larger than 15% of the yield, and linearly with the grain volume. The intersection of the parabola to zero plastic strain should occur for a stress 9% higher than the yield stress. The experimental results of THOMAS and AVERBACH [3] on 99,999% pure annealed polycrystalline copper shown in Fig. 4 substantiate this trend. They found that the yield stress was about



FIG. 4.

1000 lb/in<sup>2</sup>  $\approx$  1 kg/mm<sup>2</sup>, while continuation of the experimental parabolas intersected the  $\sigma$  axis at higher stress values. The polycrystals with grain diameters of 0.08 mm, 0.04 mm and 0.025 mm are described very well by (5.9) as shown by the drawn curves in Fig. 4. The yield tensile stress for the 0.08 mm polycrystal is  $\sigma_0 = 0.81$  kg/mm<sup>2</sup> = = 1160 lb/in<sup>2</sup>, for the 0.04 mm polycrystal  $\sigma_0 = 0.836$  kg/mm<sup>2</sup> = 1194 lb/in<sup>2</sup>, while for the 0.025 mm polycrystal,  $\sigma_0 = 0.93$  kg/mm<sup>2</sup> = 1330 lb/in<sup>2</sup>.

For copper with  $G = 4200 \text{ kg/mm}^2$  the value of  $\mathcal{N} / B^2$  in (5.9) is  $4.25 \times 10^6 / \text{mm}^3$ . A reasonable source density of  $10^7$  per cm<sup>3</sup> leads then to  $B \approx 0.1$ . For C = 2 and  $b = 2.55 \times 10^{-7}$  mm we find from (3.8)  $l_0 \approx 0.005$  mm for the average source length (distance between the nodes).

From Fig. 4 it can be seen that after the microstrain region ends another parabolic

hardening of the same type but over much larger strains [6] sets in. The flow stress whereby this second parabola begins is related to the grain diameter by

(5.10)  $\sigma_y = 0.43 D^{-1/2} - 0.12,$ 

where  $\sigma$  is in kg/mm<sup>2</sup> and D in mm.

The relation (5.10) may be taken to define the macroscopic yield stress, the definition of which is also rather arbitrary. The Eq. (5.10) resembles the Hall-Petch relation, except only that the constant is negative. This constant has often been interpretedas a friction stress but should then be positive.

# References

- 1. J. LAMBERMONT, Int. J. Engng. Sci., 7, 937, 1974.
- 2. J. LAMBERMONT, Int. J. Engng. Sci., 7, 953, 1974.
- 3. D. THOMAS, B. AVERBACH, Acta Met., 7, 69, 1959.
- 4. A. ROSENFIELD, B. AVERBACH, Acta Met., 8, 624, 1960.
- 5. N. BROWN, K. LUKENS, Acta Met., 9, 106, 1961.
- 6. J. FRIEDEL, In Dislocations, 265, Pergamon Press, 1964.
- 7. T. MITCHELL, Phil. Mag., 10, 315, 1964.
- 8. Z. BASINSKI, T. MITCHELL, Phil. Mag., 13, 103, 1966.
- 9. T. MITCHELL, R. SMIALEK, In Work Hardening, 365, Gordon and Breach, 1968.
- 10. A. ZAOUI, Mémorial de l'Artillerie Française. Sciences et Techniques de l'Armement, 1972.

INSTITUT DE MATHÉMATIQUE, AVENUE DES TILLEURS 15, B4000 LIÈGE.