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AUTHOR(S): U. F. Kocks, C. Tome, and G. R. Canova

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EFFECTIVE-CLUSTER SIMULATION OF POLYCRYSTAL PLASTICITY†

U. F. Kocks, C. Tomé* and G. R. Canova**

Center for Materials Science, Los Alamos National Laboratory, Los Alamos NM87545 USA

A model is proposed in which each grain, representative of a certain orientation and strength, is embedded in a thin shell of plastic effective medium; this assembly is called an "effective cluster". For each grain, the plastic strain increment is chosen such that the yield surface of the effective cluster gives the macroscopic stress. The results differ from uniform-strain theories only in some cases, such as in the compression of f.c.c. polycrystals, where "grain curling" occurs.

On propose un modèle où chaque grain, représentatif d'une certaine orientation ou d'une certaine dureté, est encastré dans une coquille plastique assez mince; ce multicristal est appelé un "agglomérat effectif". Chaque grain est supposé se déformer de manière à ce que la surface d'écoulement de l'agglomérat produise la contrainte macroscopique. Les résultats sont différents de ceux correspondants à une déformation uniforme dans certains cas seulement, tels que la compression des polycristaux c.f.c. où l'on observe le phénomène "grain curling".

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* Permanent address: IFIR-CONICET, Universidad Nacional de Rosario,
Pellegrini 250, 2000 Rosario, Argentina.

** Permanent address: LPMH, Fac. des Sciences, Ile du Saulcy, 57045 Metz, France.

1.- THE MODEL

The most widely used theories of polycrystal plasticity, despite many modifications, all start with the assumption of Taylor (1938): that the plastic strains are uniform throughout the body. It is well known that this is not true in fact, and cannot be true if equilibrium and yield conditions are to be satisfied everywhere (Bishop and Hill, 1951). For some of the known and expected non-uniformities, plausible arguments can be given why they might not influence the macroscopic average behavior significantly (Kocks, 1970); for others, this is not so evident. In the present paper, we propose a model to deal with one of these.

A useful picture of the elemental process of deformation in a polycrystal is this (Krüner, 1958): consider one grain and the 'hole' it was in at the start; now consider separately the deformation of the hole and of the grain and how they influence each other. The Taylor assumption is equivalent to saying that the hole deforms like the bulk and the grain follows this deformation exactly. When the particular grain chosen is, for example, stronger than the average, internal stresses are set up that help the grain meet the demanded performance -- but that are assumed not to influence the deformation of the hole. In the so-called "self-consistent" elastic-plastic treatments (Krüner, 1958, Budiansky and Wu, 1962), the elastic deformation of the hole is adjusted -- but it is not verified whether the total stress in the vicinity of the hole might exceed the yield condition there: in this respect, the model is not "self-consistent". This problem has been recognized (Hill, 1965, Berveiller and Zaoui, 1979), but not solved, in the sense that no large-strain computer code has been suggested that incorporates a plastic accommodation of heterogeneities in strength.

In the present paper, we propose a model in which the "immediate environment" of a grain is allowed to accommodate the individuality of the considered grain in a plastic response; namely, so that the grain and its immediate environment are together considered as a "cluster" which itself is now embedded in an elastic medium. This serves to average out the effect of especially different grains on a local

basis. The attempt is to provide an approximate solution rather than a rigorously self-consistent one.

A case of particular interest is when the grains are not really different in "strength" (in the sense of the size of their yield surface), but have a yield surface of very anisotropic shape. Then, certain components of strain (expressed in crystal coordinates) require an especially high stress to achieve; in sample coordinates, these "hard" components will vary from grain to grain. This could be particularly important in materials of hexagonal crystal structure (Kocks and Westlake, 1967, MacEwen et al. 1983, Tomé and Kocks, 1985). In cubic materials, there are certain situations in which plane-strain deformation is considerably easier than uniaxial deformation; then, even though uniaxial deformation be macroscopically prescribed, different grains may choose different directions of plane-strain deformation, leading to the phenomenon of 'grain curling' (Hosford, 1964).

One of the problems to be addressed is the fact that each grain is surrounded by only a dozen or so other grains: not enough to be considered representative of the average. And of course, each part of a grain feels one or two of the specific neighboring grains more strongly than it does the others. To solve this problem exactly, one would have to do a finite-element calculation. However, an elegant concept inherent in the "self-consistent" treatments (Kröner, 1958) is to assume that a representative grain, which occurs many times within a certain interval of orientation and strength, behaves as if all the various environments were averaged and thus constitute an effective medium. Thus, the non-uniformity within each grain (due to the proximity of different specific neighbors) and that from grain to grain (due to different total environments) is ignored. We shall retain the concept of a representative grain of a certain orientation (or strength, or hard component) and apply the effective-medium concept to the "immediate environment": the combination is what we call an effective cluster.

2.- THE ALGORITHM

The model has been used (Tomé et al., 1985) to modify an established computer code that simulates polycrystal plasticity (Tomé et al., 1984). Each of N grains is imagined to be surrounded by n of the other grains (picked in a systematic-random way); we have so far tried $N = 800$, $n = 12$ and $N = 200$, $n = 50$: the latter case corresponds in some way to an "effective environment"; in the former, an equivalent averaging occurs through treating more grains. The yield surface of this cluster is obtained by weighting the stresses in the following way:

$$(1) \quad \sigma_c = \left(1 - \frac{V_g}{V_c}\right) \sigma_e + \frac{V_g}{V_c} \sigma_g$$

where σ_c is the average stress in the cluster, σ_e that in the environment, and σ_g that in the (central) grain. All are in response to a postulated direction ϵ_g^0 of the strain-increment, which is initially taken to be the macroscopic one, $\bar{\epsilon}^0$, but is then iterated such as to attain

$$(2) \quad \sigma_c(\epsilon_g^0) = \bar{\sigma}(\bar{\epsilon}^0)$$

where $\bar{\sigma}$ fulfills macroscopic equilibrium conditions.

In eq. (1), V_g is the volume of the grain, V_c that of the cluster; the ratio is not equal to $1/n$, but rather an independent parameter which characterizes the range of plastic accommodation around the grain. If V_g were infinitesimally small, the influence of the grain is nil: it conforms completely to the environment and $\epsilon_g^0 \equiv \bar{\epsilon}^0$ (Taylor, 1938). On the other hand, in the limit $V_g/V_c = 1$, eq. (1) becomes equivalent to the Sachs (1928) model. We have found a value of $1/12$ to be essentially equivalent to uniform strain, and $1/4$ giving differences of the kind and magnitude that agree qualitatively with experimentally observed deviations from Taylor behavior. $V_g/V_c = 1/4$ corresponds roughly to a cluster diameter of 1.3 grain diameters.

Equations (1) and (2) were written in terms of the complete stress and strain-increment tensors. However, some of the stress and strain-increment components were exactly prescribed. Firstly, there is the major imposed strain component, which

serves as a scaling factor. (On the other hand, the major stress component was left to come out as it would.) In addition, we have used the Relaxed Constraints model (Honneff and Mecking, 1978; Kocks and Canova, 1981; Tomé et al., 1984). Here, the developing anisotropy of grain shape is taken account of by relaxing compatibility conditions on some strain components but, on the other hand, enforcing the corresponding stress components. (Van Houtte et al., 1984, have relaxed some additional components without, however, considering the interaction with the environment.)

The iteration in ε_g^0 led to rapid fulfillment of eq. (2) in many cases; it was immaterial what tolerance was allowed for the approximate relation (2). In other cases, no convergence could be obtained even after many iterations. We considered this to be a physically meaningful occurrence: sometimes, the environment will not be able to accommodate the hard component of its center grain, and the latter has to follow Taylor conditions.

So far, we have only used vertex states of the single-crystal yield surface for calculating σ_g . Thus, a change in ε_g^0 would often not give a change in σ_g (although it would change the slip system activity). In general, one should consider grain stress states along the 4th-order or 3rd-order edges of the single-crystal yield surface: a local deviation is expected to occur especially when fewer slip systems can attain a deformation similar (though not identical) to the imposed one.

To resolve ambiguities in slip system activity at vertices, we have used a vertex-rounding procedure based on the assumption of some rate sensitivity (Canova and Kocks, 1984). Improvements to this method are still in progress (Canova et al., 1985); they have no significant effect in the limit of relaxed constraints, where fewer cases of non-uniqueness occur.

3.- SOME RESULTS

Figure 1 shows the results of three different simulations of compression of a polycrystal of fcc lattice structure, in terms of the preferred direction of the normal to the compression plane in a stereographic triangle, after a true strain of

1.0, starting with a random texture. The three methods used were: (a) classical Taylor/Bishop-Hill "full-constraints" (FC) theory, using an averaging procedure to resolve ambiguities (Bishop, 1954); (b) relaxed-constraints (RC) theory, based on the evolution in grain shape with deformation and attaining tri-slip conditions in the later stages (Tomé et al., 1984); and (c) "effective-cluster" (EC) theory, as proposed here. It is seen that the last, as compared to the first, gives a wider scatter of orientations, as may well be expected; but the general shape of the direction distribution is rather similar. The RC theory (in the form used) gives a sharper texture in which, importantly, the experimentally observed main component, $\{110\}$, is missing; this has been a major problem of the RC theory and led, in fact, to the present new developments.

Fig. 1 - Inverse pole figures for the compression axis in an fcc polycrystal after a true strain of 1.0, according to calculation by (a) FC, (b) RC, (c) EC methods.

Figure 2 shows the development of the average Taylor factor, $\bar{M}$, with strain for the three cases. In the FC mode, it continues to increase, corresponding to the fact that M is larger than average in the vicinity of $\{110\}$, the developing texture component. In the RC model, FC conditions obtain initially, until the aspect ratio of the grains has become sufficiently large to relax the constraints; from then on, $\bar{M}$ decreases, since fewer slip systems are required. In the EC calculation, it decreases right from the start; this is due to the fact that an increasing number of grains elect to deform in the plane-strain mode, which ideally requires only $2/3$ of the stress--and are accommodated by the effective environment.

Fig. 2 - Development of the average Taylor factor M with compressive strain.

Since, in this model, there is a direct correlation between the strength of a grain and its behavior, we needed to assume a hardening law in the effective-cluster simulation. We have assumed it to be of the Taylor (1938) type in that the flow stress depends only on the algebraic sum of shears; the scalar hardening law uses an exponential approach to a final low (but not nil) linear hardening rate, as we have found to be appropriate for compression in copper in Tomé et al. (1984).

4.- SUMMARY

A further modification of the Taylor theory of polycrystal plasticity is proposed. The difference between the various models may be expressed in terms of the boundary conditions experienced by a grain. In the true Taylor (Full Constraints) theory, all components of strain-increment are rigorously prescribed. In the Relaxed Constraints models, only some of the strain-increment components are rigorously prescribed; on the complementary components, the stresses are rigorously prescribed. In the current model, there are two units: the grain and the "effective cluster": the grain follows rigorously the (full or relaxed) strain-increments of the cluster; but the cluster follows approximately the macroscopic stress

conditions. Only the grain is used to obtain the macroscopic average properties, but its strain may deviate from the average -- the more so the harder it is for the grain to conform, and the easier it is for the cluster to accommodate.

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