

TITLE RELIABLE MODELING OF COMPLEX BEHAVIOR

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RELIABLE MODELING OF COMPLEX BEHAVIOR†

U. F. Kocks

Center for Materials Science
Los Alamos National Laboratory
Mail Stop K765, Los Alamos, NM 87545, USA

Abstract

The status of modeling for large-strain plasticity is assessed, and this overview is used to emphasize some general points concerning modeling in Materials Science. While a physical foundation is essential in order to achieve generality and some measure of confidence in extrapolations, phenomenological constraint is equally crucial to achieve reliability and predictive value in descriptions of the macroscopic behavior despite the enormous complexity of the underlying physics. Many details that may be of interest in modeling the physical foundation lose importance in the integration to an overall materials response, which depends on few parameters and is quite reproducible. From this point of view, the current understanding of large-strain plasticity is adequate in many respects. However, some problems are highlighted in which more quantitative modeling results would impact the reliability and generality of macroscopic properties descriptions, and which seem amenable to treatment with current techniques and resources.

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Introduction

"This is just a model" is an excuse often heard when some aspects of a model do not agree with some observations or with some presumed basic knowledge. The implication is that this modeling is an intermediate exercise on the way to a full theory: then, the current model may be helpful, but should not be taken too seriously.

There are, however, many cases in Materials Science where the total set of processes and properties (the material "behavior") is so complex that a full, *ab initio* (and *ad finem!*) theory cannot be expected to be available in any foreseeable future. In this case, modeling is a task to be taken very seriously. A major part of the effort is to find an *adequate* model: one whose predictions can be relied upon (to a specified accuracy). Two criteria must be fulfilled: all features that are considered essential must be modeled well enough; and no prediction or assumption of the model can be in clear contradiction to other experimental or theoretical knowledge. (An example of the latter would be some symmetry violation.) Finally, a model earns its real merit when it is reliable not only in the measured range of variables, but can be extrapolated into a regime that is inconvenient or even inaccessible to experiment, but whose limits are at least approximately known.

These high demands on a model can be met only if, on the one hand, it captures the essence of the physics involved and, on the other, discards enough of the detail to be operationally meaningful in the end. Experience has shown that in Materials Science one is fortunate enough that the macroscopic behavior can always be described by a much smaller number of parameters or curves than one has any right to expect, given all the complex mechanisms. This decimation of information happens at every level (of length scale, time scale, dimensionality, etc.): as one progresses from one level to the next, only little information is carried forward. Each submodel at one level may be looked upon as a "black box": only its output matters at the next level. It is the purpose of this paper to assess, in this light, the current status of the modeling of large-strain plasticity.

Hierarchy of Physical Mechanisms and Macroscopic Properties

Table I shows many of the mechanisms (not necessarily all) that are involved in macroscopic plastic behavior based on dislocation glide (not involving diffusion), at various levels. It begins with atomic interactions and ends with polycrystal strain hardening; it begins with scalar properties and ends with yield surfaces in five-dimensional stress deviator space. The part we wish to concentrate on is the interaction between the various levels: each one has been given a number, and before its number appear the numbers of those "lower-level" mechanisms whose output is needed for this current one.

Let us start with atomic mechanisms (#1). Their influence on dislocation behavior is primarily through the lattice resistance (#3, "Peierls stress"), which is controlled by the dislocation core structure (#2). The number 3 appears twice later: the lattice resistance provides one of the components of the flow stress (#11); and it may determine which slip systems are active in low-symmetry crystals (#18). But the interatomic force law (#1) and the dislocation core structure (#2) do not appear ever again!

Similarly, all the various properties of individual dislocations and their interaction (numbers 4 through 7) are relevant only to the dislocation component of the flow stress (#8); once this is known, the details are not needed for understanding at a more macroscopic level (except perhaps the self stresses, #6, in the context of strain hardening, #13).

Table I: Hierarchy of Physical Mechanisms and Macroscopic Properties*

1.	Interatomic forces	
1→ 2.	Atomic arrangement in dislocation core (incl. pressure effects)	
1,2→ 3.	Lattice resistance	→ POTENTIAL SLIP SYSTEMS
<hr/>		
4.	Dislocation motion (phonon, electron, radiation drag)	
5.	Dislocation interaction with individual obstacles (incl. disl's)	
6.	Dislocation self stresses (bowing, parallel dislocations)	
7.	Thermal activation of one dislocation over obstacles	
4-7→ 8.	Interaction of one dislocation with many obstacles (percolation)	
8→ 9.	Statistics of many dislocations (pile-ups, dynamics)	
10.	Superposition of mechanisms	
3,8-10-11.		→ CRITICAL RESOLVED SHEAR STRESS
<hr/>		
8→12.	Dislocation storage	
6,12-13.	Internal stresses, plastic relaxation	
14.	Dislocation rearrangement (thermally aided)	
15.	Dipole annihilation (diffusion aided)	
11-15-16.		→ STRAIN HARDENING IN SINGLE CRYSTALS
17.		→ BAUSCHINGER EFFECT IN SINGLE CRYSTALS
<hr/>		
3-18.	Stress to activate an adequate number of slip systems in a grain	
11-19.	Interaction of grains in a polycrystal (flow around hard grains)	
18,19-20.	Averaging over GRAINS OF GIVEN DISTRIBUTION OF ORIENT. & SHAPE	
21.		→ POLYCRYSTAL YIELD SURFACE
22.		→ GRAIN-TO-GRAIN INTERACTION STRESSES
<hr/>		
19-23.	Repartition of slip systems	
24.	Kinematics of non-uniform deformations	
23,24-25.		→ TEXTURE CHANGE
<hr/>		
16-26.	Multiple-slip hardening law for representative grain	
25,26→		→ STRAIN HARDENING IN POLYCRYSTALS
17,22→		→ BAUSCHINGER EFFECT IN POLYCRYSTALS
<hr/>		
→→→→→	SIZE, SHAPE, AND LOCATION OF POLYCRYSTAL YIELD (FLOW) SURFACE	
→→→→→	for given INITIAL STATE VARIABLES, and its EVOLUTION with strain	

* Various physical mechanisms are highlighted that eventually contribute to MACROSCOPIC PROPERTIES relating to large-strain plasticity at low and intermediate temperatures. The list proceeds from small length scales to large ones, from zero-temperature mechanisms to those involving thermal activation, from scalar properties to those requiring tensor spaces. Each mechanism is assigned a number; these numbers are used to highlight where, later on in the list, this mechanism influences others. Note that many never appear again, such as #1 and #2 (except through #3), or #4 through #7 (except through #8).

Strain hardening in single crystals (or in a grain of a polycrystal - #16) depends on many detailed dislocation processes; but once its laws are known (including, for example, its dependence on strain rate and temperature), none of the underlying mechanisms are needed for an understanding of polycrystal strain hardening (#26): the only information needed in addition is the texture development (#25).

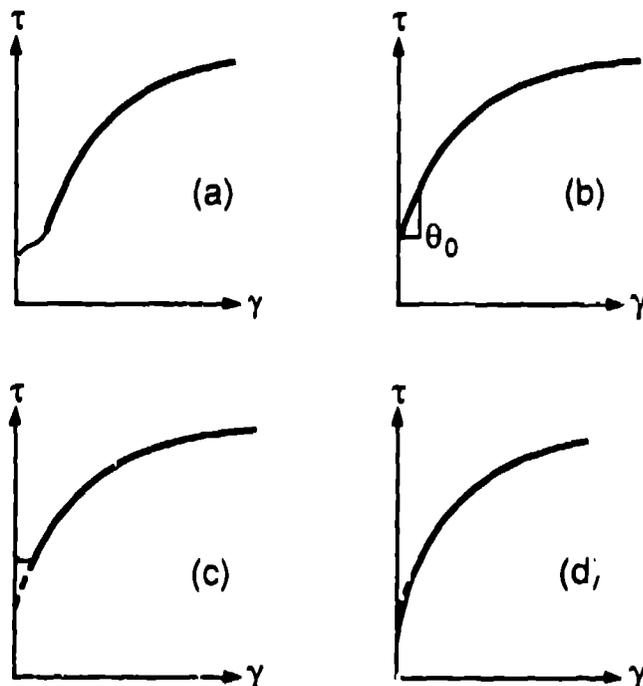
These examples illustrate a general principle of modeling: using details of a "lower-level" process, even though they may be well understood, in the description of a "higher-level" process is often unnecessary. In a certain sense, it is even undesirable: it may involve superfluous parameters; and it may falsely imply that the higher-level description must change when something has changed in the understanding of the lower-level process.

Aspects of Behavior. Classes of Materials. Regimes of Variables

One cannot expect to ever have a single unique set of laws for all plastic behavior of all materials at all temperatures, strain rates, etc. On the other hand, if Materials Science is to make any difference, one must be able to do better than have a new law (or nomogram) for each material at each temperature, each strain rate, etc. Figure 1 shows the stress/strain behavior for four different cases (all schematic). It is seen that they have a many features in common - provided that one ignores some initial behavior at low strains. Thus, "large-strain plasticity" may be an aspect of behavior that is amenable to some generalized treatment; we will come back to what "large strain" means in this context.

The four examples in Fig. 1 all refer to metals of cubic lattice structure: one single crystal and three polycrystals (one pure, one solution hardened, and one dispersion strengthened). The polycrystal stress/strain curves have been converted to resolved shear stress vs resolved shear. It does not matter, for the current discussion, how this was done or, for that matter, how accurate it is. But in order of magnitude, all show the same steepest slope, θ_0 , of order $1/200$ of the shear modulus, μ . If we use this slope as the *initial* slope of what we will label "large-strain behavior", we have

Fig. 1 - Typical stress/strain curves for FCC materials at low and intermediate temperatures: (a) pure single crystal, (b) pure polycrystal; (c) solution hardened; (d) dispersion strengthened polycrystal.



defined the "small-strain" aspects of the behavior, which for this treatment will be ignored as initial "transients". This does not mean, of course, that they are unimportant: merely that a different set of laws must be discovered for this different aspect of materials behavior.

The same reference hardening rate θ_0 can serve to delineate the regime of temperature and strain rate that can be treated by the same set of mechanisms: namely, all for which $\theta_0 \approx \mu/300$, within a factor 2 at most. This would still cover most if not all face-centered and body-centered cubic metals over a temperature range of roughly 20 K to at least half the melting point, and strain rates of at least 10^{-7} to 10^3 sec^{-1} : an enormous regime of variables, for a very large class of materials.[1]

It is this restriction to certain aspects of behavior, a certain regime of the variables, and a certain class of materials that makes it possible to specify a general, closed set of equations, rules, nomograms, etc., for the material behavior within these limits. An integral part of such a description is the specification of the limits to which it may hold, and a diagnostic technique to ascertain that one is within these limits for a particular application.

Results of Dislocation Theory

We will now give an example of a set of equations that describes the relevant results of dislocation theory sufficiently well for the reliable use in more macroscopic models. We will point out current shortcomings and, on the other hand, areas where further modeling efforts, even if successful, would not impact macroscopic applications.

First, there is the flow stress: the current yield stress of a material that may have had arbitrary previous deformations. The current flow stress may be due to many different types of dislocation interaction with a variety of obstacles to glide: we will only discuss the contribution of dislocation/dislocation interactions, which are the cause of strain hardening. (The superposition of this contribution with others is one of the problems not solved quite well enough at the present time.[2]) Flow stresses are best described as resolved shear stresses τ , and strains and strain rates are best described as shears and shear rates γ and $\dot{\gamma}$, because even in polycrystals the relation between these physical quantities and macroscopically measured ones depends on an additional, geometric quantity: the orientation of the crystal or the texture of the polycrystal. The dislocation (super-script D) component of the flow stress is

$$\tau^D = \alpha \mu b \sqrt{\rho} \cdot s(T, \dot{\gamma}) \quad (1)$$

where μ is an appropriate shear modulus [3], b the length of the Burgers vector, ρ the dislocation density, and α a constant that is empirically between 0.5 and 1.0 [4]. This relation can be derived on the basis of any type of dislocation interaction and almost any detailed definition of ρ (but best for the "forest density"[5]); it is thus an example of a relation that is quite insensitive to details of the microscopic model.

The function $s(T, \dot{\gamma})$ at the end of eq.(1) expresses the effect of the glide kinetics on the flow stress. For the purposes of later use in polycrystal models, it is opportune to introduce a "standard state", at a standard temperature T_1 and shear rate $\dot{\gamma}_1$, and express the kinetic relation as one between the flow stress τ_1 under these conditions and the values chosen for T_1 and $\dot{\gamma}_1$. (This will hold even when there are other additive terms to the flow stress in eq. 1). We choose the general form

$$\log \frac{\tau_1}{\mu} = \mathcal{F} \left[\frac{kT_1}{\mu b^3} \log \frac{\dot{\gamma}_0}{\dot{\gamma}_1} \right] \quad (2)$$

While \mathcal{F} may be an arbitrary function, its argument expresses the fundamental insight that the temperature and strain-rate dependence of glide are linked through an Arrhenius-type equation for thermal activation. An additional temperature (but not strain-rate) dependence enters through the shear modulus, and its appearance on both the left- and right-hand sides is well established. [3] Equation (2) contains one adjustable parameter, $\dot{\gamma}_0$, which is used to make all points for different temperatures and strain rates fall on the same curve.

If \mathcal{F} were a linear relation, eq. (2) would amount to a power law between strain rate and stress, which is not appropriate in this case: the power would typically be between 30 and 300. (For this reason, also, any possible stress dependence of $\dot{\gamma}_0$ is negligible.) A form of \mathcal{F} is known that is insensitive to details of the mechanism [3,6] and phenomenologically sufficient; on the other hand, an exact form would depend not only on the dislocation obstacle interaction, but also on the statistics, and therefore would be unlikely to have generality for many actual cases.

Equation (2) is known to be incomplete at very high rates of strain (greater than about 10^6 s^{-1}): then, drag on dislocations in obstacle-free regions becomes important and adds a stress dependence to the $\dot{\gamma}_0/\dot{\gamma}_1$ term. Modeling of this correction is also reasonably well advanced. [7]

Let us now return to eq.(1). It predicts the flow stress once the dislocation density is known. But the dislocation density is a difficult parameter to measure. From a phenomenological point of view, a measurement of the initial flow stress itself is much simpler and more reliable. The real application of eq.(1) comes in predicting the flow stress at a later time; i.e., from a prediction of the evolution of the dislocation density.

The differential relation for the evolution of the flow stress with strain may be written as

$$\left. \frac{\partial \tau^D}{\partial \gamma} \right|_{\dot{\gamma}, T} = \theta - \theta_0 \cdot \left\{ 1 - \mathcal{E} \left[\frac{\tau^D}{\tau_B} \right] \right\} \quad (3)$$

The current hardening rate depends on the current flow stress (not directly on the strain, which is not a state variable). The essential content of eq.(3) is that both θ and τ^D can be scaled, by the parameters θ_0 and τ_B , respectively, to bring all curves at different temperatures and strain rates into coincidence. [8] This is not always true; but it is a sufficiently good approximation for a large class of materials and a substantial regime of strain rate and temperature (as explained with the introduction of Fig. 1). The function \mathcal{E} may be arbitrary; when it is linear, the stress/strain curve follows the Voce law. In fact, it usually saturates less rapidly, and sometimes not at all ("stage IV"). Fig. 2 shows some cases derived from a match of polycrystal modeling with observations [9].

Equation (3) splits the strain hardening rate into two components: a positive, "hardening" ("stage II") contribution and a negative "dynamic recovery" ("stage III") contribution. [4] These have been modeled with fair success by dislocation theory. One result is that θ_0 should be (as it is) athermal and insensitive to material; the observed value of $\theta_0 = \mu/200$ is reasonable in light of dislocation theory [5], but the actual number

(including, for example, its slight dependence on material) has not been derived quantitatively. Here is an opportunity for further microscopic modeling - although the result is unlikely to change anything in the "output" used for macroscopic modeling. At very high strain rates, θ_0 has been observed to increase markedly; only qualitative explanations have so far been given for this effect [6].

The principal rate and temperature dependence of strain hardening resides in τ_s . This was explained early on by thermally activated cross slip and is now more generally attributed to rearrangements of the initially stored dislocation tangles into cell walls, by a combination of stress and thermal activation.[5] It therefore should follow a relation much like eq.(2):

$$\log \frac{\tau_s}{\mu} = \mathcal{S} \left(\frac{kT}{\mu b^3} \log \frac{\dot{\gamma}_{s0}}{\dot{\gamma}} \right) \quad (4)$$

again with a temperature-dependent μ . [8] The function \mathcal{S} is again arbitrary. Figure 3 shows observations for copper at elevated temperature [10]. The slope in this diagram is equivalent to the stress exponent of steady-state creep, in units of $\mu b^3/kT$. It varies from about ?? to about 4 for the data shown (meaning that strain hardening is much more rate sensitive than the flow stress).

A significant implication of eq.(4) is that the stress exponent should decrease *continuously* as the temperature is raised. While a decrease is observed experimentally, it is not well established that it is continuous rather than discontinuous (as often assumed in creep theories and deformation mechanism maps).

Another consequence of a low effective stress exponent is that any stress dependence of the adjustable parameter $\dot{\gamma}_{s0}$ would now matter, and it is indeed sometimes observed to matter at higher temperatures. An empirical relation of the type

$$\dot{\gamma}_{s0} \propto \tau_s^{n_0} \quad (5)$$

with n_0 typically between 4 and 5 has been found useful [8]; it could be explained fairly easily if the power were 1 or 2, but not higher than 3.

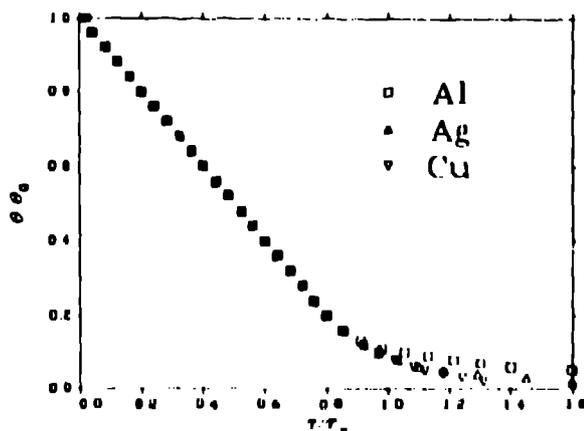


Fig. 2 - Grain hardening law: scaled hardening rate vs scaled stress, for Al, Cu, Ag [11]

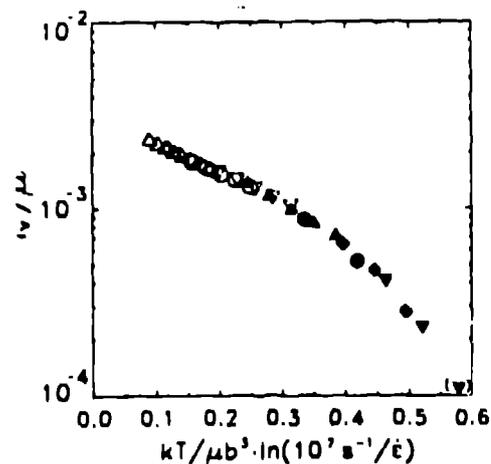


Fig. 3 - Normalized stress scaling factor vs normalized activation energy for Cu [10]

It is seen that there is a definite need for additional modeling of dynamic recovery mechanisms. Such modeling should also address the actual form of the general function ϵ above, which is not understood in sufficiently quantitative detail at low strain-hardening rates. Finally, an improved model should incorporate a physical interpretation for the known existence of a second state parameter (beyond τ^D), which controls the "long transients" (about 3 to 5 percent long) after strain-rate or temperature changes in "stage III" of strain hardening, as well as the other idiosyncrasies of stage III [4].

Significant progress could perhaps be made by modeling static recovery, which has been shown to have similar microscopic consequences as dynamic recovery; namely, a sharpening of the tangles into cell walls and eventually subboundaries [12,13]. This is clearly a local energy minimization process (even though the original laying down of dislocations into tangles during straining is not). It may involve the activation of additional ("secondary") dislocations to relax the internal stresses set up by the primarily stored ones, and this is an interesting side effect by itself. A computer study of a single tangle, and later of a single cell (with all walls), in three dimensions, might provide significant insight; it would be extensive, but not intractable. However, one should not expect any change in the equations 1 through 4 which, in this general form, are well established; only the actual form of the functions ϵ and σ might perhaps be obtained, and an understanding of the term $\dot{\gamma}_{s0}$ and its stress dependence.

Summarizing the situation in the aspects of large-strain plasticity that depend on dislocation theory, we can say the following. The flow stress at a given state, including its dependence on strain rate and temperature, needs no further modeling from an applications point-of-view, except perhaps with respect to superposition laws. The strain hardening law at very low hardening rates is not sufficiently well known, and does not seem, from experiments so far, to exhibit a general type of behavior; additional conceptual modeling is required. The processes of (static and) dynamic recovery can be well enough described phenomenologically, but lack detailed understanding of the processes involved, the dependence on material (stacking-fault energy?), and the development of local misorientations (important for plastic instabilities and subsequent recrystallization behavior). These problems can probably be addressed with current simulation techniques.

Grains in a Polycrystal

The grains in a polycrystal have complex boundary conditions imposed upon them; in that sense, they are different from single crystals, which are usually thought of as free test specimens. When one tries to derive the properties of polycrystals in terms of those of single crystals, one really means: in terms of the properties of the "representative grain". [14] These may include direct effects of the grain boundaries, which lead to grain size effects. And they may even refer to a part of a grain, if that is the smallest unit in which some degree of homogeneity can be assumed. But the most important property of the representative grain is the set of potentially active slip systems to fulfill imposed straining conditions.

Each slip systems can be characterized by the unit distortion m it causes in a sample frame R^0 [15]:

$$m_{ij}^{(s)} = R_{ik}^0 b_k^{(s)} R_{jl}^0 n_l^{(s)} \quad (6)$$

where b^s is the slip vector and n^s the slip plane normal. Then, the shear rate on that system may be expressed as

$$\dot{\gamma}^{(s)} = \dot{\gamma}_1 \left[\frac{m_{ij} \sigma_{ji}}{\tau_1^{(s)}(\sigma)} \right]^{1/m} \quad (7)$$

This is a linear approximation of eq.(2) in the neighborhood of the pair $(\dot{\gamma}_1, \tau_1)$; the scalar m (not to be confused with the matrix m) is the local rate sensitivity $(\partial \ln \tau / \partial \ln \dot{\gamma})_T$; and the resolved shear stress τ has been expressed explicitly in terms of the applied stress σ . Equation (7) does not really serve as a kinetic law: it is used only to distribute shear rates between slip systems in the overall grain deformation

$$\dot{\epsilon} = \sum \text{sym}(m^{(s)}) \dot{\gamma}^{(s)} \quad (8)$$

Slip rates that are less than 1/10 the maximum are of no concern here: that is why a power law is a sufficient approximation. The dependence of flow on the macroscopic strain rate and temperature continues to be given through the relation between τ_1 and $\dot{\gamma}_1$ in eq.(2) (or its extension to all relevant mechanisms).

The most important term in eq.(7) is $\tau_1^{(s)}$. In the rate independent limit $m=0$, it would be the "critical resolved shear stress (CRSS)" for the system s ; it may still be called that, only now in the meaning: "at a standard strain rate and temperature". But in addition, it may depend on pressure and indeed on the entire stress state σ , through its effect on the dislocation core structure and thus the Peierls stress. When a sufficient number of slip systems of negligible Peierls stress is available (as in most FCC metals), τ_1 is a constant and "the CRSS law holds". But in materials of lower symmetry, it is typically the Peierls stress that controls which slip systems are available under which conditions, and then, typically, "the CRSS law is violated", because the applied stress dependence is now more complex. The trouble is that the stress state dependence is virtually unknown; not even its sign is generally agreed upon in the practically important case of the influence of hydrostatic pressure.

It should be possible, in the foreseeable future, to model the Peierls stress quantitatively, on the basis of atomistic simulations. It would be quite instructive to know results even at zero absolute temperature: to compare different slip systems, e.g., in hexagonal metals, and to assess the stress state dependence. The simulation need only be done for a single straight screw dislocation (since screws always have the narrower core and thus the higher Peierls stress); it is thus a two-dimensional problem. The temperature dependence could later be modeled indirectly: through the simulation of a double kink on the screw dislocation (which makes it now a three-dimensional problem) in an unstable equilibrium configuration at a finite resolved stress, and the ensuing relation between this stress and the area swept out: thermal activation theory can take it from there.[3]

One further remark about eq.(7). The rate sensitivity m is meant to be taken "instantaneously" or "at constant structure". There is one case where this may be hard to assess; viz is when the rate sensitivity is negative (not truly at constant structure, but still "instantaneous" enough to lead to instability under some circumstances). The mode of deformation is then often localized, but still the distribution of slip systems may be an interesting problem that has, to the author's knowledge, not been addressed.

To summarize, the constitutive behavior of individual grains in a polycrystal, in a given state, is well described by eqs.(6) through (8); the

only quantity in need of further modeling is the Peierls stress contribution to the flow stress τ_1 , and its stress dependence.

The situation is again more complicated for the description of *evolution*. In the last section, strain hardening was described as a scalar quantity only. Under general, multiple-slip conditions, it is often described by a relation of the form

$$d\tau_i^s = h^{st} \dot{\gamma}_i^t dt \quad (9)$$

where each diagonal component of the hardening matrix h (or some other scalar combination) is the hardening rate θ defined in eq.(3); the other components describe "latent hardening". The linear appearance of the matrix equation (9) is misleading: each component of h may depend on all components of τ , which makes it nonlinear and changing with strain. Useful modeling of the hardening matrix has been undertaken only for FCC metals deforming according to the forest model [16]. Completely unknown is the interaction between slip and twinning mechanisms - but we have left deformation twinning out of the discussions in this paper.

Models for Single-phase Cubic Polycrystals

For all polycrystals that deform continuously (i.e., without grain boundary sliding or void formation), two statements are easy to prove: the macroscopic strain rate is the volume average over the strain rates in each grain (called $\dot{\epsilon}$ above); and the macroscopic stress deviator is the volume average over the stresses in each grain (called σ above), of which only the deviatoric parts enter into eq.(7) (except when τ_1 depends on pressure); the hydrostatic stress everywhere, and in the average, would follow from separate equilibrium conditions.

The problem lies in the inversion of this averaging procedure (called "localization" in mechanics): the determination of the *local* distortions and stresses from the boundary conditions, the maintenance of compatibility and equilibrium everywhere, and the material response given in eqs.(7) and (8), for a given state. One is helped by the theorem that enforcing equilibrium yields a lower bound, enforcing compatibility an upper bound to the flow stress.

The most prominent model for polycrystal plasticity is that of Taylor which states, in its most general form, that an upper bound is likely to be closer to the truth than a lower bound (for plastic strain rates large compared to elastic ones)[14]. In fact, using a uniform strain rate throughout the material gives reliable results for polycrystals of cubic lattice structure (pure metals and many solution hardened alloys), with a sufficient number of roughly equiaxed grains in the cross section, and for grain sizes large compared to those features of the substructure that determine the deformation mechanism. The crucial property of cubic metals is that there is a large number of equivalent slip systems, so that the stresses needed to activate various combinations do not vary too widely from grain to grain. For example, the Taylor factor (the deformation work) during rolling of a random FCC polycrystal has a standard deviation of the order of 10%. Thus, the violation of local equilibrium, which is inherent in the theory, appears to be not so excessive as to make the model inappropriate.

When the Taylor model is adequate, eqs.(7) and (8) can be used in an iterative procedure to determine the stress for a given strain rate. An extension of the Taylor model to very flat grains leads to mixed boundary conditions on the grain [17]; but again eqs (7) and (8) can be used to

determine the nonprescribed components of strain rate and the nonprescribed components of stress, which may then be averaged over the polycrystal.

A more difficult problem is the determination of local rotations. They are important, because the change in the grain orientation (R^*), which is needed to evaluate eq.(6) for the next step, depends on the skewsymmetric part of the local velocity gradient L^l :

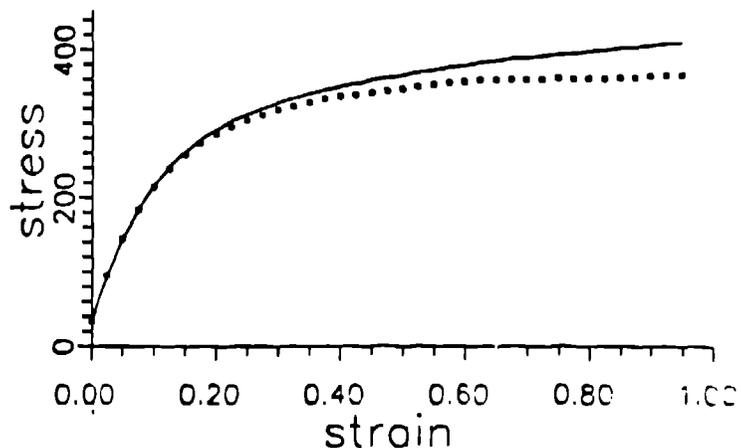
$$\dot{R}^* R^{*T} = \text{skew}(L^l) - \sum \text{skew}(m^S \dot{\gamma}^S) \quad (10)$$

It has been shown that, for the Taylor model, the local velocity gradient (not only its symmetric part) is the same as the macroscopic one; on the other hand, any local variations in shear strains automatically lead to local variations in the skewsymmetric part also.[18,19] In any case, modeling for both the original and the extended Taylor models appears to be nearly complete.

Comparison with experimental results leaves one major problem: the predicted rotations seem to be always faster than (though in the same direction as) the experimental ones. The vague truism that nature is not as deterministic as computer simulations needs fleshing out: various ideas have been proposed, but none quantitative. Another feature of cubic polycrystal deformation for which modeling has not come to a complete conclusion is the development of macroscopic shear bands in plane strain at larger strains, and their influence on texture development.

Effects of texture on macroscopic stress/strain curves can be substantial: the change of flow stress with strain, specified by eqs.(3) and (9), gets convoluted with the change in orientation of each grain, specified by eqs.(6) through (8). Figure 4 shows a simulated case for demonstration: the initial texture is assumed to be a $\langle 111 \rangle$ fiber in copper, as it would be expected in a wire-drawn or cold-rolled rod, often even after annealing. The rod is then subjected to tension (solid line), in which not much further change in texture is expected, and to compression (symbols), in which the very high initial Taylor factor would decrease substantially: this leads to classical "geometric softening" and may be very important in applications.

Fig. 4 - Influence of different texture development in tension (line) and compression (*) on FCC polycrystal with an initial $\langle 111 \rangle$ fiber texture.



The second example we wish to show (Fig. 5) is of a polycrystal yield surface projection calculated subsequent to severe rolling, under two different assumptions for the hardening matrix h . They look rather similar; but if one were particularly interested in the normal at the stress σ_{11} (that is, the "R-value" in tension in the previous rolling direction), it is substantially different in the two cases. The observation is general: strain-rate ratios are very sensitive to many details, and are the hardest

to predict. This, however, seems more of a "calibration" problem than a model problem. In any case, the first task is extensive and detailed comparisons of theory and experiment where all other properties are well predicted.

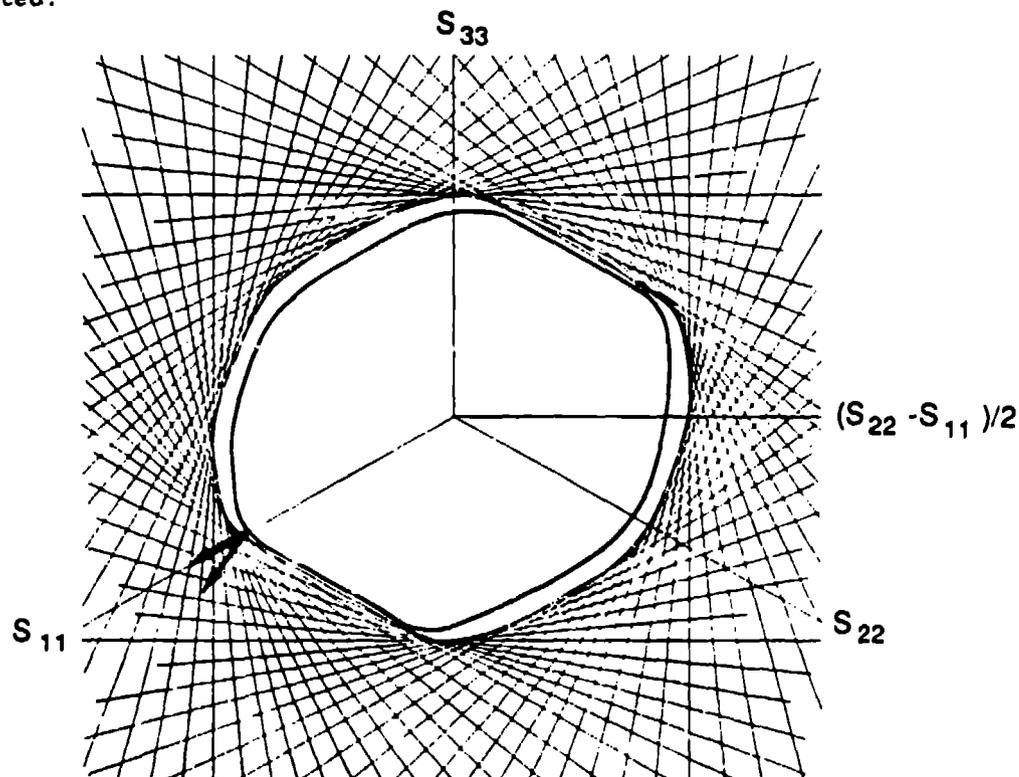


Fig. 5 - Predicted yield surface of a polycrystal rolled to a strain of 2.0 (in the 11-33 direction). Outer: with latent hardening; inner: without.

In summary, the decreased rate of texture development, the development of deformation heterogeneities, and the sensitivity of predicted strain-rate ratios to various assumptions need further understanding. The stress/strain behavior and the kinetics can, on the other hand, be predicted reliably. [11]

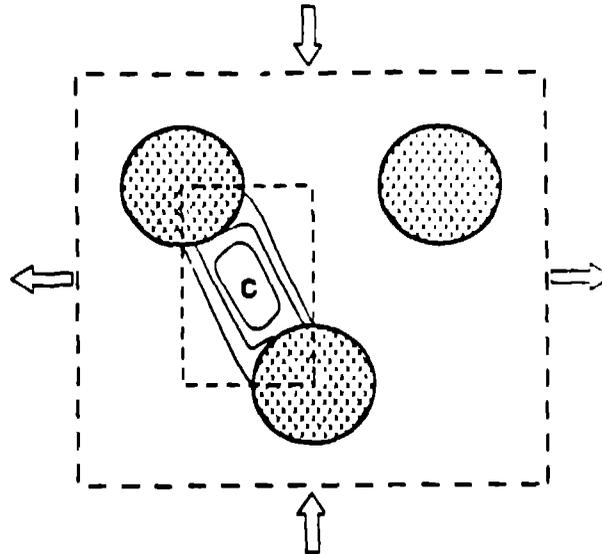
Models for Two-phase or Low-symmetry Polycrystals

When the variation in stress from grain to grain, which would follow from an assumption of uniform strain rate, is very large, the assumption must be wrong and straining must develop heterogeneities. An example of this situation that is relatively easy to assess, is a cubic metal matrix with nondeformable, isolated inclusions. The most obvious approach to this problem is to assume that the lacking deformation in a particular inclusion will be compensated for by extra deformation in its neighborhood. The effect will decay with distance and, provided the inclusions are sufficiently far apart, the material will decompose into "clusters" that do, as a whole, behave like a grain in a Taylor model.

This model does not seem to be appropriate, at least not in general. There have been a number of finite-element calculations (generally two-dimensional) that indicate this. Figure 6 shows a result from one of these, for a 20 volume percent concentration of nondeformable wires aligned with the transverse direction in a plane-strain test. [20] The particular quantity contoured does not matter for the current discussion (it is the current local spin of the principal strain-rate axes with respect to the current local "rigid-body spin", all after a strain of about 40%.) The point is

that in the region labeled C, the deviations from the macroscopic conditions are the greatest. This is more-or-less half-way between particles, not near particles. It is true that there are also strong deviations in the very neighborhood of the particles, but they comprise a very small volume fraction of the material. The most important effect seems to be a behavior akin to fluid flow between the particles. These predictions have recently been verified for the case of tungsten wires in a copper matrix [21].

Fig. 6 - Schematic "unit cell" of fiber composite modeled by FEM. The cross-hatched wires are undeformable. The flow pattern in the matrix is changed: most severely at C, far away from the wires.



There is, at present, no model that takes some general account of this situation, and thus would lead to general predictions about local (and average) hardening and texture development. It would get especially interesting for concentrations where both phases are continuous (in three dimensions): perhaps some percolation model of macroscopic plasticity, akin to that for dislocation percolation through a slip plane, could be developed.

A similar, but even more difficult problem is posed by materials in which the slip (and twinning) flow stresses are very disparate for different systems: then, certain straining requirements imposed on a grain by its surroundings cannot be easily fulfilled and substantial internal stresses must develop. But these internal stresses would be different in tensor character from grain to grain; thus it may be possible for the "hard" modes in one grain to be compensated by soft modes in the surroundings: again, this could lead to a percolation problem.

Summary Assessment

Large-strain plasticity is a prime example of complex behavior: reliable macroscopic descriptions can be obtained only by judicious modeling of the many physical processes occurring at various levels of length, time, and dimensional scale. Much of the detailed physical information gets lost in the progression from microscopic to the macroscopic properties, but some essential features are retained and provide the means to extrapolate known behavior into regimes in which less macroscopic information is available. From this point of view, modeling of large-strain plasticity, for a large class of materials and in a wide regime of variables, is far advanced: the results are reliable in many respects, and in these respects, further modeling is not likely to have significant impact. On the other hand, there are some glaring holes in our overall understanding of plasticity. We highlight one each on the atomistic, dislocation, and macroscopic scales.

1. Calculation of the Peierls stress for various slip systems in non-cubic materials, including effects of pressure and other stress components. This is one case where there is a direct connection between modeling at the atomistic scale and properties at the macro-scale. The principal obstacle is that even the best available interatomic potentials and calculation methods do not seem to be quite good enough for this sensitive application.

2. Dynamic recovery of dislocation structures in deformed materials, under the action of their own internal stresses and thermal activation. This problem has been addressed by various simplified mechanisms since the fifties. Progress could now be made by a simulation of realistic dislocation tangles and cell walls. The macroscopic output could be a more quantitative description of strain hardening at very large strains, of its temperature and rate dependence, and of its contribution to local misorientations.

3. Plastic flow in macroscopically heterogeneous polycrystals, in which the strength, at least in some directions, varies widely from grain to grain. Here, further finite-element simulations, for various geometries, could help assess the situation for some special cases, but the real need is for conceptual modeling: some abstraction that will lead to a set of general rules.

All of these problems require extensive use of computers; but their requirements are not orders of magnitude away from current possibilities.

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