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Approach to the Theoretical Strength of Materials.

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**Dislocation Accumulation at Large Plastic Strains-an Approach to the
Theoretical Strength of Materials.**

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Introduction:

The usual method of introducing engineers to the concept of dislocations and their role in plastic flow is to compare an estimate of the theoretical strength of solid (of order $\mu/30$ where μ is the shear modulus) [1] and the observed strength of either single crystals ($\mu/10^4$) or practical engineering material such as structural steels where the yield stress in shear is of order $\mu/10^3$. However, if we consider the problem in reverse, we can consider the accumulation of dislocations as one important mechanism by which we can produce engineering materials in which the strength level approaches the theoretical strength. If we assume that the flow stress can be expressed in terms of the mean free path between stored dislocations or as the square root of the global dislocation density, then we can see the influence of dislocation density in a diagrammatic form as in Figure 1.

We are interested both in the understanding of the physics of deformation in materials with a high density of dislocations and in the development of ultra high strength materials with useful combinations of properties such as strength and ductility, strength and toughness, strength and electrical conductivity, etc. The salient factors to be considered in this regard is that in a number of systems with increasing imposed strain both the tensile strength and the ductility (measured by the reduction in area) increase [2] as exemplified in Table I.

Table I Tensile Strength (TS) and Reduction in Area at Fracture (RA) of
0.2wt%Cr0.96wt%C hypereutectoid Steels [3]

Isothermal Transformation Temperature (°C)	TS before Drawn (Mpa)	TS after Drawn (Mpa)	RA (%) before Drawn (Mpa)	RA (%) after Drawn (Mpa)
575	1500	3910	31.6	38.6

It is clear that the strengthening by dislocation accumulation due to large imposed plastic strains represents an important approach both to the development of new, potentially valuable, engineering materials and an important area of basic understanding in terms of the mechanical response of materials close to their theoretical strength. Thus, this article will survey some of the factors which influence dislocation accumulation at large strains and the consequences of such accumulation processes.

Survey of Large Strain Deformation Processes

In considering strengthening due to large strain deformation, we can consider the influence either of the process or of the materials. Thus, in processing, attention can be given to factors such as stress state, strain rate, temperature or strain path. In the materials, we can consider factors such as grain size, the presence of interphase interfaces, solute content and a variety of aspects of thermodynamic stability of the materials. This includes the tendency to undergo martensite transitions, dynamic precipitation, the optimization of two-phase microstructures, and the possibility that plastic flow aids the dissolution of second-phase particles in some systems. The catalogue of both processes and material variables are summarized in the schematic diagram in Figure 2. It is clearly not possible to review in detail all these factors in the current overview. Hence some specific aspects of hardening or dislocation accumulation in a variety of systems will be covered. Some general points should be emphasized prior to discussing specific materials. In regard to the state of stress, this may have a major role in suppressing competitive processes such as fracture and damage accumulation [3] and thus enable large plastic strains to be attained. This is essential in the wire drawing of two-phase systems. The level of hydrostatic stresses may also vary with stress state and may influence features such as the extent of martensite transformation in the drawing of stainless steels [4, 5].

Dislocation Accumulation in Single Phase Materials.

It is appropriate to describe the process of dislocation accumulation in single phase materials as a template on which to superimpose additional hardening processes. There exists an enormous literature on both the detailed dislocation

structures observed in deformed single-phase crystals and polycrystals [6] and on constitutive laws to describe the work hardening process over a wide range of temperatures and strain rates [7][8][9]. Various authors have used either the dislocation density or a mechanical threshold stress as an internal state variable. Following the seminal work of Kocks [10], Mecking and Gil Sevillano[11] a general model of structure evolution can be considered in terms of the net strain hardening rate θ ($=d\sigma/d\varepsilon$, where σ and ε are the flow stress and the strain, respectively.) which results from the summation of hardening rate θ_0 and a dynamic recovery term $\theta_r(T, \dot{\varepsilon})$

$$\theta = \theta_0 - \theta_r(T, \dot{\varepsilon}) \quad (1)$$

where T is the temperature and $\dot{\varepsilon}$ is the strain rate. It is usually assumed that θ_0 is independent of temperature and $\dot{\varepsilon}$ and can be considered proportional to the stage II hardening rate in single crystals. An empirical form of this equation can be written as:

$$\theta = \theta_0 (1 - \sigma / \sigma_s) \quad (2)$$

where σ is the current flow stress and σ_s is a "saturation stress" for the material. Much data can be plotted in this form [12] (Figure 3) and although it ignores the existence of stage IV hardening, it does provide a guide for estimation the maximum flow stress or dislocation density which can be achieved at a given combination of strain rate and temperature. It can be extended to large strain by adding the stage IV hardening to give:

$$\begin{aligned} \theta &= \theta_0 (1 - \sigma / \sigma_s) & \sigma \leq \sigma_s \\ \theta &= \theta_{IV} & \sigma > \sigma_s \end{aligned} \quad (3).$$

Let us examine ways in which we can extend the process of dislocation storage by decreasing the dynamic recovery rate either by deforming at very high strain rates or at low temperatures.

In recent experiments, Niewczas et al [13] have shown that copper polycrystals can achieve tensile strengths of order 1.4-2.6GPa at fracture when deformed at 4.2K as shown in Table II. This is a very remarkable result because it is very close to the value of the tensile stress obtained for [100] Cu whiskers (where were dislocation free) by Brenner [14]. This raises speculation about the detailed atomic mechanism by which ductile materials containing extremely high dislocation density can fail at very high stress in the absence of heterogeneous events such as void nucleation at second phase particles.

Table II Tensile Test Data Obtained at 4.2K

Grain Size (μm)	Ultimate Tensile Strength (Mpa)	Dislocation Density $\times 10^{11}(\text{cm}^{-2})$	Fracture Strength (Mpa)	Dislocation Density at Fracture $\times 10^{13}(\text{cm}^{-2})$
29	623	11.05	2613	1.5
99	643	11.25	1625	0.7
413	463	6.3	1680	0.8
742	426	7.2	1427	0.8

Let us consider now the process of dislocation accumulation in copper at high strain rates. Stress strain curves for various strain rates including shock loading at 20GPa [15] are shown in Figure 4. It is clear that at high strain rates and strains of order 1 copper can achieve strengths of order 700 MPa and thus much higher density of dislocations are stored than in normal tensile processes. It should be noted that related modeling of high strain rate deformation by Follansbee et al [15] suggests that at strain rates of $5 \times 10^4 \text{sec}^{-1}$ the hardening rate θ_0 in equation 2 may increase due to dislocation being trapped after travelling small distances.

From the basic framework for the behavior of single phase materials given by equations (2) and (3) empirical approaches can be developed to include additive constitutions to the strength such as role of grain size or dispersion strengthening. A number of such models have been discussed by Estrin and Mecking, Gil Sevillano and others [11, 16]. The behavior is summarized in the schematic in Figure 6, which indicates that at low strain, some materials exhibit a grain size dependent hardening term which is additive to the statistical storage of dislocations. This can be considered as a grain size dependent gradient plasticity term which influences the initial role of dislocation storage but not the final dislocation density which can be attained.

Production of additional Obstacles during Deformation

In addition to the storage of dislocations during plastic flow, we can consider two other situations in which additional obstacles are produced as consequences of

plastic flow. These are a) the case where twins or martensite plates are produced as a consequence of flow and b) The case of deformation of supersaturated solid solutions where dynamic precipitation can occur during plastic flow. These cases differ from the case described in Figure 6 for polycrystals where an additional set of obstacles are present at the onset of plasticity because in both twinning (or martensite reactions) and dynamic precipitation the density of additional obstacles increases during the flow process itself.

There are a variety of ways in which large strain deformation can influence the thermodynamic stability of the material during deformation. In the case of solid solutions such as Al-Mg where precipitation of a second phase does not occur dynamic strain aging can occur. The interaction between dislocations and solute atoms (which is dependent on both temperature and strain rate) results in a drastic decrease in the dynamic recovery rate and thus an increase in work hardening and thus dislocation storage relative to pure aluminum. This is illustrated (in Figure 7) from the work of Stout and Rollett [17, 18] who used torsion tests to obtain shear stress shear strain data. Figure 7 shows the data both in the form of τ - γ and θ - τ plots. It is important to note that dynamic strain aging decreases the role of dynamic recovery but the overall hardening rate does not exceed θ_0 (equation 2) although the dislocation arrangement in materials undergoing dynamic strain aging may show much less evidence of cell structure than those observed in pure materials. In contrast if supersaturated solid solutions are deformed this may result in dynamic precipitation such that additional obstacles are formed in addition to the storage of dislocations and thus the resultant strain hardening rate may be higher than θ_0 even at low temperatures where dynamic recovery is negligible. An example of this behavior

taken from the work of Deschamp et al [19] is shown in Figure 7 which indicates that at 4.2 K the deformation of a supersaturated solution of Al achieves a stress of 600 Mpa which is very similar to the value which can be attained by optimum precipitation hardening in this alloy system. Deschamps et al also measured the evolution of resistivity with plastic flow at 4.2K for both pure Al and the supersaturated Al-Zn-Mg alloys (Figure 8). If dislocations were the only obstacles stored, the resistivity should be proportional to the square of the increase in flow as indicated for pure Al in Figure 8. Thus, the strong non-linear relation for the supersaturated Al-Zn-Mg alloy suggests that even at 4.2K, dynamic precipitation occurs and a second set of obstacles is produced by the process of plastic flow.

Other systems such as MP35N [20] and Inconel 718 [21] also exhibit interaction between plastic flow and precipitation. The detailed mechanisms are not clearly understood in most case but an example of the behavior of MP35N (a 35wt%Co, 35wt%Ni, 20wt%Cr and 10wt%Mo alloy) is shown in Figure 9(a) and (b) to illustrate the strength levels which can be achieved in these materials and related structures.

Twinning and Martensitic Transformations

The transformation to either twins or martensite platelets during deformation can strengthen the material in a variety of ways. The production of interfaces may provide additional barriers to plastic flow and hence strengthen the materials. The dislocation structure accumulated may in part be transformed to sessile dislocations [22] within the twins and hence harden the material. Also the transformed region,

e.g. the martensite may be a complex structure which acts as a strengthening region to which load is transformed as thus the material is in essence transformed to a composite material due to the strain induced transformation.

As an illustration of the importance of transformation hardening let us consider the behavior of a series of stainless steels (type 304, 316 and 301) subject to large strains. From the data in Figure 10 [4], it can be seen that the material which transforms most readily to martensite has the highest hardening rate and attains the highest strength. We can provide a simple empirical model to describe this behavior by assuming that the martensite is a hard phase compared with the matrix and adds a strengthening term $\sigma_m f(\epsilon)$ to the strength of the matrix, where σ_m is the intrinsic strength of the martensite, and $f(\epsilon)$ is the volume fraction of the martensite which is itself a function of strain. Thus we can modify equation 2 to add an additional hardening term due to the martensite production viz:

$$\sigma = \sigma_0 (1 - \sigma / \sigma_s)(1-f) + \sigma_m df(\epsilon)/d\epsilon \quad (4)$$

The data for a number of stainless steels are shown in figure 11. It should be emphasized that a number of materials such as brass and Hadfields manganese steels show rapid strengthening due to twin formation and that this may be a very important strengthening mechanism particularly if combined with cryogenic deformation processing.

Large Strain Deformation of Multiphase Materials

It has been known for several decades that a variety of two phase materials can be deformed to strength levels close to the theoretical strength. The existence work

of Embury and Fisher [23], Langford [24], Bevk [25] and Gil Sevillano [26] has given an experimental basis for understanding both the stress strain relationship up to large strains in these materials and the relationship of the strength to the scale of the microstructure. For a wide variety of materials, the strengthening can be expressed as an exponential function of the imposed strain as shown in Figure 12 .

A variety of interpretation of this type of strengthening have been proposed including dislocation storage [²⁷, ²⁸, ²⁹], the creation of interfaces and the development of what are essentially embedded whisker structures by mechanical refinement of the scale of the microstructure. However, any complete description of the structure property relationship for heavy deformed multiphase material must take cognizance of two important additional facts viz. the nature of the interphase interfaces which are developed by deformation and the complex, short wavelength, internal stresses which are developed by codeformation. These features are illustrated in Figures 13 and 14.

As a final example, let us consider the classical case of drawn pearlite which can achieve very high strength which can be achieved by drawing. Consideration must be given to the competitive processes such as fracture which can occur in the carbide plate and the difference in behavior between carbides present in lamellar pearlite and those present as coarse grain boundary carbides. The very comprehensive review by Lesuer et al [³⁰] outlines in a very clear manner how the various microstructure features can be optimized as summarized in Table III. The resultant strength levels achieved by Ochai and coworkers for very fine diameter wires range up to nearly 6GPa or E/35 as shown in Figure 15. This is a beautiful example of microstructure design to achieve an increase in strength which is of great potential engineering value.

Table III Optimization of Various Microstructure Features by Alloy Additions

Elements	Eutectoid Steel	Hypereutectoid Steel
Cr	Refines lamellar spacing	Refines lamellar spacing
Si	Increases lamellar spacing Dissolves in ferrite and strengthens it	Suppresses proeutectoid carbide formation
Mn	Promote lamellar formation at low carbon content (0.3-0.5wt%)	Refines lamellar spacing
C		Refines lamellar spacing
Co		Suppresses proeutectoid carbide formation

Drawn carbide steels also exhibit an additional aspect of the interaction of plastic flow and the thermodynamic stability of the material. In Fe-C the interaction energy between dislocation and C is of order of 0.5eV which is comparable with the solution pressure of small carbides. Thus as the scale of the structure is refined by imposed strain, carbon can be driven into solution and is thus available for subsequent strain aging and several studies of the strain aging response of drawn pearlitic steels have been reported [31][32][33].

Sometimes, because of the excessive temperature during deformation, the strength of the materials increases faster than in the standard practice and dynamic strain aging is considered to occur during the drawing process. Such aging is a function of highest temperature attained by the materials during the deformation and

the length of time at that temperature. As more work is needed for plastic deformation of high strength feed stock during the deformation, more heat will be produced and the temperature of the wire will be raised. Thus, dynamic aging is likely to be enhanced during the deformation of ultra-high strength steels.

Discussion

From the results outlined for a variety of materials, it is clear that large strain deformation provides a mechanism for the attainment of strengths close to the theoretical strength. The detailed mechanisms by which these strength levels are attained are not completely clear and careful microstructural studies are needed in many cases. However, a general frame work for the understanding of ultra high strength material can be constructed based on the basic concepts of dislocation accumulation and annihilation outlined by Kocks and Mecking plus the process of stage IV hardening at large plastic strains discussed by a number o authors. In pure materials, the hardening rate in stage IV, θ_{IV} is of order of $5 \times 10^{-4} \mu$, which is much less than θ_0 so we can express the hardening rate over a wide range of strain in equation (3). As shown schematically in Figure 15(a), (b) and (c), we can now examine the various mechanisms by which strength of order $E/100$ to $E/50$ can be attained.

- a) By cryogenic deformation at 4.2K dynamic recovery is reduced to that dislocation can be stored up to a density of order 10^{12} - 10^{13} cm^{-2} as shown in Figure 15(a).
- b) We can add an additional hardening term by the creation of twins or martensite plate which adds to the hardening rage at large strain such that :

$$\theta = \theta_0 ((1 - \sigma / \sigma_s) + \theta_{IV})(1-f) + (\sigma_m - \sigma) df(\epsilon) / d\epsilon \quad (5)$$

as shown in Figure 15 (b).

(c) In dynamic precipitation, we can again have a situation where a new set of obstacle can be created as a function of plastic deformation. If we approximate these as a separate set of point obstacles which require bending the dislocation to angle ϕ to break them, the extra strength $\Delta\sigma$ is of order:

$$\Delta\sigma = (\mu b/L)(\cos(\phi/2))^{3/2}(0.8 + \phi/5\pi) \quad (6)$$

where L can be approximately related to the number of obstacles per unit area by $L \approx n^{-1/2}$

$$\text{Thus, } \Delta\sigma = A\mu b n^{-1/2} \quad (7)$$

And if we assume that n is proportional to the imposed strain. This gives an additional rate of hardening which is very significant at low strains and decreased with strain accord with the data described in Figure 6.

In the case of two phase materials we can consider that as the scale of the structure decreases, we create additional interface energy so that we consider not only simply the hardening rate but the rate of dislocation storage $\sigma d\sigma/d\varepsilon$. We have two stored energy terms as a function of strain one due to dislocations in which the rate of energy storage decreases with strain and one due to interfaces which increases with strain. This concept is outlined in Figure 15(c) and compared with data for Cu-Nb [34].

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Figure 1. The influence of dislocation density on the flow stress of pure copper tested under different conditions.

Process Factors

Structure Factors

Figure 2. Schematic diagram to summarize the processes and material variables.

Figure 3. Cu polycrystals data [12] plotted showing the relationship between θ and σ as indicated by equation (2).

Figure. 4. Stress strain curves of Cu for various strain rates including shock loading at 20GPa [15].

Figure 5. Schematic diagram showing the relationship between θ and σ as indicated by equation (3) and role of grain size or dispersion strengthening on the work hardening using additive constitutions.

a.

b.

Figure 6. Data from Rollett [] both in the form of τ - γ and θ - τ plots of solid solutions Al-Mg where precipitation of a second phase does not occur dynamic strain aging can occur.

a. Stress-strain curves.

b. Work hardening rate.

Figure 7. Comparison of the deformation of pure Al and supersaturated solution of Al-6wt%Zn-2.3wt%Mg at 4.2K.

Figure 8. Evolution of resistivity with plastic flow at 4.2K for both pure Al and the supersaturated Al-Zn-Mg alloys.

a.

b.

Figure 9. The strength levels which can be achieved in MP35N (a 35wt%Co, 35wt%Ni, 20wt%Cr and 10wt%Mo alloy) (a) and related structures (b).

Fig. 10 Effect of cold rolling on the 0.2% proof stress and martensite content of austenitic stainless steels [1].

a. Work hardening rate with strain.

b. Martensite content variation with strain.

Fig. 11. The data for stainless steels showing the relationship between work hardening rate θ , martensite content and strain.

Fig. 12. The strengthening can be expressed as an exponential function of the imposed strain for alloyed pearlite [25].

Fig. 13. HRTEM image of Cu-Ag showing the nature of the interphase interfaces

Fig. 14. Short wavelength internal strain measured by neutron diffraction in Cu-Nb materials. The internal strains are developed by codeformation.

Figure 15. The resultant strength levels achieved by Ochai and coworkers for very fine diameter wires.

(a) By cryogenic deformation at 4.2K dynamic recovery is reduced so that high work hardening rate can be achieved due to the storage of dislocation (10^{12} - 10^{13} cm^{-2}).

(b) An additional hardening term by the creation of twins or martensite plate which adds to the hardening rate at large strain.

(c) Consideration of both the hardening rate, the rate of dislocation storage and increase of the interface energy during the deformation in Cu-Nb [28].

Figure 16. Examination of various mechanisms by which strength of order $E/100$ to $E/50$ can be attained.

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