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Plasticity Theory at Small Scales

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Synonyms

Higher-order plasticity theory (https://doi.org/10.1007/978-90-481-9751-4_100296); Strain gradient plasticity theory (https://doi.org/10.1007/978-90-481-9751-4_100798)

Definition

Plasticity theory is the mathematical formalism that describes the constitutive model of a material undergoing permanent deformation upon loading. For polycrystalline metals at low temperature and strain rate, the J_2 theory is the simplest adequate model. Classic plasticity theory does not include any explicit length scale, and as a result, the constitutive behavior is independent of the sample dimensions. As the characteristic length of a sample is reduced to the micro (and nano) scale, careful experimental observations clearly reveal the presence of a size effect that is not accounted for by the classical theory. Strain gradient plasticity is a formalism devised to extend plasticity theory to these smaller scales. For most metals, strain gradient plasticity is intended to apply to objects in the range from roughly 100 nm to 100 μm. Above 100 μm, the theory converges with the classical theory and below 100 nm surface and grain boundary effects not accounted for in the theory begin to dominate the behavior. By assuming that the plastic work (or in some theories, the yield strength) depends not only on strain but also on strain gradients (a hypothesis physically grounded in dislocation theory and, in particular, in the notion of geometrically necessary dislocations (GND) associated with incompatibility due to strain gradients), an intrinsic length scale is naturally introduced, allowing the theory to capture size effects. According to most theories, the intrinsic length scale is of the order of the distance between dislocation-clipping obstacles or cellular dislocation structures (typically, submicron to tens of microns). This continuum theory is appropriate for length scales that remain large relative to the distance between dislocations. As the sample length scale is dropped below this level, dislocations must be modeled individually, and discrete dislocations simulations (DSS) are the preferred approach. At even smaller scales, molecular dynamics (MD) becomes the applicable tool. This article presents a brief overview of one of the simplest continuum strain gradient plasticity theories that reduces to the classical J_2 theory when the scale of the deformation becomes large compared to the material length scale. This simple theory captures the essence of the experimental trends observed to date regarding size effects in submicron to micron scale plasticity.

Plastic Flow of Materials and the Emergence of Size Effects at Small Scales

When ductile materials are loaded beyond their elastic limit, permanent deformation will result, involving long-range displacement of atoms (i.e., displacements much larger than the atomic spacing). In metals, this deformation occurs through the motion of dislocations. A typical stress–strain curve for uniaxial tensile loading is depicted in Fig. 1. In polycrystalline samples at low temperatures ($T < 0.5\,T_m$, with T_m the melting point of the material on the absolute scale) and relatively low strain rates ($\dot{\epsilon} < 10/s$), a simple constitutive equation relating uniaxial stress to uniaxial strain is typically adequate. The flow stress can be defined as:

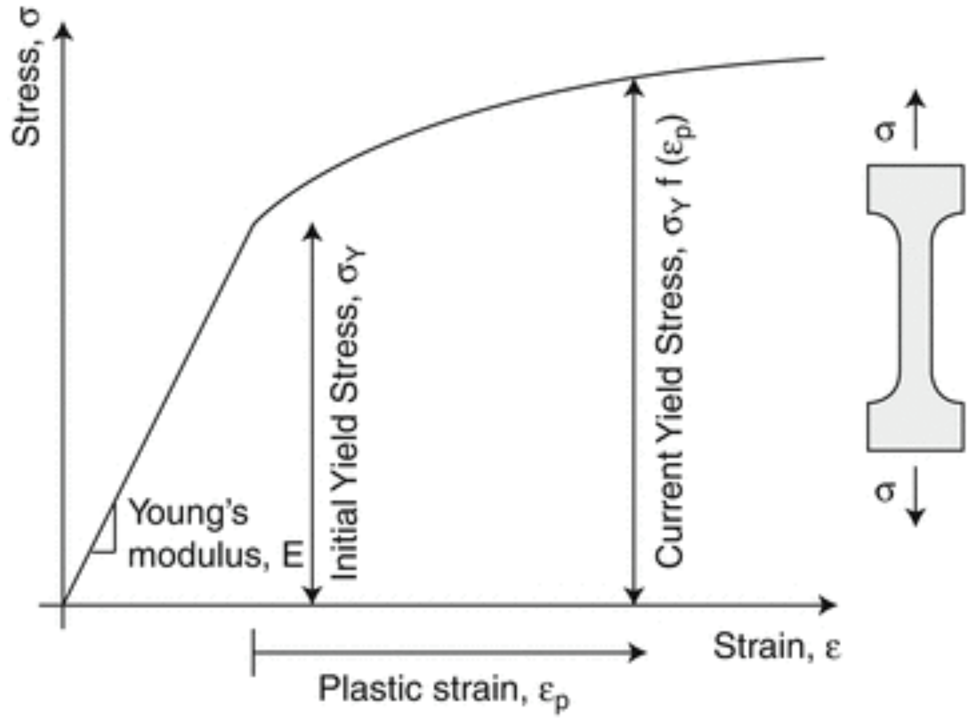
$$\sigma = \sigma_Y f\left(\epsilon_p\right)$$

(1)

with σ_Y the initial yield strength, ϵ_p as the uniaxial plastic strain, and $f\left(\epsilon_p\right)$ the hardening function. A power-law expression for f is often adequate. The plastic work per unit volume can be expressed as:

$$U_P\left(\epsilon_p\right) = \int_0^{\epsilon_p} \sigma d\epsilon_p = \sigma_Y \int_0^{\epsilon_p} f\left(\epsilon_p\right) d\epsilon_p$$

(2)



Plasticity Theory at Small Scales, Fig. 1

Typical stress–strain curve for an elastoplastic material in uniaxial tension. Young modulus, initial yield strength, and hardening behavior are illustrated

Generalization of this behavior to general three-dimensional states of stress and strain is the objective of plasticity theories and is reviewed in the next section.

For samples with characteristic dimensions larger than 10–100 μm (depending on the material), yield strength and hardening are independent of sample dimension, rendering (1) scale independent. Traditional plasticity theories embody this critical concept. Over the past two decades, though, as technological advances allowed measurements of mechanical properties in smaller and smaller systems, unexpected size effects became evident, typically suggesting that smaller samples are stronger. A large body of experimental literature supports this finding. Here, for the sake of conciseness, three key observations are reviewed. For a more exhaustive list, see [1].

1. (a)

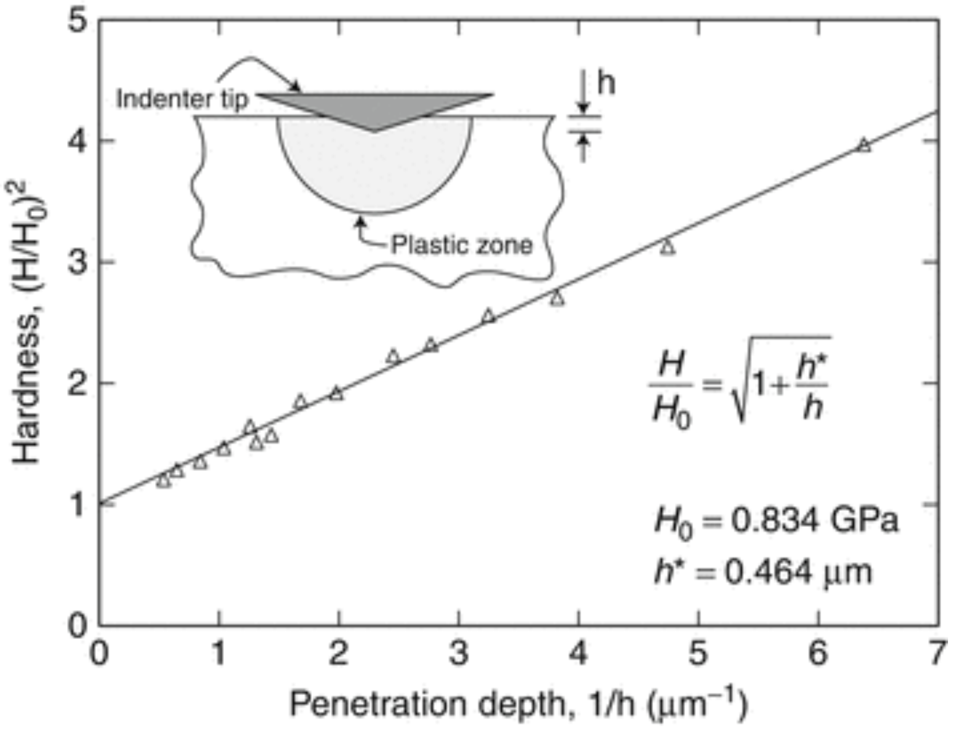
   Materials are harder when indented at smaller depths [2]. A number of careful nanoindentation experiments were conducted and compiled by Nix and Gao [2], revealing a linear dependence of hardness on indentation depth: $(H/H_0)^2 = 1 + (h^*/h)$, where H is the hardness for a given depth of indentation, H_o the hardness in the limit of infinite depth, and h^* a characteristic length of order 1 μ that depends on the shape of the indenter, the shear modulus of the material, and H_o (Fig. 2). The effect becomes negligible as the indentation depth is increased to a depth well beyond h^*.

2. (b)

   Thinner foils are stronger in bending than thicker ones [3]. Experiments conducted by bending thin nickel foils around a mandrel revealed that thinner samples are stronger and strain harden more than thicker samples. Scaling arguments based on classic plasticity theory predict that the normalized moment, M/bh^2 (with b and h the foil width and thickness, respectively), should depend uniquely on the plastic strain at the foil surface, $\epsilon_b = h/2R_0$, with R_o the mandrel radius. For foils of different thickness but identical material, the results should superimpose in the absence of an intrinsic length scale, a conclusion clearly negated by experimental evidence for foil thicknesses between 12.5 and 50 μm (Fig. 3). Importantly, an opposite (albeit less significant) trend is observed in tension, i.e., thinner samples are weaker. Although this conclusion has not been fully rationalized, it clearly demonstrates that strengthening at small length scales entails the presence of strain gradients.

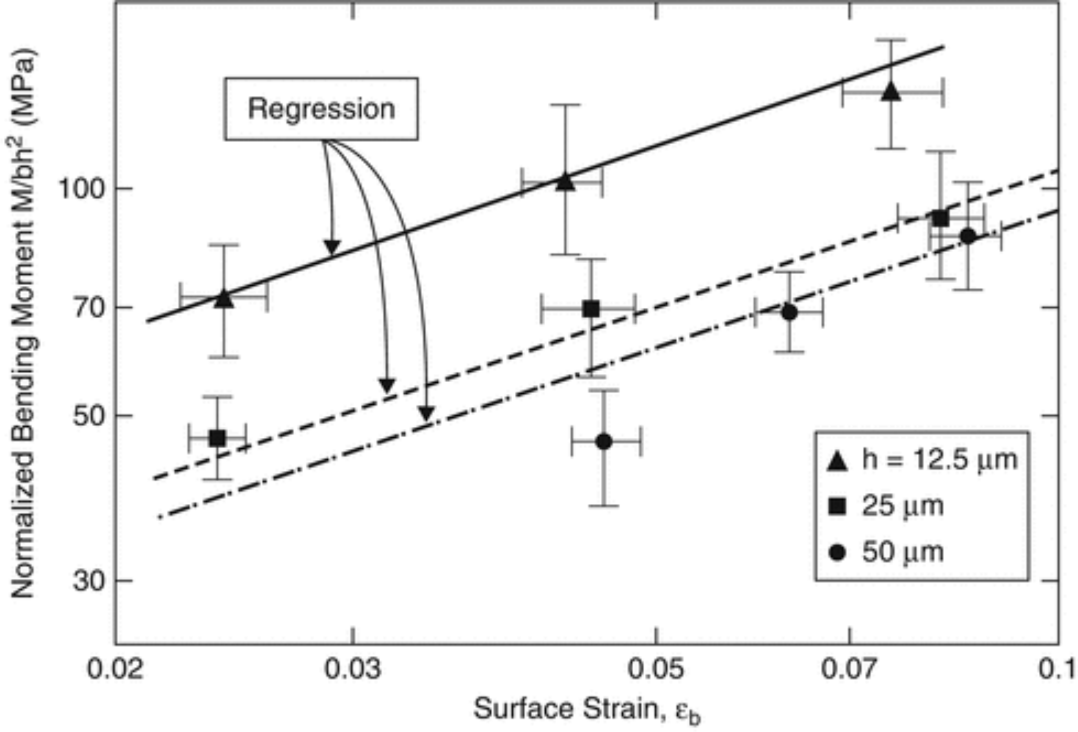
3. (c)

Thinner wires are stronger in torsion than thicker ones [4]. In this classic experiment by Fleck et al. spearheading intense activity in the development of strain gradient plasticity theories, thin copper wires in diameters ranging from 15 to 170 μ were tested in tension and torsion. Dimensional analysis based on conventional plasticity theory predicts a dependence of the normalized torque, T/a^3 (with a the wire radius), on the plastic shear strain at the surface of the wire, $\gamma_s = \kappa a$, with κ the angle of twist per unit length. Again, data from samples of different radius should superimpose, when plotted in these coordinates. Experimental results clearly contrast with this prediction (Fig. 4a). Once again, tensile tests do not show the same trend (Fig. 4b), confirming that the strengthening is associated with the presence of strain gradients.



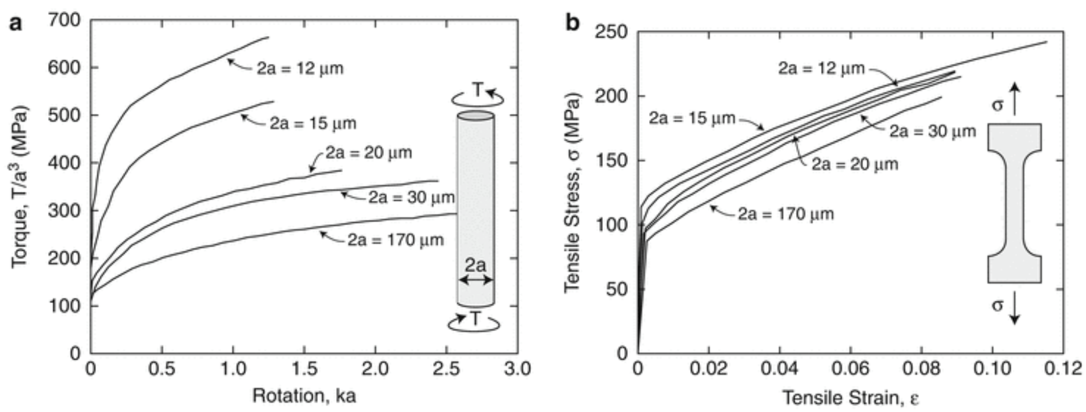
Plasticity Theory at Small Scales, Fig. 2

Dependence of hardness of cold worked polycrystalline copper on the indentation depth. The data fit a linear model almost perfectly (Modified from [2])



Plasticity Theory at Small Scales, Fig. 3

Size effect in bending on thin nickel foils. Substantial strengthening is observed for thinner films, consistently with predictions from SGP theories. Importantly, the same effect is not observed in tension (Reprinted from [3])



Plasticity Theory at Small Scales, Fig. 4

Experimentally measured size effect in torsion of thin copper wires. (**a**) A significant size effect is reported for pure torsion. (**b**) Nearly no size effect is observed in uniaxial tension, confirming that the strengthening entails the presence of strain gradients (Modified from [4])

A constitutive theory incorporating an explicit dependence of the stress on strain gradients (in addition to strain) could in principle explain all the size effects described above. An elementary theory encompassing this principle is discussed below. As explained above, observations (b) and (c) clearly indicate that the strengthening effect disappears as the gradients are removed. It is important to mention that this conclusion changes as the sample size is reduced to sub-micrometric dimensions: in these regimes, substantial size-dependent strengthening is observed under uniform stresses in single crystals (see entry on " Size-dependent Plasticity of Single Crystalline Metallic Nanostructures (https://doi.org/10.1007/978-90-481-9751-4_287)" in this volume).

Conventional Plasticity Theory (J_2 Deformation Theory)

The goal of plasticity theories is the generalization of the one-dimensional model to general, three-dimensional states of stress and strain. For the sake of simplicity, in this article the attention is limited to plastically isotropic materials (i.e., materials for which the flow stress and hardening behavior are independent of the orientation of the coordinate system). It is also assumed that the loading is monotonic and proportional ($\sigma_{ij} = \lambda\sigma_{ij}^0$, with σ_{ij}^0 a constant stress state and λ a loading parameter; throughout this article, indicial notation is adopted: when two indices appear in one term of an equation, summation over those indices is implicitly assumed; see [5] for details) at least approximately. This condition justifies the use of deformation theory, a constitutive model relating plastic strain to stress independently of the loading path. For more general loading scenarios (including all cyclic loadings), a more elaborate theory relating increments of stress and plastic strain (flow theory) is required [5, 6].

The yield point in a uniaxial tensile test (Fig. 1) generalizes to a yield surface, defined in a six-dimensional stress space as the envelope of all stress states resulting in elastic deformation: $f\left(\sigma_{ij}\right) = 0$. If $f < 0$, the behavior is completely elastic, whereas if $f = 0$ plastic deformation occurs.

Under the common assumption that a hydrostatic state of stress ($\sigma_{ij} = -p\,\delta_{ij}$) can be neglected in characterizing plastic behavior, f is taken as a function of the deviatoric stress tensor ($s_{ij} = \sigma_{ij} - (1/3)\sigma_{kk}\delta_{ij}$). For isotropic materials, the most general dependence can be expressed as $f\,(J_2,\ J_3) = 0$, where $J_2 = (1/2)s_{ij}s_{ij}$ and $J_3 = (1/3)s_{ij}s_{jk}s_{ki}$ are the second and third invariants of the deviatoric stress tensor. In the J_2 theory of plasticity, the dependence of f on J_3 is ignored, and thus the yield surface can be simply represented as $f\,(J_2) = 0$. From (1), we have $J_2 = \sigma_Y^2/3$, with σ_Y the yield strength in uniaxial tension. This is the well-known Von Mises criterion [7]. Similarly, the hardening function f can be chosen as an isotropic function of the plastic strain tensor, ϵ_{ij}^p (isotropic hardening). In the simplest theories, it is also common to assume that hardening depends only on the second invariant of ϵ_{ij}^p, with $\epsilon_{kk}^p = 0$ (plastic incompressibility). Thus, the yielding condition for an isotropic material in a general state of stress can be still written in scalar form as:

$$\sigma_e = \sigma_Y f\left(\epsilon_p\right)$$

(3)

with:

$$\sigma_e = \sqrt{\frac{3}{2}s_{ij}s_{ij}} \quad \text{and} \quad \epsilon_p = \sqrt{\frac{2}{3}\epsilon_{ij}^p\epsilon_{ij}^p}$$

(4)

The numerical factors 2/3 and 3/2 are introduced so that the equivalent stress, σ_e, and the plastic strain magnitude, ϵ_p, coincide with stress and plastic strain for uniaxial tensile loading.

The plastic work per unit volume can then be expressed as:

$$U_p\left(\epsilon_p\right) = \int_0^{\epsilon_p} \sigma_e \, d\epsilon_p = \sigma_Y \int_0^{\epsilon_p} f\left(\epsilon_p\right) d\epsilon_p$$

(5)

which is identical to (2), as long as stress and plastic strain are defined as in (4).

As the Cauchy stress tensor σ_{ij} and the strain tensor ϵ_{ij} are work-conjugate, the plastic strain tensor can be expressed as:

$$\epsilon_{ij}^p = \frac{\partial U_p}{\partial \sigma_{ij}} = \frac{\partial U_p}{\partial J_2}\frac{\partial J_2}{\partial \sigma_{ij}} = \frac{\partial U_p}{\partial J_2} s_{ij} = \frac{3}{2}\frac{\epsilon_p}{\sigma_e} s_{ij}$$

(6)

where the relation $J_2 = \sigma_e^2/3$ was adopted. The implication is that according to J_2 deformation theory, the plastic strain tensor is codirectional with the stress deviator.

Strain Gradient Plasticity Theories

As mentioned earlier, the theory presented in the previous section does not contain any intrinsic length scale, and is thus incapable of predicting the size effects depicted in Figs. 2–4. The most natural way of introducing a length scale in the constitutive model is to assume that the plastic work is a function of an enhanced strain measure that incorporates both the plastic strain, ϵ_{ij}^p, and the plastic strain gradients, $\epsilon_{ij,k}^p$. The deformation version intended for application to proportional or near-proportional loading was introduced by Fleck and Hutchinson [4] and represents the application to plasticity theory of higher-order elasticity theories first introduced by Toupin [8] and Mindlin [9]. The simplest implementation defines the plastic work per unit volume as:

$$U_p\left(E_p\right) = \int_0^{E_p} \sigma_e \, d\epsilon_p$$

(7)

where:

$$E_p = \left(\left(\epsilon_p\right)^\mu + \left(\ell \epsilon_p^*\right)^\mu\right)^{1/\mu}$$

(8)

The measure of the plastic strain gradient, ϵ_p^*, can be defined in many different ways [10, 11]. Here the representation $\epsilon_p^* = \sqrt{\epsilon_{p,i}\epsilon_{p,i}}$, based on the choice made by Zibb and Aifantis [12], is adopted for mathematical convenience. Based on dimensional considerations, the dependence of E_p on ϵ_p^* requires the introduction of an intrinsic length scale ℓ. This definition generates a family of theories, as a function of the parameter μ. The choice $\mu = 1$ appears to give the best agreement with experimental observations (e.g., it predicts the linear dependence of hardness on indentation depth, Fig. 2 [1]), but most formulations have used $\mu = 2$ for mathematical reasons. This section surveys the basic predictions and general trends of such theories. A physical interpretation of the intrinsic length scale ℓ is provided in the following section.

The general trends predicted by this theory are easily elucidated. Imagine a perfectly plastic object ($f\left(\epsilon_p\right)=1$) of characteristic dimension h, subject to an average plastic strain, ϵ_p. Dimensionally, the plastic strain gradient is given by $\epsilon_p^* = c\ \epsilon_p/h$, with $c \approx 1$. According to (7) and (8), the plastic work per unit volume can be expressed as:

$$U_p = \sigma_Y \left(1 + c\ell/h\right) \epsilon_p$$

(9)

Comparing (9) to the classic J_2 theory prediction, $U_p = \sigma_Y \epsilon_p$, one concludes that this strain gradient plasticity theory predicts a yield strength elevation of $1 + c\ell/h$. As the length scale of the object, h, approaches the characteristic materials length scale, ℓ, the yield strength elevation becomes significant.

In general, the potential energy functional can be written as:

$$\Phi = \int_V \left(\frac{1}{2} C_{ijkl} \epsilon_{ij}^e \epsilon_{kl}^e + U_p\left(E_p\right)\right) dV - \int_{S_T} \left(T_i u_i + t\epsilon_p\right) dS$$

(10)

with $\epsilon_{ij}^e = \epsilon_{ij} - \epsilon_{ij}^p = \epsilon_{ij} - \frac{3}{2}\frac{\epsilon_p}{\sigma_e} s_{ij}$. Here, C_{ijkl} are the elastic moduli (isotropic here) with $\sigma_{ij} = C_{ijkl}\epsilon_{kl}^e$ and where T_i and $t = \tau_i n_i$ are prescribed on S_T. This class of theories, referred to as higher-order theories, inevitably introduces a new stress measure, τ_i, that is work-conjugate to the plastic strain gradient, i.e., $\tau_i = \partial U_p / \partial \epsilon_{p,\ i}$. Specification of an additional boundary condition is required, involving t, ϵ_p or a combination of both, thus allowing solution to a wider variety of problems, intractable with conventional plasticity theory. For example, passivation layers can be applied on the surface of a solid, forcing the plastic strain to vanish at the surface. (For more details, see [11].)

The solution to (10) represents a minimum with respect to u_i and ϵ_p, assuming a monotonic uniaxial stress–strain curve (1). The material length scale, ℓ, must be obtained by fitting one set of experimental data that brings in strain gradient effects.

Application to the torsion problem presented in Fig. 4 illustrates the predictive capability of the theory. Full details of the analysis are presented in [1]. Elastic strains constitute a very small contribution to the tensile and torsion data in Fig. 4, justifying the adoption of a power-law tensile stress–strain curve of the form $\sigma_e = \sigma_0 \epsilon_p^N$. The strain measure ϵ_p must be replaced by E_p for all loading cases involving strain gradients, as explained above. The ensuing plastic work can then be expressed as:

$$U_p(E_p) = \frac{1}{N+1} \sigma_0 {E_p}^{N+1}$$

(11)

In torsion, with κ as the twist/length, the shear strain varies with distance, r, from the center of the wire according to $\gamma = \kappa r$, such that $\epsilon_p = \kappa r/\sqrt{3}$ (with $\kappa > 0$),

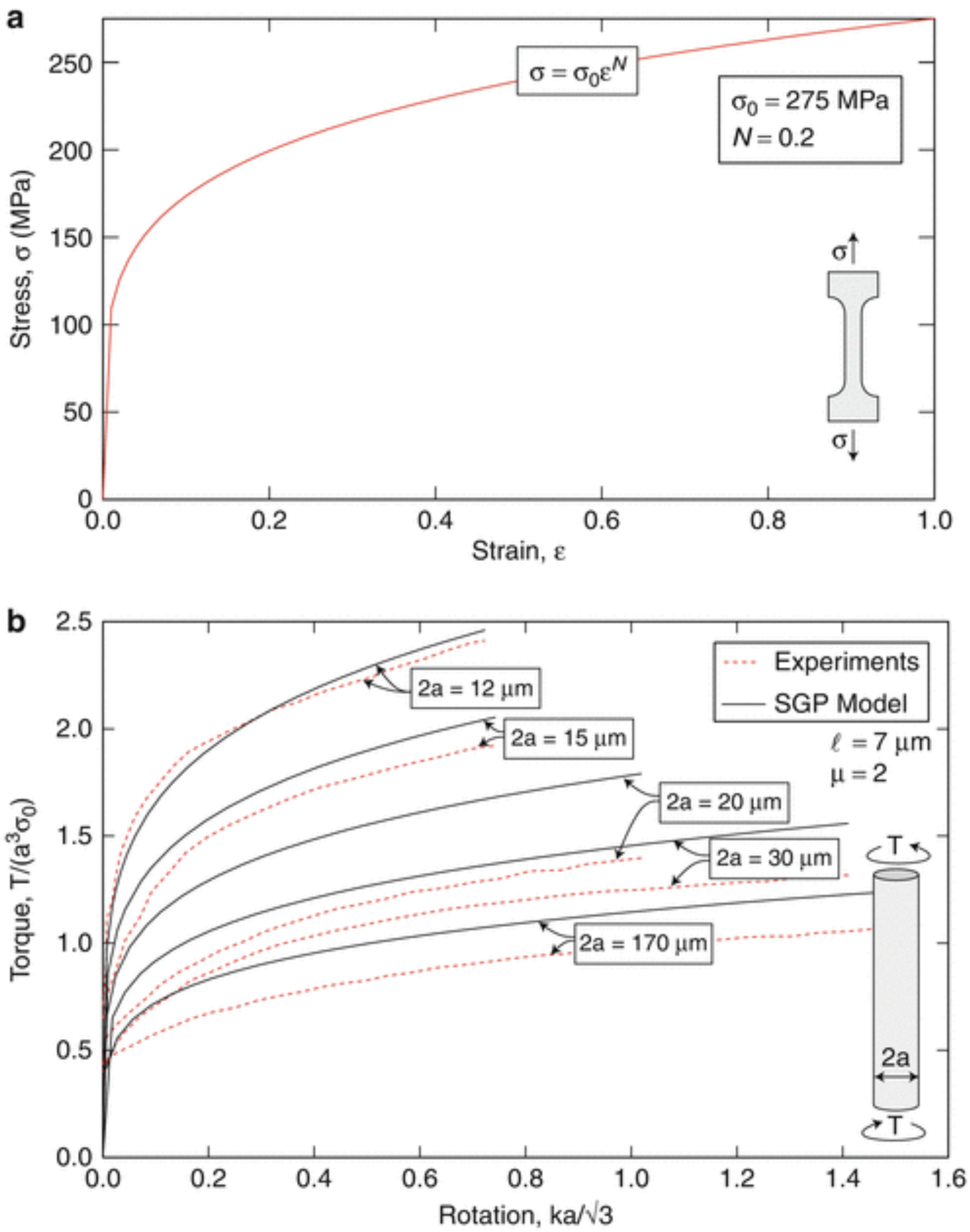
$\epsilon_p^* = \kappa/\sqrt{3}$, and $E_p = \frac{\kappa}{\sqrt{3}}[r^\mu + \ell^\mu]^{1/\mu}$. The torque, T, under monotonically increasing κ is:

$$\frac{T}{\sigma_0 a^3} = \left(\frac{\kappa a}{\sqrt{3}}\right)^N \frac{2\pi}{\sqrt{3}} \int_0^1 \left[\varsigma^\mu + (\ell/a)^\mu\right]^{\frac{N+1}{\mu}} \varsigma d\varsigma$$

(12)

where a is the radius of the wire.

The tensile stress–strain curve in Fig. 5a is plotted with $\sigma_0 = 275MPa$ and $N = 0.2$, giving an approximate fit to the experimental curves in Fig. 4a. With these same values and with the choice $\ell = 7\mu$m, the trends of the experimental torsion data in Fig. 4a are approximately captured by the theoretical curves from (12) in Fig. 5b. $\mu = 2$ was chosen for all calculations.



Plasticity Theory at Small Scales, Fig. 5

(**a**) Power-law stress–strain curve in pure tension (extrapolated at large strains), giving an approximate fit to the data in Fig. 4a. (**b**) Strain gradient plasticity prediction ((12), with $\ell = 7\mu$m, $\mu = 2$) for the torsion data of Fig. 4b, based on the stress–strain law in (**a**)

Although in this brief survey the attention was limited to the deformation theory version of strain gradient plasticity (both for mathematical convenience and transparency of scaling effects), more general flow theory versions (relating plastic strain increments to the increments of stress in a manner which has intrinsic strain-path dependence) have been developed [13, 14, 15, 16]. The constitutive behavior based on flow theory is applicable to any loading history (including cyclic loading, in principle, although none of the existing versions have been vetted for such loadings) and almost always requires a finite element formulation to analyze problems of interest.

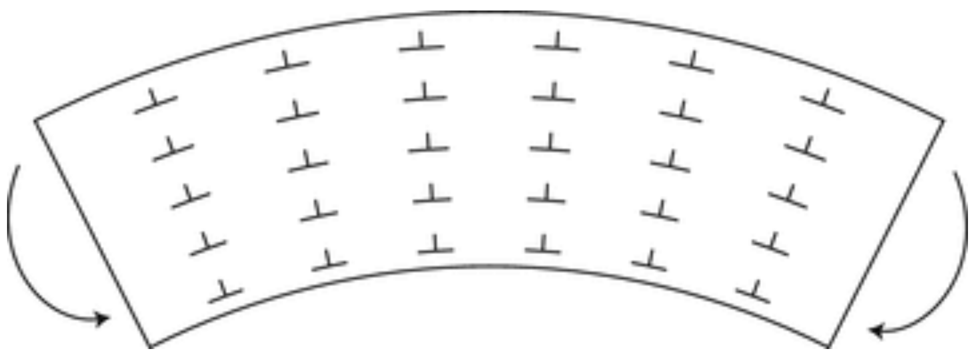
In the next section, the intrinsic length scale ℓ will be qualitatively related to basic notions from dislocation theory.

Physical Interpretation of the Intrinsic Material Length Scale

Conventional strain hardening and yield stress elevation are attributed to the interaction of mobile dislocations with relative immobile *statistically stored dislocations* (SSD). The density of SSD, ρ_{SSD}, increases proportionally to the accumulated plastic strain, according to $\epsilon_p \approx \rho_{SSD} bd$, with b the burger's vector and d the average distance traveled by a dislocation (defined by the spacing of obstacles). As emphasized by Ashby [17], accumulation of plastic strain gradients requires the introduction of additional dislocations to ensure geometric compatibility (Fig. 6): unlike SSDs, these *geometrically necessary dislocations* (GND) must be arranged in space to accommodate the incompatibility associated with the plastic strain gradient and scale as $\epsilon_p^* \approx \rho_{\mathrm{GND}} b$. The motion of both families of dislocations contributes to the plastic work. If one assumes that SSD and GND do not strongly interact, a simple additive contribution is appropriate. According to this model, the plastic work can be expressed as:

$$U_p \approx \sigma_Y \left(\rho_{\mathrm{SSD}} bd + \rho_{\mathrm{GND}} bd\right) \approx \sigma_Y \left(\epsilon_p + d\epsilon_p^*\right)$$

(13)



Plasticity Theory at Small Scales, Fig. 6

Cartoon illustrating the formation of geometrically necessary dislocations (GND) in pure bending

Comparison with (9) immediately reveals $\ell \approx d$. As the average distance traveled by a dislocation is comparable to the average spacing between obstacles, this simple analysis suggests that usually $\ell \approx 1 - 20\mu\text{m}$, consistent with experimental results and modeling prediction (Fig. 5).

Modeling Plasticity of Very Small Samples

The strain gradient plasticity theory described in this entry is still a continuum theory (i.e., it does not model individual dislocations). As the size of the sample is reduced to the point that only a handful of dislocations exist across the characteristic length scale, this fundamental assumption breaks down. In this case, numerical approaches which explicitly model dislocation interactions are required. Molecular dynamics (MD) is a natural modeling strategy, but its application is limited to relatively small samples and extremely high strain rates. Discrete dislocations simulations (DDS) present an approach that bridges the two theories [18, 19, 20]. These models generally utilize a FE continuum framework to solve for stresses, strains, and displacements, and treat dislocations as singularities, which both affect and are affected by the global strain and stress fields. Dislocations motion is governed by the Peach–Koehler equation and standard dislocation–dislocation interaction laws. Dislocation sources like Frank–Read and single-arm sources are introduced at statistically random locations. These models (both in two-dimensional and three-dimensional) are computationally more efficient than full-scale MD simulations, but have not yet fully succeeded in duplicating key aspects of the experimentally measured size effects in plasticity [21].

Open Issues, Future Developments, and Final Considerations

One reason why strain gradient plasticity theories have not been widely embraced is the ambiguity surrounding the definition of the intrinsic length scale. Although the scaling arguments presented in this article ascribe its physical basis and define its order of magnitude, a quantitative physical model allowing expression of ℓ as a function of measurable materials parameters is still lacking. Attempts to define such a model based on dislocation theory are still ongoing. At the same time, efforts are still underway in developing a fully consistent flow theory version of strain gradient plasticity and in implementing such theories in finite element codes.

Cross-References

Ab Initio DFT Simulations of Nanostructures (https://doi.org/10.1007/978-90-481-9751-4_243)

Finite Element Methods for Computational Nano-Optics (https://doi.org/10.1007/978-90-481-9751-4_17)

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