Scaling confirmation of the thermodynamic dislocation theory

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The thermodynamic dislocation theory (TDT) is based on two highly unconventional assumptions: first, that driven systems containing large numbers of dislocations are subject to the second law of thermodynamics and second, that the controlling inverse timescale for these systems is the thermally activated rate at which entangled pairs of dislocations become unpinned from each other. Here, we show that these two assumptions predict a scaling relation for steady-state stress as a function of strain rate and that this relation is accurately obeyed over a wide range of experimental data for aluminum and copper. This scaling relation poses a stringent test for the validity of the TDT. The fact that the TDT passes this test means that a wide range of problems in solid mechanics, previously thought to be fundamentally intractable, can now be addressed with confidence.

dislocations | thermodynamics | effective temperature | nonequilibrium deformation | thermal activation

For almost a century, the dislocation theory of crystalline deformation has played a central role in materials science. Unfortunately, this theory has made only modest progress for about seven decades. Although crystalline solids are essential in engineering applications and although modern experimental techniques have provided a wealth of information about dislocations in these solids, the theories developed to explain dislocation-driven phenomena have been primarily phenomenological. They describe phenomena mathematically but do not explain them; they are not predictive.

The cause of this theoretical failure is clear. Dislocation-driven deformations of solids are complex nonequilibrium processes involving macroscopic numbers of dynamical degrees of freedom. Theoretical physicists know that they must use statistical methods to deal with such situations. Especially important is the second law of thermodynamics, which states that driven complex systems must move toward their most probable configurations (i.e., that their entropies must be nondecreasing functions of time). However, leading materials scientists since the 1950s have asserted that dislocation energies are too large, and that dislocation entropies are too small, for the second law to be applicable (1, 2).

We have argued for a decade that those assertions are wrong. The thermodynamic dislocation theory (TDT) is based directly on the second law. It was introduced in 2010 (3) and has been shown in a series of publications since then (4–13) to be capable of solving a wide range of the most important problems in solid mechanics including strain hardening, elastic–plastic yielding, shear banding, grain-size effects, and the like. Those problems were out of reach of the conventional approaches. However, questions remain. How sure are we that the TDT is more reliable than the observation-based phenomenologies? Can we use it confidently to solve important materials problems that have been left untouched by the conventional methods?

To test the reliability of the TDT, we have used it to derive a scaling law for steady-state deformations. Such scaling laws have been proposed in the past. For example, Kocks and Mecking (14)

devoted much of their review article to the search for scaling relations based on experimental data and phenomenological strain-hardening formulas. The TDT-based scaling relation, however, is derived directly from first principles. As we shall show, it is accurately obeyed over a wide-enough range of experimental data to make it seem highly unlikely that there is anything fundamentally incorrect about its underlying assumptions. Our increased confidence in the TDT now leads us to raise some issues that urgently need to be addressed for both basic and applied reasons.

The thermodynamic basis of the TDT has been presented in earlier publications (especially refs. 3, 7, and 9). Its main premise is that the dislocations in a deforming crystalline solid can be described—indeed, must be described—by an effective temperature T_{eff} that differs greatly from the ordinary, ambient temperature T. T_{eff} is truly a "temperature" in the conventional sense of that word; it is derived by invoking the second law of thermodynamics. It is also a true temperature in the sense that, as energy flows through an externally driven system containing dislocations, effective heat is converted to ordinary heat and dissipated. Thus, this driven, nonequilibrium system should be visualized as consisting of two weakly coupled subsystems: the dislocations at temperature T_{eff} and the rest of the system playing the role of a thermal reservoir at temperature T.

For present purposes, we need to know only that, in steady-state shear flow, the areal density of dislocations is given by the usual Boltzmann formula:

$$\rho_{ss} = \frac{1}{a^2} \exp\left[-\frac{e_D}{k_B \, T_{eff}^{ss}}\right], \quad \text{[1]}$$

Significance

Conventional theories of the deformation of crystalline solids assume that the second law of thermodynamics is inapplicable to dislocations. As a result, they have been only descriptive and nonpredictive. In contrast, the thermodynamic dislocation theory (TDT), based directly on the second law, has proven capable of solving problems that are out of reach of conventional approaches. Examples include strain hardening, elastic–plastic yielding, shear banding, etc. We show that the fundamental assumptions of TDT predict a scaling relation and that this relation is confirmed by experiment. Our increased confidence in the TDT leads us to raise issues that need to be addressed for both basic and applied reasons. One example is the unsolved problem of fracture toughness in crystalline solids.

where a is a minimum spacing between dislocations, e_D is a characteristic dislocation energy, and T_{eff}^{ss} is the steady-state effective temperature. The quantity $k_B T_{eff}^{ss}/e_D$, usually denoted by the symbol $\tilde{\chi}_{ss}$, is a measure of the degree of disorder of the subsystem of dislocations. It is determined by the rate at which this subsystem is being driven at the strain rate $\dot{\epsilon}$. If that driving rate is slow enough that irreversible atomic rearrangements have time to relax before the strain has changed appreciably, then $\tilde{\chi}_{ss}$ must be independent of the strain rate. Typical timescales for atomic motions are of the order of $10^{-10}s$. Thus, $\tilde{\chi}_{ss}$ must be a constant for strain rates up to $10^6/s$ or even higher. It then follows from Eq. **1** that steady-state dislocation densities must also be constant across this range of driving rates, which includes most ordinary applications. In ref. 3, we used a Lindemann-like argument to estimate that $\tilde{\chi}_{ss} \sim 0.25$, which turns out to be roughly correct.

The second core ingredient of the TDT is the depinning ("double-exponential") formula, which also is based on a comparison of timescales. We know that the dislocations in a deforming solid, under a wide range of circumstances, are locked together in an entangled mesh that can deform only via thermally activated depinning of pairwise junctions. The pinning times are very much longer than the times taken by dislocation segments to jump from one pinning site to another. Thus, the depinning rate controls the deformation rate, and no other rates are relevant in this approximation.

To be more specific, define the depinning rate to be $\tau_P^{-1} = \tau_0^{-1} \exp[-U_P(\sigma)/k_B T]$, where τ_0 is a microscopic timescale and U_P is a pinning energy that depends on the applied stress σ. Write this energy in the form $U_P(\sigma) = k_B T_P \exp[-\sigma/\sigma_T(\rho,T)]$, where $\sigma_T(\rho,T)$ is a characteristic stress that determines the magnitude of σ necessary to reduce the pinning barrier by a factor of $1/e$. If a' is the separation between dislocations needed to produce this reduction and $1/\sqrt{\rho}$ is the average distance between dislocations, then $a'\sqrt{\rho}$ is a strain, and $\sigma_T(\rho,T) = \mu(T) a'\sqrt{\rho}$ is a stress, where $\mu(T)$ is the (temperature-dependent) shear modulus. In fact, $\sigma_T(\rho,T)$ is the Taylor stress. To compute the plastic strain rate, use the Orowan formula $\dot{\epsilon}^{pl} = \rho b v$, where b is the magnitude of the Burgers vector and v is the average dislocation speed $1/(\tau_P \sqrt{\rho})$. The result is

$$\dot{\epsilon}^{pl} = \frac{b}{\tau_0}\sqrt{\rho}\exp\left[-\frac{T_P}{T}e^{-\sigma/\sigma_T(\rho,T)}\right] \qquad [2]$$

or equivalently,

$$\frac{\sigma}{\sigma_T(\rho,T)} = -\ln\left[\frac{T}{T_P}\ln\left(\frac{\dot{\epsilon}_0(\rho)}{\dot{\epsilon}^{pl}}\right)\right], \qquad [3]$$

where $\dot{\epsilon}_0(\rho) \equiv b\sqrt{\rho}/\tau_0$. This is the scaling relation.

For steady-state situations in which $\rho = \rho_{ss}$ remains constant, Eq. **3** contains three system-dependent but theoretically strain rate-independent parameters: $\sigma_T^{ss} \equiv \sigma_T(\rho_{ss},T)$, $\dot{\epsilon}_0^{ss} \equiv \dot{\epsilon}_0(\rho_{ss})$, and T_P. Thus, plots of measured values of σ/σ_T^{ss} as functions of $(T/T_P)\ln(\dot{\epsilon}_0^{ss}/\dot{\epsilon}^{pl})$ should collapse onto a single curve after we have identified the values of those three parameters, which we can do by using known values of the modulus $\mu(T)$ and using a least-squares method to find the best fit between the parameters and the scaling curve.

To check this scaling prediction, we have used a set of compression measurements by Samanta (15). These are old results, but they have the special advantage for us of using two different materials and testing them at different temperatures and strain rates under otherwise identical conditions. Our scaling graph shown in Fig. 1 contains 32 points: 12 for pure copper at three temperatures in the range (600 °C to 900 °C) and four strain rates (960 /s to 2,300 /s) and 20 for pure aluminum at
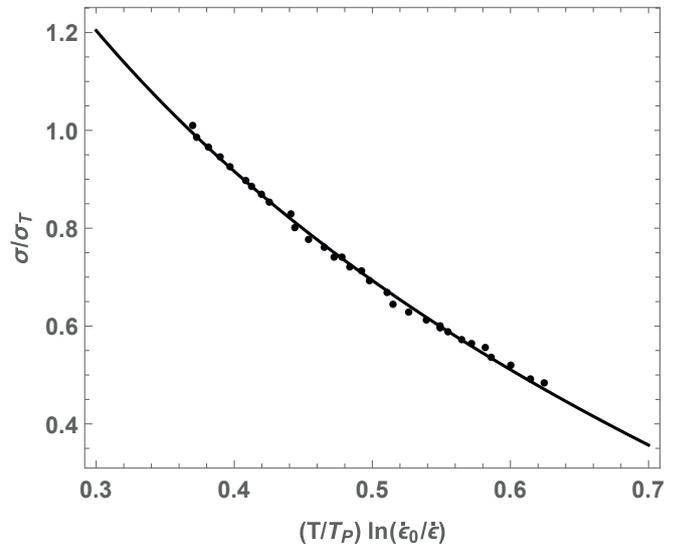

Fig. 1. Scaling relation given by Eq. 3. The solid curve is the function $f(x) = \ln(1/x)$, with $x = (T/T_P)\ln(\dot{\epsilon}_0^{ss}/\dot{\epsilon}^{pl})$. The data points are from ref. 15 as interpreted in ref. 16.

temperatures in the range (250 °C to 550 °C) and five strain rates (520 /s to 2,200 /s). Clearly, these points fall very accurately on the smooth curve predicted by the TDT analysis, which adds greatly to our confidence in this theory. The most physically interesting fitting parameters are $T_P = 45,000$ K for copper and $T_P = 27,800$ K for aluminum, which differ somewhat from previous estimates, possibly because of differing sample preparations or measurement techniques.

The time-dependent TDT consists of three physics-based equations of motion. The first is Hooke's law with the ("hypo-elasto-plastic") assumption that elastic and plastic shear rates are additive:

$$\dot{\sigma} = 2\mu(1+\nu)(\dot{\epsilon}^{tot} - \dot{\epsilon}^{pl}), \qquad [4]$$

where ν is Poisson's ratio and $\dot{\epsilon}^{tot}$ is the total elastic plus plastic strain rate. $\dot{\epsilon}^{pl}$ is given by Eq. **2**, making this a highly nonlinear equation.

Second is an equation of motion for ρ, which is a statement of energy conservation:

$$\dot{\rho} = \kappa_\rho \frac{\sigma \dot{\epsilon}^{pl}}{\gamma_D}\left[1 - \frac{\rho}{\rho_{ss}(\tilde{\chi})}\right]. \qquad [5]$$

Here, γ_D is the dislocation energy per unit length, and κ_ρ is the fraction of the input power $\sigma\dot{\epsilon}^{pl}$ that is converted into dislocations. The second term inside the square brackets determines the rate at which dislocations are annihilated. It does this by invoking a detailed balance approximation using the effective temperature $\tilde{\chi}$; that is, it says that the density ρ must approach the value given by Eq. **1** but with the steady-state $\tilde{\chi}_{ss}$ replaced by a time-dependent $\tilde{\chi}$ during the approach to steady-state deformation.

Finally, the equation of motion for $\tilde{\chi}$ is a statement of the first law of thermodynamics:

$$c_{eff} e_D \dot{\tilde{\chi}} = \sigma \dot{\epsilon}^{pl}\left(1 - \frac{\tilde{\chi}}{\tilde{\chi}_{ss}}\right) - \gamma_D \dot{\rho}, \qquad [6]$$

where c_{eff} is the effective specific heat. The second term in the parentheses is proportional to the rate at which effective heat is
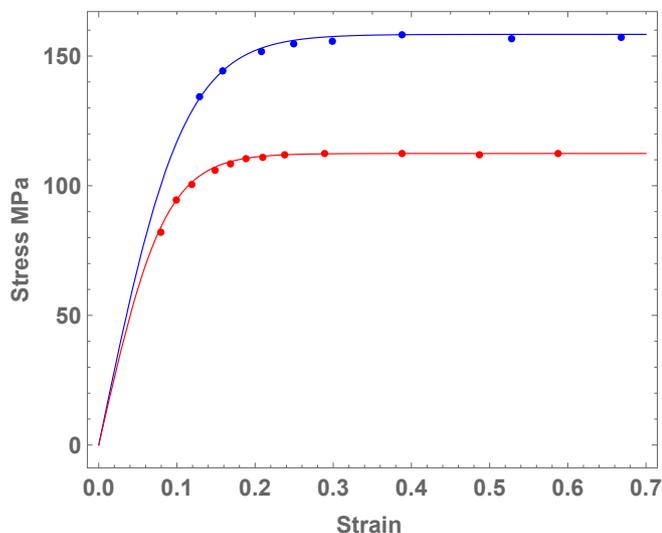
Fig. 2. Strain hardening curves for Cu: $T = 1,023\,\mathrm{K}$, $\dot{\epsilon} = 1,800/s$ (upper blue) and $T = 1,173\,\mathrm{K}$, $\dot{\epsilon} = 960/s$ (lower red). The data points are from ref. 15.

converted to ordinary heat, which reminds us that $\tilde{\chi}$ is a thermodynamically well-defined temperature. Like the comparable term in Eq. **5**, this is a detailed balance approximation. The last term on the right-hand side accounts for energy stored in the form of dislocations.

To illustrate the solutions of these equations of motion, we show in Fig. 2 just 2 of Samanta's 32 stress–strain datasets, compared here with the TDT predictions. The agreement between theory and experiment shown here is reassuringly excellent. Ref. 16 has details about how the TDT equations were reformulated for numerical purposes and how parameter values were chosen for comparing their predictions with the experiments. In computing the curves shown in Fig. 2, we simplified the analysis by neglecting Eq. **6** for $\tilde{\chi}$ and simply solving Eq. **5** with $\tilde{\chi} = \tilde{\chi}_{ss} = 0.23$, consistent with our observation in ref. 3 that $\tilde{\chi} \to \tilde{\chi}_{ss}$ very rapidly at high temperatures T. Our measured value of $\tilde{\chi}_{ss}$ is roughly consistent with our original guess that $\tilde{\chi}_{ss} \sim 0.25$. The graphs in Fig. 2 are almost identical to those shown for wider ranges of temperatures and strain rates in the early TDT papers. They also illustrate the invariance of the onset slopes for non-prehardened copper discovered experimentally by Kocks and Mecking (14) and explained theoretically in refs. 3 and 7.

We emphasize that these equations of motion are based entirely on fundamental principles—the laws of thermodynamics, energy conservation, and dimensional analysis. Specific phenomena such as hardening, grain-size effects, or yielding transitions play no role in deriving them. Those phenomena are predicted by the equations. The associated physical mechanisms are contained in the derivation of the double-exponential depinning formula, Eq. **2**, and in the conversion factors κ_ρ and c_{eff} in Eqs. **5** and **6**. For example, the extreme stress sensitivity of the strain rate in Eq. **2** naturally explains the ρ and T dependences of yield stresses; the phenomenological concept of a "yield surface" is unnecessary. In a more specific way, the physically understandable grain-size dependence of the conversion factor κ_ρ in Eq. **5** provides a simple explanation of Hall–Petch effects. Both of these predictions are discussed in ref. 7.

One of the most remarkable aspects of these results is how many ingredients of conventional dislocation theories are completely absent in this elementary version of the theory. The TDT dislocations are simply lines. We do not ask whether they are

edge dislocations or screw dislocations or whether they are excess dislocations or geometrically necessary ones. There are no partial dislocations. The crystals through which they move have no specific symmetries. Their motions are unaffected by crystalline orientations, slip planes, or stacking faults. They do not undergo cross-slip. They interact with each other only at the pinning junctions and not via long-ranged elastic forces.

Apparently, we can go remarkably far with only this TDT caricature, but there must be limits. Finding and understanding those limits should be a high priority for new investigations. After we see what important physics is missing, we should be able to put realistic features back into the theory in fundamentally consistent ways and thereby understand what roles they play and how important those roles may be.

This process of making the TDT more realistic should help us distinguish useful phenomenological concepts from those that are unrealistic. Our candidates for the "unrealistic" category include distinctions between "mobile" and "immobile" dislocations, distinctions between different "stages" of strain hardening, and the idea that large flow stresses at high strain rates can be explained by something called "phonon drag." At present, we see no scientific basis for any of those conventional ideas, but surely we are mistaken in some cases. We expect to learn a great deal by finding clear counterexamples or missing ingredients in the TDT.

Similarly, there must be many limits to the validity of our scaling analysis. Here is an already obvious one. We have pointed out that the assumption of constant $\tilde{\chi}_{ss}$, and thus, constant ρ_{ss}, must be changed at physically plausible, high strain rates. Already, in ref. 3, we showed how a simple strain rate dependence of $\tilde{\chi}_{ss}$ with a corresponding increase in ρ_{ss} can explain the high stresses observed in strong-shock experiments. We thus found agreement between TDT and experiment over 15 decades of strain rate. This kind of analysis of high strain rates was also applied in ref. 8 to interpret molecular dynamics simulations of crystalline deformation (17). We consider those simulations to have been especially important in the development of the present theory.

There are many other open issues, but most of them seem to be minor technicalities in comparison with a far more important question: what is the physics of brittle and ductile fracture in crystalline solids? Basic theoretical research in this area has been at a decades-long standstill comparable with that which has afflicted theories of strain hardening.

Consider the following. We know that solids are stronger when they are colder; their yield stresses and flow stresses decrease with increasing temperature. This behavior is now predicted by the TDT as seen in Eq. **2** and its applications. However, we also know that solids become more brittle (i.e., they break more easily) at lower temperatures despite the fact that they are stronger. How can these properties be consistent with each other?

This basic question has not been answered. So far as we know, it is seldom even asked in the solid mechanics literature. The conventional model used for studying brittle or ductile crack initiation is one in which dislocations are emitted from infinitely sharp crack tips and move out along well-defined slip planes (18, 19). These dislocations either move freely, supposedly implying brittle behavior, or become dense enough to shield the crack tip and somehow produce ductility and toughness. Agreement with experiment is modest at best. As stated in a recent experimental paper by Ast et al. (20), an "understanding of the controlling deformation mechanism is still lacking." Finding a predictive theory of fracture toughness in crystalline solids should now be feasible and should be a high priority for materials theorists.

Data Availability. All study data are included in the article.

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