Analytic Model of the Remobilization of Pinned Glide Dislocations from Quasi-static to High Strain Rates

A. Hunter*, D. L. Preston

*Los Alamos National Laboratory
Los Alamos, NM 87545, USA*

Abstract

In this paper, we construct an analytic model describing mobile-immobile dislocation intersections using a mean-first-passage-time (MFPT) framework. By applying MFPT theory to dislocation intersection, the deformation mechanics at high strain rates is more reliably described than in traditional models based on Van't Hoff-Arrhenius thermal activation. The plastic strain rate is expressed as a function of the applied stress, mobile and immobile dislocation densities, material density, and temperature. This kinetic equation is applicable at strain rates from quasi-static to rates in excess of 10^{12} s^{-1} , pressures from ambient to about 1000 GPa, and temperatures ranging from zero to the melt temperature.

Keywords:

dislocation intersections, mean-first-passage-time (MFPT) theory, plastic flow, shock loading

1. Introduction

Plastic constitutive models, i.e., material strength models, applicable at strain rates of roughly 10^5 s^{-1} and higher, are essential for simulations of explosively-driven systems, hypervelocity impacts, and more generally, material deformation and failure under shock wave loading. As plastic strain rates increase to 10^5 s^{-1} and above, the majority of rate-dependent plastic flow models (Seeger, 1954a,b,c, 1955b; Follansbee and Kocks, 1988; Hoge and Mukherjee, 1977; Steinberg and Lund, 1989; Zerilli and Armstrong, 1987) exhibit a progressive drop in fidelity, in some cases leading to explicit failure, because the rate-controlling intersections of non-coplanar, attractive mobile and immobile (forest) dislocations are described by Van't Hoff-Arrhenius thermal activation theory, which breaks down at high stresses. The main result of this paper, our kinetic equation, is an analytic model of mobile-immobile dislocation intersection that generalizes the standard low-strain-rate relation $\dot{\epsilon} = \dot{\epsilon}_0 \exp(-E(\sigma)/kT)$ up to strain rates of roughly 10^{12} s^{-1} . This equation describes the formation and dissolution of dislocation-dislocation intersection nodes and short junctions, and relates plastic strain rate to the stress, mobile and immobile dislocation densities, material density, and temperature. Our kinetic equation is applicable at plastic strain rates from quasi-static to rates of order 10^{12} s^{-1} , temperatures from zero to melt, and pressures greater than 1000 GPa. It is intended to be used in conjunction with a model for the evolution of mobile and immobile dislocation densities.

It is well known that metals and alloys exhibit a significant increase in strain rate sensitivity at rates $\sim 10^4\text{--}10^5 \text{ s}^{-1}$. This behavior is usually interpreted as a change in the rate-controlling mechanism from thermally-activated glide at low rates, as described by a Van't Hoff-Arrhenius equation, to dislocation drag at high rates. Conversely, our kinetic equation, predicts an increase in strain rate sensitivity at high rates by correctly accounting for the effects of thermal fluctuations at dislocation intersections, i.e. in the absence of dislocation drag. Of course, at high rates ($> 10^5 \text{ s}^{-1}$), drag and relativistic effects must also be included to accurately model high rate material behavior.

*Los Alamos National Laboratory
P.O. Box 1663 MS T086
Los Alamos, NM 87545, USA
ahunter@lanl.gov

Figure 1: Intersections of attractive mobile and immobile dislocations can result in the formation of either (a) a junction, or (b) a crossed-state or node.

Consider a crystal with total dislocation density ρ_{tot} , which can be decomposed into mobile and immobile (also called network or forest) components: $\rho_{tot} = \rho_m + \rho_i$. As an attractive pair of dislocations approach one another, the configuration evolves in a complex way due to the tensor interaction between the dislocations. We limit this discussion to pairwise interactions, which have been shown to predominate the work hardening process (Friedel, 1964); thus, we neglect interactions involving three or more dislocations, including multi-junction formation by dislocation intersection with a junction previously formed by pairwise intersection (Bulatov et al., 2006). When two dislocation cores are within a critical distance, the attraction is unstable, resulting in the formation of either a junction, i.e. a straight segment branching into the two reacting dislocations at both of its ends (Figure 1(a)), or a crossed state, a single node that does not zip up to form a junction (Figure 1(b)) (Wickham et al., 1999). Furthermore, simulations completed by Wickham et al. (1999) indicate that crossed states or dislocation nodes are formed considerably more frequently than junctions. Hence, we focus on accurately describing dislocation node (crossed-state) formation and dissolution. For a more detailed discussion on the physical origin of the crossed states see Madec et al. (2002b).

At finite temperatures, atomic oscillations produce local stress fluctuations that can assist the applied stress to move mobile dislocations past short-ranged obstacles, such as forest dislocations (Friedel, 1964; Becker, 1925; Orowan, 1934a,b,c). In other words, the combination of applied stress and temperature-induced stress fluctuations can result in node dissociation. The lifetime of the node, Γ , is universally calculated on the basis of the well-known Van't Hoff-Arrhenius rate equation (Van't Hoff, 1896; Arrhenius, 1889), which originated from studies of chemical reaction rates and was first applied to dislocations by Becker (1925), Orowan (1934a,b,c), and Eyring (1936). The Van't Hoff-Arrhenius rate equation calculates the inverse of the node lifetime as

$$\Gamma^{-1} = f_a \exp\left(-\frac{E}{k_B T}\right), \quad (1)$$

where E is the activation (Gibbs free) energy, f_a is an "attempt frequency", k_B is the Boltzmann constant, and T is the temperature. Neglecting dislocation drag, the equivalent plastic strain rate, $\dot{\epsilon}$, is directly proportional to Γ^{-1} . Intersecting mobile and immobile dislocations are in a metastable state (local potential minimum) that is separated by an energy barrier with amplitude E from the dissociated state in which the mobile dislocation is remobilized. The node oscillates around the potential minimum due to thermal noise and eventually escapes over the energy barrier after absorbing a sufficient amount of thermal energy. In other words, if the applied stress is not large enough to dissociate the node, the node can still be destroyed by thermal fluctuations. Equation 1 gives the decay rate of the metastable state due to thermal fluctuations. The calculation of such rates is the subject of reaction rate theory (Hänggi et al., 1990) which encompasses classical transition state theory (TST) (Eyring, 1935; Vineyard, 1957) and Kramer's theory for chemical reaction rates (Kramers, 1940); both lead to Equation 1 for the rate of a chemical reaction, or of plastic deformation. For an excellent account of reaction rate theory see Pollak and Talkner (Pollak and Talkner, 2005).

Equation 1 has served as the foundation for the majority of continuum-scale models constructed by the materials science community to describe thermally-activated plastic flow (Seeger, 1954a,b,c, 1955b; Follansbee and Kocks, 1988; Hoge and Mukherjee, 1977; Steinberg and Lund, 1989; Zerilli and Armstrong, 1987; Preston et al., 2003; Langer et al., 2010; Austin and McDowell, 2011, 2012). However, the Van't Hoff-Arrhenius equation is valid only

when the height of the potential barrier is large in comparison with the thermal energy: $E/k_B T \gg 1$. The derivation of Equation 1 from either TST or Kramer's theory requires a separation of time scales: the time scale for escape over the barrier must be much greater than any other time scale (noise correlation time, transition time ...). In other words, the conditions for escape over the potential barrier must be quasi-stationary (to a high degree of accuracy a Maxwell-Boltzmann distribution obtains in the neighborhood of the initial minimum), meaning that there will be a very slow diffusion of particles, or dislocations, across the saddle point to another energetic minimum in comparison to other time scales. Under these assumptions, Chandrasekhar (1943) carried out a clear, elegant derivation of Equation 1 from the Smoluchowski equation over 70 years ago, a derivation which rests on the assumption that $E/k_B T \gg 1$. The requirement that $E/k_B T \gg 1$ is a serious limitation if Equation 1 is to be applied to intersecting dislocations at high strain rates. The energy barrier E that must be overcome for node dissociation must decrease with increasing applied stress to ensure that the plastic strain rate will also increase. At sufficiently high stresses the potential barrier becomes comparable to the thermal energy, thus, the constraint $E/k_B T \gg 1$ is no longer satisfied. Hence, Equation 1 will not give the correct node lifetime or plastic strain rate at very high stresses, and therefore, models based on Equation 1 break down in this regime. To explicitly illustrate the limitations of Arrhenius-based models at high plastic strain rates or stresses, we briefly discuss two such models, a 1954 model developed by Seeger (1954a,b,c, 1955b) and the more recent mechanical threshold stress (MTS) model of Follansbee and Kocks (1988).

Seeger (1954a,b,c, 1955b) modeled the temperature, stress, and strain dependence of the strain rate as

$$\dot{\epsilon} = \dot{\epsilon}_0 \exp\left(-\frac{U - v(\epsilon)(\sigma - \sigma_b)}{k_B T}\right), \quad (2)$$

where σ_b is the mean internal shear stress opposing glide due to neighboring dislocations or other obstacles (back stress), $v = bd/\sqrt{\rho_f}$ is the activation volume, d is the dislocation core width (stacking fault width in fcc metals), b is the Burgers vector, and ρ_f is the strain-dependent forest dislocation density. Seeger solved Equation 1 for the stress and expressed the result in the form

$$\sigma = \sigma_b + \frac{U}{v} \left(1 - \frac{T}{T_c}\right), \quad (3)$$

where

$$T_c = \frac{U}{k_B \ln(\dot{\epsilon}_0/\dot{\epsilon})} \quad (4)$$

is a critical temperature. If $T > T_c$ then $\sigma < \sigma_b$, which is unphysical. This deficiency was rectified by means of the *ad hoc* inclusion of a factor, $\theta(T_c - T)$, in the second term of Equation 3. If the applied stress in Equation 2 increases to $\sigma_b + U/v$, the activation energy vanishes and the strain rate goes to $\dot{\epsilon}_0$. If the strain rate is increased further, $T_c < 0$ and the flow stress becomes fixed at σ_b . Clearly, this model does not produce reliable results at very high strain rates.

The MTS model involves a single internal state variable, the zero-temperature flow stress, and is also an Arrhenius-based model with a simple phenomenological relation for the activation energy (Follansbee and Kocks, 1988). Follansbee and Kocks determined $\dot{\epsilon}_0 = 10^7 \text{s}^{-1}$ for OFE copper by fitting to uniaxial compression data for strain rates ranging from 10^{-4}s^{-1} to 10^4s^{-1} and true strains up to 0.25. This model predicts $E/k_B T = 7, 5, 3, 1$ for $\dot{\epsilon} = 9.1 \times 10^3 \text{s}^{-1}$, $6.7 \times 10^4 \text{s}^{-1}$, $5.0 \times 10^5 \text{s}^{-1}$, $3.7 \times 10^6 \text{s}^{-1}$ respectively. Clearly the assumption that $E/k_B T \gg 1$ breaks down at the higher strain rates. Evidently the MTS model, based as it is on standard thermal activation theory, cannot be applied at rates as high as 10^6s^{-1} .

A host of other plastic flow models based on the Van't Hoff-Arrhenius equation have been constructed, most notably the Hoge and Mukherjee (1977), Steinberg and Lund (1989), Zerilli and Armstrong (1987), Preston-Tonks-Wallace (PTW) (Preston et al., 2003), Langer-Bouchbinder-Lookman (LBL) (Langer et al., 2010), and Austin and McDowell (2011, 2012) models, and, most recently, the model of Yanilkin et al. (2014). The first three break down at high strain rates, but PTW and LBL can be applied at rates up to 10^{12}s^{-1} . In the PTW model, Arrhenius thermal activation is replaced at high rates by a constitutive relation obtained from overdriven shock wave theory. On the other hand, the LBL model utilizes an Arrhenius-like relation between the strain rate and an effective dislocation temperature at all strain rates. The dislocation-based model of Austin-McDowell is applicable to fcc polycrystals at strain rates of 10^5s^{-1} to 10^8s^{-1} , rates characteristic of weak shock waves. While this model incorporates an advanced treatment of dislocation evolution, the dislocation-obstacle waiting time is described using a conventional Van't Hoff-Arrhenius form (Austin and McDowell, 2011). In subsequent work, the model is extended to higher plastic strain

rates (higher shock stresses) but still utilizes standard Van't Hoff-Arrhenius thermal activation (Austin and McDowell, 2012). The Yanilkin et al. (2014) model is applicable at strain rates greater than 10^5s^{-1} but again employs a Van't Hoff-Arrhenius-type expression for the waiting time.

Two notable exceptions to these Arrhenius-based models are the multiscale strength model of Barton et al. (2011), and the dislocation-based model of Krasnikov et al. (2010, 2011). In the multiscale model, thermal activation is represented by a functional form derived from molecular dynamics simulations. The plastic flow model of Krasnikov et al. (2010, 2011) was developed to describe plastic flow at very high rates (up to $\sim 10^8 \text{s}^{-1}$). Thermally-activated glide is not encoded in the model *"because the thermal fluctuation mechanism of overcoming of obstacles has not managed to operate in contrast to the case of quasi-static deformation."* However, our improved description of thermal activation exhibits an increase in rate sensitivity at very high rates, so it may be important to include the effects of thermal fluctuations, in addition to drag (which is included in the Krasnikov et al. (2010, 2011) model), at shock wave deformation rates.

Finally, we mention the work of Fan et al. (2012) who also present a formalism for the onset of the non-Arrhenius response at high strain rates, specifically the well-known upturn in stress vs. strain rate curves at rates in the range of 10^3 to 10^7s^{-1} . Notably, the approach of Fan et al. (2012) relies on a functional form of the stress-dependent activation barrier that does not follow from the formalism. Rather, it must be chosen to fit experimental data. Fan et al. (2012) choose the same functional form as that used by Follansbee and Kocks for the activation free energy of the MTS model (Follansbee and Kocks, 1988); the free energy parameters, which are not physically-based, are determined by means of atomistic simulations. In contrast to the Fan et al. (2012) formalism, our approach is self-contained; it is not necessary to specify a parameterized functional form in our analytic kinetic equation, yet the non-Arrhenius response at high strain rates is still captured.

In view of the limitations inherent in using the Van't Hoff-Arrhenius rate equation to correctly predict the lifetimes of mobile-immobile dislocation intersection nodes at large stresses, we depart from such a formulation and instead develop a mean-first-passage-time (MFPT) framework *specific* to intersecting dislocations. Our replacement for Equation 1 correctly accounts for the effects of thermal fluctuations on nodes at arbitrarily high stresses and strain rates. The microphysics is encoded in the kinetic equation, which relates the plastic strain rate to the applied stress, the network and mobile dislocation densities, the material density, and the temperature. Furthermore, we show that our MFPT-based stress-strain response exhibits the sharp, non-Arrhenius upturn without including high-rate phonon drag.

For a stochastic process, $f(t)$, with or without memory, the MFPT, $t_\Omega(f_0)$, is the average time required for the process starting at $f_0 = f(0)$ to first leave a prescribed open domain, Ω . Such a process can be described by the conditional probability, $P_\Omega(f, t|f_0)$, of visiting the point f at time t if it started at f_0 at $t = 0$ and never left Ω . In terms of this probability the MFPT reads (Hänggi et al., 1990)

$$t_\Omega(f_0) = \int_0^\infty \int_\Omega P_\Omega(f, t|f_0) df dt. \quad (5)$$

In this paper, $f(t)$ is the thermally-driven stochastic component of the force between intersecting dislocations, t_Ω is the mean time it takes to remobilize a mobile dislocation trapped at a node, i.e. the mean lifetime of a node, and $\Omega(t)$ is the time-dependent open interval $(-\infty, f_c(t))$, where $f_c(t)$ is a time-dependent critical value of the stochastic component of the force. We do not explicitly calculate $P_\Omega(f, t|f_0)$. Instead, its integral over Ω is related to the integral of the probability distribution of f over the complement of Ω . For intersecting dislocations, t_Ω is independent of $f(0) \in \Omega$, but of course $t_\Omega(f_0) = 0 \forall f_0 \in \partial\Omega$.

Section 2 discusses the critical shear stress (to dissociate nodes at zero temperature), the back stress, and the effective stress. Thermally-driven force (stress) fluctuations at dislocation nodes, including their autocorrelations, are addressed in Section 3 in terms of localized modes. The total force between intersecting dislocations is the sum of the force due to line tension during bow-out and that arising from thermal fluctuations. When this force reaches a critical value the node will dissociate. In Section 4, we carry out a MFPT derivation of the mean lifetime of a dislocation intersection node or short junction. This result is a conceptual and theoretical advancement over standard (Arrhenius) thermal activation that generalizes the description of thermal fluctuations at dislocation nodes and short junctions to very high strain rates, and thereby enables the formulation of our kinetic equation (stress versus strain rate, dislocation and material densities, and temperature), described in Section 5. The density dependencies of all quantities appearing

Figure 2: Schematic of mobile dislocation bow-out when pinned by two immobile dislocations intersecting the glide plane.

in the kinetic equation are discussed in Section 6. In Section 7 we show that our kinetic equation predicts viscous solid flow at very high stresses and strain rates. Finally, our concluding comments appear in Section 8.

2. Critical Shear, Back, and Effective Stresses

In this section we discuss the critical applied shear stress required to dissociate nodes at zero temperature, and the back and effective stresses.

Consider Figure 2, a schematic of a mobile dislocation pinned by two forest dislocations intersecting the glide plane. The mean distance between nodes, $\mathcal{L}_i$, is equal to the mean separation of immobile dislocations. To a good approximation, $\mathcal{L}_i$ equals the inverse square root of the immobile dislocation density, ρ_i ,

$$\mathcal{L}_i = \frac{1}{\sqrt{\rho_i}}. \quad (6)$$

During dislocation bow-out around a node at $T = 0$, the force, $\mathcal{F}$, between the dislocations is clearly equal to $2\mathcal{T} \sin \phi$, where $\mathcal{T}$ is the dislocation line tension, ϕ is the angle between the initial straight line direction and the tangent to the dislocation line at the node, and the factor of two accounts for bow-out of the dislocation around both sides of the node (see Figure 2). Assuming small bow-out, we have $\sin \phi \approx \phi$, hence the time-dependent force between the intersecting dislocations is approximately

$$\mathcal{F}(t) = 2\mathcal{T} \phi(t). \quad (7)$$

At zero temperature, the node will be destroyed if the force between the dislocations exceeds the critical value

$$\mathcal{F}_c = 2\mathcal{T} \phi_c = \sigma_c b \mathcal{L}_i, \quad (8)$$

where b is the Burgers vector, σ_c is the critical shear stress, and ϕ_c is the critical bow-out angle.

The line tension is given by Hirth and Lothe (1992)

$$\mathcal{T}(\beta, \nu) = \frac{G b^2}{4\pi(1-\nu)} \left\{ (1+\nu) \cos^2 \beta + (1-2\nu) \sin^2 \beta \right\} \ln \left(\frac{\mathcal{L}_i}{b} \right), \quad (9)$$

where G is the temperature- and density-dependent shear modulus, ν is the Poisson ratio with a mean value of about $1/3$, and β is the angle between the dislocation line direction and the Burgers vector. Note: in Equation 9 (also Equation (6-82) in Hirth and Lothe (Hirth and Lothe, 1992)) we have used b as a reasonable approximation of the dislocation core width, replacing the product $e\rho$ in Hirth and Lothe (Hirth and Lothe, 1992), where $e = 2.71828 \dots$ and ρ is a cutoff parameter. Averaging over the angle β and setting ν equal to $1/3$ yields the mean line tension

$$\mathcal{T} \equiv \langle \mathcal{T}(\beta, 1/3) \rangle = \frac{5}{16\pi} G b^2 \ln \left(\frac{\mathcal{L}_i}{b} \right). \quad (10)$$

Evidently this expression breaks down when $\rho_i \sim b^{-2}$; for copper at zero pressure this corresponds to $\rho_i = 1.6 \times 10^{15} \text{cm}^{-2}$.

Equation 8 holds at $T = 0$. However, the second equality in that equation can be used to define the critical stress at finite T . Combining Equations 8 and 10 results in

$$\sigma_c(T) = \frac{2\mathcal{T}(T)\phi_c}{b\mathcal{L}_i} = \frac{5}{8\pi}\phi_c G(T)b\mathcal{L}_i^{-1}\ln\left(\frac{\mathcal{L}_i}{b}\right), \quad (11)$$

and

$$\mathcal{F}_c = \frac{5}{8\pi}\phi_c G(T)b^2\ln\left(\frac{\mathcal{L}_i}{b}\right). \quad (12)$$

Madec, Devincere, and Kubin (Madec et al., 2002a) have carried out large-scale 3D dislocation dynamics (DD) simulations on copper to obtain the critical stress for crossed-state junction rupture

$$\sigma_c^{MDK} = kGb\mathcal{L}_i^{-1}\ln\left(\frac{\mathcal{L}_i}{b}\right). \quad (13)$$

They find that $k = 1/10$ produces excellent fits to numerical data. Comparison of Equations 11 and 13 shows that

$$\phi_c = \frac{4\pi}{25} = 0.503 = 28.8^\circ \quad \text{copper}. \quad (14)$$

Since $\sin\phi_c = 0.482$, the critical angle is small, at least for copper; hence, the small bow-out approximation is quite accurate. Henceforth, we take $\phi_c = 1/2$ for copper. Equation 12 then gives, for copper, $\mathcal{F}_c = 0.00034, 0.00023, 0.00012$ dyne for $\rho_i = 10^6, 10^9, 10^{12} \text{ cm}^{-2}$, respectively.

In addition to the core-core interaction between dislocations, there are the long-range internal stresses due to other dislocations. Over the years, there has been much discussion as to whether or not these long-range interactions can act as a 'back stress' opposing dislocation motion. As early as 1935, W.G. and J.M. Burgers recognized that immobile dislocations may "give rise to an 'interior' field . . . of a stress τ_i increasing with the number of dislocations formed" (Burgers and Burgers, 1935). About twenty years later, A. Seeger argued that, in addition to the applied stress, moving dislocations are subject to an opposing stress arising from the surrounding dislocations, and that the main contribution is from dislocations roughly parallel to the mobile dislocation and having the same Burgers vector (Seeger, 1955a). For a density N of such dislocations, he proposed that this internal stress is given by

$$\sigma_b^{Seeger} = \alpha b G(\rho, T) \sqrt{N}, \quad (15)$$

where ρ is the material density, and " α is a constant of the order of $1/5$ whose exact value depends on the details of the dislocation arrangement, Poisson's ratio ν , and the character of the dislocations involved". Recently, Groma et al. (2003) investigated the collective behavior of straight, parallel dislocations and found that the effect of correlations on the dislocation dynamics can be described by a local back stress that is the sum of two contributions of the same sign, one which varies as the square root of the dislocation density but with a stress-dependent pre-factor (not evaluated by Groma et al.), plus a term which is proportional to the gradient of the density of geometrically necessary dislocations (GND), i.e. a diffusion-like term. A back stress proportional to the gradient of the GND density has also been derived by other groups (Yefimov et al., 2004; Yefimov and Van der Giessen, 2005; Bayley et al., 2006). We remind the reader that GND, first proposed by Ashby, are dislocations that must appear in order to accommodate deformation gradients in the microstructure (Ashby, 1970). For the case of polycrystal deformation, where GND accumulate along the grain boundaries, an explicit expression for the corresponding contribution to the back stress has yet to be derived. However, experimental measurements of GND densities have been carried out recently (Kysar et al., 2010; Dahlberg et al., 2014).

Experiments show that back stresses exist in metals and can impact the mechanical response. However, there are several reported sources of back stress, and in the opinion of the authors, theoretical results to date on the back stress are inconclusive; additional research is needed, which is beyond the scope of this paper. For our purposes it is sufficient to use a rough estimate of the back stress, and for that we borrow from Seeger, but replace N by the immobile dislocation density and α by a constant of order $1/5$

$$\sigma_b = g_b b G(\rho, T) \sqrt{\rho_i}. \quad (16)$$

The effective applied stress, $\hat{\sigma}$, is the difference between the true applied stress, σ , and the back stress, σ_b , for $\sigma > \sigma_b$, but vanishes if $\sigma \leq \sigma_b$ (θ is the unit step function):

$$\hat{\sigma} = (\sigma - \sigma_b) \theta(\sigma - \sigma_b). \quad (17)$$

3. Thermally-Driven Force Fluctuations at Dislocation Nodes

The node formed during mobile-immobile dislocation intersection acts as an extended defect within the crystal. In order to calculate the node dissociation rate as a function of applied stress and temperature, we consider localized vibrational modes of the node and show that the distribution of the corresponding force fluctuations between the dislocations is nearly Gaussian.

The localized vibrational modes exhibited by point defects (impurities, vacancies, and interstitials) in a monatomic lattice with only nearest-neighbor interactions were first studied theoretically by Montroll and Potts (1955). The localized mode frequencies for defects are shifted above the frequency band of the perfect lattice. The amplitudes of the localized modes die out rapidly with increasing distance, r , from the point defects – in a simple cubic lattice the amplitude decreases as $r^{-1} \exp(-Ar)$ (Montroll and Potts, 1955) – and the attenuation distance is decreased as the displacement of the localized mode frequency above the band increases (Maradudin et al., 1958). For example, vacancies pulsate at a frequency $\omega = \omega_L P / (2\sqrt{P-1})$, where $P = \gamma'/\gamma > 2$ is the ratio of the force constant, γ' , for neighbors of the vacancy to that of the perfect lattice, γ , and $\omega_L = \sqrt{4\gamma/M}$ (M is the atomic mass) is the highest normal mode frequency on the zone boundary. Note that $\omega > \omega_L$, that is, the frequency of the pulsating mode lies above the maximum frequency of the perfect lattice. Similarly, if the force constant for an atom is increased but the mass is left unchanged, then again a localized mode appears with a frequency above ω_L ; for $P \geq 1$, $\omega = \omega_L [1 + 2(P-1)^2]$. If $\gamma' < \gamma$ ($P < 1$), the mode frequency then lies within the band and attenuation will not occur, i.e. the mode is not localized. In general, an increase (decrease) of a single force constant has the same effect as a decrease (increase) of a single mass (Bjork, 1957). More importantly, the amplitude of a localized mode around a point defect is much larger than the amplitudes of the perfect-crystal modes (Bjork, 1957; Rosenstock and Kilck, 1960). When a strongly localized mode is present, the other modes avoid the impurity (Bjork, 1957). Consequently, the motions of the defect and its near neighbors are well-approximated by the localized modes alone.

Montroll and Potts also considered the interaction of a pair of point defects. Identical isolated defects have the same localized mode frequency, but as they are brought together this degeneracy is split: the defect pair has two localized mode frequencies, one above and the other below the frequency of a single point defect (Montroll and Potts, 1955). As another example, the breaking of crystal symmetry in the cores of dislocations also results in the appearance of localized modes (Schuck et al., 2009). In fcc crystals, both edge and screw dislocations have strong localized peaks but almost no resonance peaks (intradband frequencies).

The node formed by intersecting dislocations is a compact extended lattice defect; it is comprised of a small number of atoms, N . As in the case of point defects, the node oscillations should be accurately described in terms of only the localized modes since the ordinary modes (phonons) avoid the node. The node, like a point defect, drives the crystal at a frequency above its band of normal mode frequencies and this high-frequency driven wave is attenuated in a short distance. As mentioned previously, a pair of point defects in a linear chain has two localized mode frequencies. Generalizing to N atoms and three dimensions, we conclude that the dislocation-dislocation node can oscillate in $n = 3N$ localized (normal) modes. In contrast to a free N -atom molecule with $3N - 6$ modes, the N -atom node is embedded in and interacts with the lattice, hence the six degrees of freedom associated with translational and rotational invariance should not be subtracted. Rather than describing the vibrations of the node in terms of $3N$ rectangular coordinates, it is more convenient to employ generalized or internal coordinates, q_i ($i = 1, \dots, n$), such as interatomic distances or interband angles, or alternatively, normal coordinates, Q_i , one for each localized normal mode. The normal coordinate,

$$Q_i(t) = \sqrt{\epsilon_i} \cos(\omega_i t + \phi_i), \quad (18)$$

describes motion in a single localized mode of frequency ω_i , energy ϵ_i , and phase ϕ_i . The Q_i are normalized so that the potential energy is simply $\sum_i Q_i^2$. The generalized coordinates are linear combinations of the normal coordinates

$$q_i = \sum_{j=1}^n c_{ij} \sqrt{\epsilon_j} \cos(\omega_j t + \phi_j), \quad i = 1, \dots, n. \quad (19)$$

In any normal mode, say j , all of the generalized coordinates, q_i ($i = 1, \dots, n$), have frequency ω_j and phase ϕ_j , but, in general, differing amplitudes, $c_{ij} \sqrt{\epsilon_j}$.

We assume that we can define generalized coordinates such that the set of critical configurations, i.e. node configurations resulting in dissolution of the node, is completely specified by q_1 attaining a critical value (Slater, 1959). This coordinate is our reaction coordinate, that is, the coordinate along the reaction path. This is the path of steepest descent on the potential energy surface (Born-Oppenheimer electronic energy) from its saddle point or node dissolution configuration, to its minimum, $V = 0$, which corresponds to a zero-temperature node at the time of its formation, i.e., for zero glide bow-out. We approximate the crystal potential, V , as harmonic in the generalized coordinates; anharmonic corrections are important only in the immediate vicinity of the saddle point. The results of Bjork (Bjork, 1957) and Rosenstock/Klick (Rosenstock and Kilck, 1960) on point defects indicate that the localized modes suppress the ordinary modes (phonons) in the vicinity of the node, hence, the node oscillations are, to a very good approximation, superpositions of its localized modes. Thus, the phonon contributions to V can be neglected. Furthermore, the potential includes a term linear in the reaction coordinate that accounts for the decrease in the potential barrier with increased bow-out of the dislocation line; terms linear in $q_2, \dots, q_n$ would deform the reaction path, which would be inconsistent with q_1 as the reaction coordinate. We also point out that the localized modes of the individual dislocations are strongly attenuated at the node, and may therefore be neglected. The potential assumes the form

$$V \approx \frac{1}{2} b_{11} q_1^2 + \frac{1}{2} \sum_{r,s} (b_{rs} - \delta_{r1} \delta_{s1}) q_r q_s - 2\mathcal{T} \phi q_1, \quad (20)$$

where δ_{ij} is the Kronecker delta. The negative gradient along the reaction coordinate gives the total force between the dislocations acting to dissociate the node

$$-\frac{\partial V}{\partial q_1} = 2\mathcal{T} \phi(t) - b_{11} q_1(t). \quad (21)$$

The first term on the right hand side (RHS) is the force between the dislocations arising from bow-out; this force is $\mathcal{F}(t)$, as defined in Equation 7. The second term on the RHS is the fluctuating contribution to the force between the dislocations due to thermal vibrations of the N -atom node in superpositions of its localized modes. Upon defining $a_i = b_{11} c_{1i}$ and absorbing the overall minus sign in the phase, ϕ_i , this term can be expressed as

$$f(t) = \sum_{i=1}^n a_i \sqrt{\epsilon_i} \cos(\omega_i t + \phi_i). \quad (22)$$

The energies and amplitudes of the localized modes are comparable to those of the ordinary modes, thus ϵ_i is directly proportional to $k_B T$. Since $k_B T$ has the dimensions of force times distance, the coefficient a_i must have units of square root of force per unit length, and for intersecting dislocations both the force and the unit of length must be characteristic of dislocations, hence we choose the ratio of force to distance to be $\mathcal{T}/b$. Therefore,

$$a_i \sqrt{\epsilon_i} = \alpha_i \sqrt{\mathcal{T} k_B T / b}, \quad (23)$$

where the α_i are dimensionless, and

$$f(t) = \sqrt{\mathcal{T} k_B T / b} \sum_i^n \alpha_i \cos(\omega_i t + \phi_i). \quad (24)$$

The time scale for the force fluctuations is the reciprocal of the mean localized mode frequency $\bar{\nu}_{loc} = \bar{\omega}_{loc}/2\pi$, which is larger than but on the order of the maximum acoustic phonon frequency; in the Debye approximation this is $\nu_D = \omega_D/2\pi$, where ω_D is the Debye frequency. In the case of copper, for example, $\nu_D^{Cu} = 7.2 \times 10^{12} \text{s}^{-1}$. In general, $\bar{\nu}_{loc} \sim 10^{13} \text{s}^{-1}$.

The probability density of $f(t)$ averaged over time and phases is given by

$$\mathcal{P}(f) = \frac{1}{\pi} \int_0^\infty \cos(fx) \prod_i^n J_0(\sqrt{\mathcal{T} k_B T / b} \alpha_i x) dx; \quad (25)$$

for the lengthy derivation of this result see Slater, Chapter 4 (Slater, 1959). If we use the approximation

$$J_0(z) \approx \exp(-z^2/4), \quad (26)$$

we obtain

$$\mathcal{P}(f) \approx \frac{1}{\sqrt{2\pi\langle f^2 \rangle}} \exp\left\{-\frac{f^2}{2\langle f^2 \rangle}\right\}, \quad (27)$$

where

$$\langle f^2 \rangle = \frac{1}{2} \frac{\mathcal{T}}{b} k_B T \sum_{i=1}^n \alpha_i^2 \equiv \frac{2}{\kappa} \frac{\mathcal{T}}{b} k_B T. \quad (28)$$

Equation 27 is the Gaussian approximation for the distribution of the stochastic component of the force at the dislocation node. Its failure is manifest when f is near its maximum value,

$$f_{\max} = \sqrt{\mathcal{T} k_B T / b} \sum_{i=1}^n \alpha_i, \quad (29)$$

because $\mathcal{P}(f) = 0$ for $f > f_{\max}$. However, the Gaussian distribution rapidly approaches zero for $f \sim f_{\max}$, and is a very good approximation for relatively small values of n , the number of localized modes, and improves with increasing n . For example, if $\sqrt{\mathcal{T} k_B T / b} \alpha_i = 1 \forall i$ and $n = 10$ ($\langle f^2 \rangle = 5$), the Gaussian approximation differs from the exact $\mathcal{P}(f)$ by at most 10% for $f < 6$; for larger f the error grows but the absolute difference decreases to $\sim 10^{-5}$ at $f = 10$.

3.1. Autocorrelation of Force Fluctuations

As time increases, $f(t)$ becomes more weakly correlated to its initial value. The time scale over which $f(t)$ becomes statistically independent of $f(0)$ is provided by the autocorrelation function of $f(t)$. Using Equation 24 for $f(t)$, we can determine the autocorrelation function for a large class of physically reasonable distributions of the α_i . As we shall see, the autocorrelation decays either as τ/t or as $\exp(-t/\tau)$, where τ^{-1} is on the order of the range of localized mode frequencies, $\Delta\omega$.

The dimensionless amplitudes, α_i , may be regarded as the values of a C^∞ function, $\alpha(\omega)$, on the set of localized mode frequencies, $\{\omega_i\}$. We assume that the ω_i are densely distributed over the interval $[\omega_1, \omega_N]$, and that the phases, ϕ_i , are randomly and uniformly distributed on $[0, 2\pi)$. Let $n(\omega) d\omega$ be the number of localized mode frequencies on $(\omega, \omega + d\omega)$ and the integral of $n(\omega)$ over $[0, \infty)$ is N . We define the amplitude spectrum

$$E(\omega) = \frac{1}{2} \alpha^2(\omega) n(\omega), \quad (30)$$

with the dimension of inverse frequency. The autocorrelation function is related to the amplitude spectrum according to (Longuet-Higgins, 1958)

$$\langle f(t) f(t + \Delta t) \rangle = \frac{\mathcal{T}}{b} k_B T \int_0^\infty E(\omega) \cos(\omega \Delta t) d\omega. \quad (31)$$

The amplitude spectrum is not currently known for dislocation-dislocation nodes, but we can, nevertheless, draw general conclusions about the dependence of the autocorrelation on the functional form of $E(\omega)$. Toward that end, we consider the following three-parameter amplitude spectrum

$$E(\omega) = \frac{\alpha}{1 + p \cosh \left[\cosh^{-1} (1/p) (\omega - \bar{\omega}) / \Delta\omega \right]}. \quad (32)$$

Here $\Delta\omega = (\omega_N - \omega_1)/2$ is the half-width of the spectrum, approximated as symmetric around the mean frequency $\bar{\omega}$, and $p \leq 1$ controls the curvature at $E(\bar{\omega})$. For p near 1, $E(\omega)$ is Gaussian-like, but as p decreases the peak broadens, becoming a square pulse in the limit $p \rightarrow 0$. In order to evaluate the autocorrelation analytically, it is necessary to extend the lower limit of the ω integration in Equation 31 from 0 to $-\infty$. This is a good approximation because $E(\omega)$

must have its support on $\omega > 0$. Applying Equation 32 and integrating, we obtain (Gradshteyn and Ryzhik, 1994; Gröbner and Hofreiter, 1958)

$$\langle f(t) f(t + \Delta t) \rangle = \frac{\mathcal{T}}{b} k_B T \frac{\alpha \pi}{\sqrt{1-p^2} \cosh^{-1}(1/p)} \frac{\Delta \omega \cos(\bar{\omega} \Delta t) \sin(\Delta \omega \Delta t)}{\sinh[\pi \Delta \omega \Delta t / \cosh^{-1}(1/p)]}. \quad (33)$$

For $\Delta t \gg (\Delta \omega)^{-1}$,

$$\frac{\langle f(t) f(t + \Delta t) \rangle}{\langle f(t)^2 \rangle} \sim \frac{2\pi \cos(\bar{\omega} \Delta t) \sin(\Delta \omega \Delta t)}{\cosh^{-1}(1/p)} \exp\left\{-\frac{\Delta t}{(\pi \Delta \omega)^{-1} \cosh^{-1}(1/p)}\right\}. \quad (34)$$

The correlation time is of order $(\Delta \omega)^{-1}$ for $0 < p \leq \frac{1}{2}$; as $p \rightarrow 1$ the correlation time goes to zero. In the limit $p \rightarrow 0$

$$\frac{\langle f(t) f(t + \Delta t) \rangle}{\langle f(t)^2 \rangle} \sim \frac{\cos(\bar{\omega} \Delta t) \sin(\Delta \omega \Delta t)}{\Delta \omega \Delta t}, \quad (35)$$

which decreases from unity as $(\Delta t)^{-1}$ on a time scale $(\Delta \omega)^{-1}$. The previous equations hold for $E(\omega)$ symmetric about the mean frequency $\bar{\omega}$. Now consider the asymmetric spectrum

$$E(\omega) = \frac{\alpha (\omega - \omega_1) \theta(\omega - \omega_1) \theta(\omega_N - \omega)}{(\omega_N - \omega_1)^2}, \quad (36)$$

which is normalized to $\alpha/2$. For $\Delta t \gg (\Delta \omega)^{-1}$

$$\frac{\langle f(t) f(t + \Delta t) \rangle}{\langle f(t)^2 \rangle} \sim \frac{\sin(\omega_N \Delta t)}{\Delta \omega \Delta t}, \quad (37)$$

and again we see that the autocorrelation decreases as $(\Delta t)^{-1}$ on a time scale $(\Delta \omega)^{-1}$.

We conclude that, in general, $f(t)$ becomes weakly correlated with $f(0)$ on a time scale, τ , of order $(\Delta \omega)^{-1}$, where $\Delta \omega$ is the half-width of the range of localized mode frequencies and must be on the order of the mean phonon frequency, $\bar{\nu}$; consequently, $\tau \sim \bar{\nu}^{-1} \sim 10^{-13} s$.

3.2. Remobilization Conditions

Consider dislocation intersection at zero temperature where the only force between the dislocations is $\mathcal{F} = 2\mathcal{T}\phi$ due to bow-out. The bow-out angle ϕ (see Figure 2) is a monotonically increasing function of time

$$\phi(t) = \phi_m \tilde{\phi}(t) = \frac{\hat{\sigma} b \mathcal{L}_i}{2\mathcal{T}} \tilde{\phi}(t), \quad (38)$$

where ϕ_m is the maximum bow-out angle, $\tilde{\phi}(0) = 0$, and $\tilde{\phi}(t) \sim 1$ as $t \rightarrow \infty$; $\tilde{\phi}(t)$ is calculated in Section 4. The force between the dislocations during bow-out is

$$\mathcal{F}(\hat{\sigma}, t) = 2\mathcal{T}\phi(t) = b \mathcal{L}_i \hat{\sigma} \tilde{\phi}(t). \quad (39)$$

As discussed in Section 2, the node will dissociate if the external stress field is strong enough that the force $\mathcal{F}(t)$ exceeds the critical value $\mathcal{F}_c(t) = 2\mathcal{T}\phi_c$. Thus, the condition for remobilization of the stalled mobile dislocation is

$$\mathcal{F}(\hat{\sigma}, t) \geq \mathcal{F}_c, \quad T = 0. \quad (40)$$

As $\mathcal{F}(\sigma, \sigma_b, t)$ increases, the potential landscape changes and, in particular, the depth of the initial minimum in the crystal potential decreases. When Equation 40 is satisfied the energy minimum is eliminated and the stalled mobile dislocation will remobilize.

At finite T , the total force between the dislocations is $\mathcal{F}(\hat{\sigma}, t) + f(t)$. The condition to destroy the node and remobilize the dislocation is generalized to

$$\mathcal{F}(\hat{\sigma}, t) + f(t) \geq \mathcal{F}_c, \quad T > 0. \quad (41)$$

This condition may also be expressed as

$$f(t) \geq f_c(\hat{\sigma}, t) \equiv \mathcal{F}_c - \mathcal{F}(\hat{\sigma}, t), \quad (42)$$

which defines the critical force fluctuation, $f_c(\hat{\sigma}, t)$. This critical fluctuation is time-dependent due to dislocation drag.

In weak external stress fields, thermal fluctuations can induce reverse motion of the mobile dislocations. The condition for reverse (negative) remobilization is

$$\mathcal{F}(\hat{\sigma}, t) + f(t) \leq -\mathcal{F}_c, \quad (43)$$

However, from the definition, Equation 39, of $\mathcal{F}(\hat{\sigma}, t)$ it follows that

$$\mathcal{F}(\hat{\sigma}, t) = -\mathcal{F}(-\hat{\sigma}, t). \quad (44)$$

Using Equation 44 and the definition, Equation 42, of $f_c(\hat{\sigma}, t)$, Equation 43 may be written

$$f(t) \leq -f_c(-\hat{\sigma}, t). \quad (45)$$

4. Mean Remobilization Time

In this section, we calculate the mean lifetime of a dislocation intersection node, the probability of node formation, and the mean time required for remobilization.

We first consider forward (positive) glide of the mobile dislocation following node dissociation. The dependence of the critical force on stress will be implicit: $f_c(t) \equiv f_c(\hat{\sigma}, t)$. The condition $f(t) \in \Omega(t) = (-\infty, f_c(t))$ is assumed to be satisfied, i.e. a node exists at time t . The probability that the node is dissociated and the stalled dislocation is remobilized at time $t + \tau$ can be written

$$\begin{aligned} \mathcal{D}_\tau(t) &\equiv \text{Prob}(f(t + \tau) > f_c(t + \tau) | f(t) < f_c(t)) \\ &= \int_{f_c(t+\tau)}^{\infty} \mathcal{P}(f) df, \end{aligned} \quad (46)$$

where $\text{Prob}(a|b)$ is the conditional probability of a given b , and $\mathcal{P}(f)$ is defined previously in Equation 27.

As stated in Section 2, we assume small bow-out, which is described by

$$B \frac{\partial y}{\partial t} = \mathcal{T} \frac{\partial^2 y}{\partial x^2} + \hat{\sigma} b, \quad (47)$$

where y is the dislocation displacement in the direction of bow-out, B is the dislocation drag coefficient, and $\hat{\sigma} = \sigma - \sigma_b$ is the effective applied stress. At a pinning point x_p , $y'(x_p, t) = \tan \phi(t) \approx \phi(t)$. For a dislocation pinned at two points a distance $\mathcal{L}_i$ apart:

$$\phi(t) = \phi_m \left\{ 1 - \frac{8}{\pi^2} \sum_{n=1}^{\infty} (2n-1)^{-2} \exp \left[- (2n-1)^2 \frac{t}{t_B} \right] \right\} \quad (48)$$

where

$$\begin{aligned} \phi_m &= \frac{\hat{\sigma} b \mathcal{L}_i}{2\mathcal{T}} = \frac{\hat{\sigma}}{\sigma_c} \phi_c, \\ t_B &= \frac{B \mathcal{L}_i^2}{\pi^2 \mathcal{T}}. \end{aligned} \quad (49)$$

Note that the time scale for bow-out, t_B , is independent of the applied stress. Equation 48 is well approximated by

$$\phi(t) \approx \phi_m \left(1 - e^{-t/t_B} \right). \quad (50)$$

Using values of G and b for copper, $B = 0.0005$ Poise (Al'shitz and Indenbom, 1975), and $\rho_i = 10^6, 10^8, 10^{10}, 10^{12} \text{ cm}^{-2}$, the corresponding bow-out times are 145, 1.8, 0.025, and 0.0005 ns, respectively. Since $\tau \sim 10^{-13} \text{ s} = 0.0001 \text{ ns}$, we conclude that, to a good approximation, we can take τ/t_B to be negligible.

Using Equations 7, 8, and 50, the time-dependent critical force fluctuation, Equation 42, can be written

$$\begin{aligned} f_c(t) &= 2\mathcal{T}[\phi_c - \phi(t)] \\ &= b\mathcal{L}_i\{\sigma_c - \hat{\sigma}(1 - e^{-t/t_B})\}. \end{aligned} \quad (51)$$

The change in the critical force fluctuation on the time scale, τ , of the force fluctuations is

$$f_c(t + \tau) - f_c(t) = -b\mathcal{L}_i\hat{\sigma}e^{-t/t_B}(1 - e^{-\tau/t_B}), \quad (52)$$

which is of order τ/t_B and therefore negligible. With $f_c(t + \tau) \rightarrow f_c(t)$ we now carry out the integration in Equation 46 to obtain

$$\mathcal{D}_\tau(t) = \frac{1}{2} \left\{ 1 - \text{erf} \left[\sqrt{\frac{\mathcal{E}}{k_B T}} \left(1 - \frac{\hat{\sigma}}{\sigma_c} (1 - e^{-t/t_B}) \right) \right] \right\} \quad (53)$$

where

$$\mathcal{E} = \frac{\kappa \sigma_c^2 b^3}{4\mathcal{T}\rho_i} = \kappa \phi_c^2 \mathcal{T} b = \frac{5}{16\pi} \kappa \phi_c^2 G b^3 \ln \left(\frac{1}{b \sqrt{\rho_i}} \right) \quad (54)$$

is the activation energy at $\hat{\sigma} = 0$ (see Section 4.3), and the dimensionless material parameter κ is defined by Equation 28. For plotting purposes, in later sections we have taken $\kappa \sim 1$.

Given an intact node at time t , the probability of node dissolution within a time Δt is

$$\mathcal{D}_{\Delta t}(t) = \mathcal{D}_\tau(t) \frac{\Delta t}{\tau}, \quad (55)$$

and the corresponding probability of node survival over the time interval Δt is $1 - \mathcal{D}_{\Delta t}(t)$. The probability that the node survives to $t = n\Delta t$ is the product of the survival probabilities for each of the n intervals of length Δt

$$\mathcal{S}(t, n) = \prod_{j=1}^n [1 - \mathcal{D}_{\Delta t}(j\Delta t)] = \prod_{j=1}^n \left[1 - \mathcal{D}_\tau(j\Delta t) \frac{\Delta t}{\tau} \right]. \quad (56)$$

Converting the product in Equation 56 into a summation gives

$$\ln(\mathcal{S}(t, n)) = \sum_{j=1}^n \ln \left\{ 1 - \mathcal{D}_\tau \left(\frac{j}{n} t \right) \frac{t}{n\tau} \right\}. \quad (57)$$

For fixed t and $n \gg 1$ ($\Delta t \rightarrow 0$) we utilize the approximation

$$\ln \left\{ 1 - \mathcal{D}_\tau \left(\frac{j}{n} t \right) \frac{t}{n\tau} \right\} \approx -\frac{t}{n\tau} \mathcal{D}_\tau \left(\frac{j}{n} t \right). \quad (58)$$

Using Equations 57 and 58 we get

$$\begin{aligned} \ln(\mathcal{S}(t)) &\equiv \lim_{n \rightarrow \infty} \ln(\mathcal{S}(t, n)) = -\frac{t}{\tau} \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{j=1}^n \mathcal{D}_\tau \left(\frac{j}{n} t \right) \\ &= -\frac{t}{\tau} \lim_{n \rightarrow \infty} \frac{1}{n} \int_0^n \mathcal{D}_\tau \left(\frac{x}{n} t \right) dx. \end{aligned} \quad (59)$$

We now change the integration variable to $t' = xt/n$ and take the limit $n \rightarrow \infty$ to obtain the probability of node survival until time t :

$$\begin{aligned} \mathcal{S}(t) &= \exp \left\{ -\frac{1}{\tau} \int_0^t \mathcal{D}_\tau(t') dt' \right\} \\ &= \exp \left\{ -\frac{1}{\tau} \int_0^t \frac{1}{2} \left\{ 1 - \text{erf} \left[\sqrt{\frac{\mathcal{E}}{k_B T}} \left(1 - \frac{\hat{\sigma}}{\sigma_c} (1 - e^{-t'/t_B}) \right) \right] \right\} dt' \right\}. \end{aligned} \quad (60)$$

The probability of node dissociation on the time interval $[t, t + \Delta t]$, which we denote $\mathcal{D}(t)\Delta t$, is the product of the probability of survival until time t , Equation 60, and $\mathcal{D}_{\Delta t}$, the probability of dissociation within time Δt given by Equation 55; cancelling Δt we obtain

$$\mathcal{D}(t) = \frac{1}{\tau} \mathcal{S}(t) \mathcal{D}_{\tau}(t). \quad (61)$$

As a check, we verify that the probability of node decay at some time is unity by integrating the node dissociation probability density $\mathcal{D}(t)$ from zero to infinity:

$$\begin{aligned} \int_0^{\infty} \mathcal{D}(t) dt &= \frac{1}{\tau} \int_0^{\infty} \mathcal{S}(t) \mathcal{D}_{\tau}(t) dt \\ &= \frac{1}{\tau} \int_0^{\infty} \exp\left\{-\frac{1}{\tau} \int_0^t \mathcal{D}_{\tau}(t') dt'\right\} \mathcal{D}_{\tau}(t) dt \\ &= \int_0^{\infty} \exp(-z) dz = 1. \end{aligned} \quad (62)$$

We calculate the mean node lifetime by integrating by parts:

$$\begin{aligned} \int_0^{\infty} t \mathcal{D}(t) dt &= \frac{1}{\tau} \int_0^{\infty} t \exp\left\{-\frac{1}{\tau} \int_0^t \mathcal{D}_{\tau}(t') dt'\right\} \mathcal{D}_{\tau}(t) dt \\ &= - \int_0^{\infty} t \frac{d}{dt} \exp\left\{-\frac{1}{\tau} \int_0^t \mathcal{D}_{\tau}(t') dt'\right\} dt \\ &= -t \exp\left\{-\frac{1}{\tau} \int_0^t \mathcal{D}_{\tau}(t') dt'\right\} \Big|_0^{\infty} \\ &\quad + \int_0^{\infty} \exp\left\{-\frac{1}{\tau} \int_0^t \mathcal{D}_{\tau}(t') dt'\right\} dt. \end{aligned} \quad (63)$$

Since

$$\mathcal{D}_{\tau}(t) \sim \frac{1}{2} \left\{ 1 - \operatorname{erf} \left[\sqrt{\frac{\mathcal{E}}{k_B T}} \left(1 - \frac{\hat{\sigma}}{\sigma_c} \right) \right] \right\}, \quad t \rightarrow \infty, \quad (64)$$

is a positive constant, the upper limit of the first term of Equation 63 varies as $t \exp(-\mathcal{D}_{\tau} t / \tau)$ for large t , and therefore vanishes for $t \rightarrow \infty$. The lower limit of the first term is likewise equal to zero. Thus, the mean node lifetime is

$$\int_0^{\infty} \exp\left\{-\frac{1}{\tau} \int_0^t \mathcal{D}_{\tau}(t') dt'\right\} dt = \int_0^{\infty} \mathcal{S}(t) dt. \quad (65)$$

This result can be understood as follows. Consider a set of $N \gg 1$ nodes, and two times, t and $t' > t$. The number of nodes that dissociate between t and t' is obviously the number that have survived until t , $N \mathcal{S}(t)$, minus the number that have survived until t' , $N \mathcal{S}(t')$; hence, the probability of dissociation between t and t' is $\mathcal{S}(t) - \mathcal{S}(t')$. For $t' = t + dt$, it follows that the dissociation probability is $-\mathcal{S}'(t) dt$. Note that the integral of $-\mathcal{S}'(t)$ from 0 to ∞ gives $\mathcal{S}(0) - \mathcal{S}(\infty) = 1 - 0 = 1$, as required. The mean node lifetime is the average of the time, t , weighted by the dissociation probability density, i.e. $-\mathcal{S}'(t)$:

$$- \int_0^{\infty} t \mathcal{S}'(t) dt = - \lim_{t \rightarrow \infty} t \mathcal{S}(t) + \int_0^{\infty} \mathcal{S}(t) dt. \quad (66)$$

Assuming $\mathcal{S}(t)$ approaches 0 faster than t^{-1} as $t \rightarrow \infty$, which is necessary for the integral of $\mathcal{S}(t)$ to exist, we recover the RHS of Equation 65.

We now briefly pause to relate the computations of this section to MFPT theory. The mean first-passage time, t_{Ω} , is the mean node lifetime. As mentioned in Section 1 following Equation 5, we do not explicitly calculate the conditional probability $P_{\Omega}(f, t|f_0)$, but only its integral over Ω . Comparison of Equations 5 and 65 shows that

$$\mathcal{S}(t) = \int_{\Omega} P_{\Omega}(f, t|f_0) df. \quad (67)$$

Note that $\mathcal{S}(t)$, thus t_Ω , is independent of $f_0 \in \Omega(0)$.

When intersecting dislocations first come into contact ($t = 0$) there is a finite probability that $f(0) > f_c(0)$, that is, no node is formed. This probability is the integral of the distribution $\mathcal{P}(f)$ from $f_c(0)$ to ∞ , which is identical to $\mathcal{D}_\tau(0)$. Averaging over all intersection events, the mean time until the mobile dislocation remobilizes, the mean remobilization time, t_r , is the product of the probability that $f_0 \in \Omega(0)$, that is, the probability of node formation

$$1 - \mathcal{D}_\tau(0) = \frac{1}{2} \left(1 + \operatorname{erf} \sqrt{\frac{\mathcal{E}}{k_B T}} \right) \quad (68)$$

and the mean node lifetime:

$$t_r = \frac{1}{2} \left(1 + \operatorname{erf} \sqrt{\frac{\mathcal{E}}{k_B T}} \right) \int_0^\infty \exp \left\{ -\frac{1}{\tau} \int_0^t \mathcal{D}_\tau(t') dt' \right\} dt. \quad (69)$$

4.1. Reverse Motion

For reverse dislocation motion, the probability that $f(t + \tau) < -f_c(-\hat{\sigma}, t + \tau)$ given $f(t) > -f_c(-\hat{\sigma}, t)$ is obtained by integrating $\mathcal{P}(f)$ over all $f < -f_c(-\hat{\sigma}, t)$; compare with Equation 46 and the subsequent discussion on forward motion. Since $\mathcal{P}(f)$ is an even function, the integration can also be taken from $f_c(-\hat{\sigma}, t)$ to ∞ , which is the same as for positive motion but with $\hat{\sigma} \rightarrow -\hat{\sigma}$. Thus the mean remobilization time for negative (reverse) motion is obtained from that for forward motion by simply reversing the sign of the effective applied stress.

4.2. Instantaneous Bow-out

Here we consider node dissolution for the simplified case of instantaneous bow-out or $B = 0$, neglecting inertial effects. Taking the limit $B \rightarrow 0$ ($t_B \rightarrow 0$) in Equation 53 gives

$$\mathcal{D}_\tau(\hat{\sigma}) = \frac{1}{2} \left\{ 1 - \operatorname{erf} \left[\sqrt{\frac{\mathcal{E}}{k_B T}} \left(1 - \frac{\hat{\sigma}}{\sigma_c} \right) \right] \right\}. \quad (70)$$

The corresponding mean node lifetime for positive glide is

$$\begin{aligned} \int_0^\infty t \mathcal{D}(t) dt &= \int_0^\infty t \exp \left(-\mathcal{D}_\tau(\hat{\sigma}) \frac{t}{\tau} \right) \mathcal{D}_\tau(\hat{\sigma}) \frac{dt}{\tau} \\ &= \frac{\tau}{\mathcal{D}_\tau(\hat{\sigma})}. \end{aligned} \quad (71)$$

Recall that the mean remobilization time is the product of the probability of node formation, $1 - \mathcal{D}_\tau(t = 0)$, and the mean node lifetime. We note that that $\mathcal{D}_\tau(t = 0) = \mathcal{D}_\tau(\hat{\sigma} = 0)$. The remobilization time for $B = 0$ (instantaneous bow-out) is

$$t_r = \frac{1 - \mathcal{D}_\tau(0)}{\mathcal{D}_\tau(\hat{\sigma})} \tau. \quad (72)$$

for positive glide; for reverse motion, $\hat{\sigma} \rightarrow -\hat{\sigma}$.

4.3. Low and High Stress Limits

We now consider the mean remobilization time from forward motion in two limiting cases: $\hat{\sigma}/\sigma_c \ll 1$ and $\hat{\sigma}/\sigma_c \gg 1$. The remobilization time is given by substituting Equation 53 into Equation 69. To streamline the notation, let $A = \sqrt{\mathcal{E}/k_B T}$, and change the integration variables to $z = t/t_B$, $z' = t'/t_B$. We obtain

$$t_r = \frac{1}{2} (1 + \operatorname{erf} A) t_B \int_0^\infty \exp \left[-\frac{t_B}{\tau} \int_0^z \frac{1}{2} \left\{ 1 - \operatorname{erf} \left[A \left(1 - \frac{\hat{\sigma}}{\sigma_c} (1 - e^{-z'}) \right) \right] \right\} dz' \right] dz. \quad (73)$$

Low Stress Limit . Here we obtain the mean remobilization time for low applied stresses, $\hat{\sigma}/\sigma_c \ll 1$. We can drop the $\exp(-z')$ dependence from the error function appearing in Equation 73. For cases of interest, A is a few times unity, thus $(1 + \text{erf} A)/2 \approx 1$, and $A(1 - \hat{\sigma}/\sigma_c)$ is sufficiently large that the error function is well approximated by its asymptotic expansion

$$\text{erf}(x) \sim 1 - \frac{1}{\sqrt{\pi}} \left\{ \frac{1}{x} - \frac{1}{2x^3} + \dots \right\} e^{-x^2}, x \rightarrow \infty. \quad (74)$$

We find

$$\frac{t_r}{\tau} = 2\sqrt{\pi}A \left(1 - \frac{\hat{\sigma}}{\sigma_c}\right) \exp \left\{ A^2 \left(1 - \frac{\hat{\sigma}}{\sigma_c}\right)^2 \right\} \quad (75)$$

Because $\hat{\sigma}/\sigma_c$ is much smaller than 1, it can be dropped from the factor $1 - \hat{\sigma}/\sigma_c$, and $(\hat{\sigma}/\sigma_c)^2$ can be dropped from the exponential. The remobilization time becomes

$$t_r^{-1} = \frac{1}{2\tau} \left(\frac{k_B T}{\pi \mathcal{E}} \right)^{\frac{1}{2}} \exp \left\{ -\frac{\mathcal{E}}{k_B T} \left(1 - 2\frac{\hat{\sigma}}{\sigma_c}\right) \right\}. \quad (76)$$

Neglecting dislocation drag, a reasonable approximation at low stresses, the strain rate is:

$$\dot{\epsilon} = \rho_m b \mathcal{L}_i t_r^{-1} = \frac{b \rho_m}{2\tau \sqrt{\pi \rho_i}} \left(\frac{k_B T}{\mathcal{E}} \right)^{\frac{1}{2}} \exp \left\{ -\frac{\mathcal{E}}{k_B T} \left(1 - 2\frac{\hat{\sigma}}{\sigma_c}\right) \right\}. \quad (77)$$

Equation 77 shows that we have recovered the usual Van't Hoff-Arrhenius exponential with $\mathcal{E}$ as the activation energy at $\hat{\sigma} = 0$ with the exception that our model includes an additional $\sqrt{T/\mathcal{E}}$ prefactor. This additional prefactor does not present significant deviations from TST in the applicable regime. This is discussed in detail in Appendix A. We would like to note that Equation 77 cannot be applied in the limit $\hat{\sigma} \rightarrow 0$ because reverse glide must be included so that $\dot{\epsilon} \rightarrow 0$ in the limit.

High Stress Limit . At very large stresses, $\hat{\sigma}/\sigma_c \gg 1$, we start with Equation 73 and approximate the z' integrand by expanding $1 - e^{-z'}$ to first order in z' :

$$\begin{aligned} & \frac{1}{2} \left\{ 1 - \text{erf} \left[A \left(1 - \frac{\hat{\sigma}}{\sigma_c} (1 - e^{-z'})\right) \right] \right\} \\ & \approx \frac{1}{2} \left\{ 1 - \text{erf} \left[A \left(1 - \frac{\hat{\sigma}}{\sigma_c} z'\right) \right] \right\}. \end{aligned} \quad (78)$$

Figure 3 shows that this is a good approximation and becomes more accurate as the stress increases.

If we let $s = \hat{\sigma}/\sigma_c$, $x' = sz'$, and $x = sz$, the remobilization time for large stresses may be written

$$t_r = \frac{t_B}{s} \int_0^\infty \exp \left[-\frac{t_B}{\tau s} \int_0^x \frac{1}{2} \{1 - \text{erf}[A(1 - x')]\} dx' \right] dx; \quad (79)$$

the x' integration can be carried out analytically:

$$\int_0^x \frac{1}{2} \{1 - \text{erf}[A(1 - x')]\} dx' = \frac{1}{2} \left\{ x + (1 - x) \text{erf}[A(1 - x)] - \text{erf} A + \frac{1}{A\sqrt{\pi}} \left[e^{-A^2(1-x)^2} - e^{-A^2} \right] \right\}. \quad (80)$$

For $x \ll 1$, we can substitute the asymptotic expansions of the error functions to obtain

$$\int_0^x \frac{1}{2} \{1 - \text{erf}[A(1 - x')]\} dx' \approx \frac{e^{-A^2}}{4\sqrt{\pi}A^3} (e^{2A^2x} - 1) \approx 0. \quad (81)$$

Similarly, for $x \gg 1$ we have

Figure 3: Comparison of integrand and approximation. The dashed red curve is the exact z' integrand, and the solid blue curve is our approximation. $A = 4$ in both cases.

$$\int_0^x \frac{1}{2} \{1 - \text{erf}[A(1 - x')]\} dx' \approx x - 1. \quad (82)$$

Using the approximations in Equations 81 and 82, we obtain

$$t_r \approx \frac{t_B}{s} \left\{ \int_0^1 \exp\left[-\frac{t_B}{\tau s} \cdot 0\right] dx + \int_1^\infty \exp\left[-\frac{t_B}{\tau s} (x - 1)\right] dx \right\} = \frac{t_B}{s} + \tau \quad (83)$$

Finally, we write the mean remobilization time for $\hat{\sigma}/\sigma_c \gg 1$ as:

$$\frac{t_r}{\tau} = \frac{t_B}{\tau} \frac{\sigma_c}{\hat{\sigma}} + 1 \quad (84)$$

5. Kinetic Equation

In this section we express the plastic strain rate in terms of the mean remobilization time derived in the previous section and the drag-limited transit time between network dislocations.

The standard prescription for calculating the mean dislocation velocity is

$$v = \frac{\mathcal{L}_i}{t_r + t_{T0}}, \quad (85)$$

where $\mathcal{L}_i = 1/\sqrt{\rho_i}$, t_r is given by Equation 69, and

$$t_{T0} = \frac{B\mathcal{L}_i}{b\hat{\sigma}} \quad (86)$$

is the nominal transit time, which is defined as the time required for a dislocation subject to effective applied stress $\hat{\sigma} > 0$, and drag force Bv , to glide the distance $\mathcal{L}_i$ to the nearest obstacles. Dislocation inertial effects are neglected in Equation 86. However, after bowing toward the next obstacles (forest dislocations) for time t_r , the actual transit time,

t_T , is less than t_{T0} ; hence, Equation 85 underestimates the mean dislocation velocity and plastic strain rate. The time t_T is calculated with a simple model in Appendix B and we obtain a reasonable estimate of the correction factor,

$$\zeta \equiv \frac{t_r + t_{T0}}{t_r + t_T} \geq 1, \quad (87)$$

that should be applied to Equation 85. We find

$$\zeta^{-1}(\hat{\sigma}) \approx 1 - \frac{1}{4} \exp \left\{ -\log_{10}^2 \left[\frac{t_r(\hat{\sigma})}{t_{T0}(\hat{\sigma})} \right] \right\}. \quad (88)$$

The mean dislocation velocity, and therefore the strain rate, is underestimated by approximately 25% for $t_r \approx t_{T0}$, but ζ approaches unity as the difference between t_r and t_{T0} increases.

As mentioned in Section 3.2, reverse dislocation glide due to the thermally-driven force fluctuations can be important at very low stresses. It was shown in Section 4 that the mean remobilization time for negative (reverse) motion is obtained from that for forward glide by simply reversing the sign of the applied effective stress. Therefore, for $B = 0$ and $\zeta = 1$, the mean dislocation velocity is

$$v = \mathcal{L}_i \left\{ \frac{1}{t_r(\hat{\sigma})} - \frac{1}{t_r(-\hat{\sigma})} \right\} \equiv \frac{\mathcal{L}_i}{t_r^{eff}(\hat{\sigma})}, \quad (89)$$

where the effective remobilization time $t_r^{eff}(\hat{\sigma})$ accounts for both forward and reverse dislocation glide. For $\hat{\sigma}/\sigma_c \ll (\mathcal{E}/k_B T)^{-1}$ it is simply

$$t_r^{eff}(\hat{\sigma}) = \frac{\tau}{2} \sqrt{\frac{\pi k_B T}{\mathcal{E}}} \exp \left(\frac{\mathcal{E}}{k_B T} \right) \frac{\sigma_c}{\hat{\sigma}}, \quad (90)$$

thus the velocity vanishes as $\hat{\sigma} \rightarrow 0$, as it should. For $B > 0$, Equation 89 is generalized to

$$v = \frac{\mathcal{L}_i}{t_r^{eff}(\hat{\sigma}) + B \mathcal{L}_i / b \hat{\sigma}}. \quad (91)$$

The correction factor ζ is trivially generalized to account for reverse glide by replacing $t_r(\hat{\sigma})$ in Equation 88 by $t_r^{eff}(\hat{\sigma})$. The Orowan equation with $v \rightarrow \zeta v$ and t_r from Equation 69 yields our kinetic equation

$$\dot{\epsilon} = \frac{\zeta b \rho_m}{\sqrt{\rho_i} t_r^{eff}(\hat{\sigma}) + B/b \hat{\sigma}}. \quad (92)$$

Both ζ and t_r^{eff} are functions of $\hat{\sigma}, \rho_m, \rho_i, \rho$ and T . The drag coefficient B depends on the mass density, the temperature, and the dislocation velocity during transit to the next immobile dislocation

$$v_T = \frac{b \hat{\sigma}}{B(v_T, \rho, T)}. \quad (93)$$

The solution of Equation 93 for v_T gives $B(v_T, \rho, T)$ in Equation 92. Recent MD simulations show that, at least in Al, Ni, and Al/Mg alloys, the fixed- T drag coefficient is constant at low velocities, but increases significantly and becomes velocity dependent at velocities of order half the transverse sound speed (Olmsted et al., 2005). However, a general understanding of the velocity dependence of B up to pressures of order 1000 GPa and temperatures from zero to the melt temperature has yet to be achieved. For this reason, and because the focus of this work is intersection node dissociation, we simply take B to be a constant. The generalization to a velocity-dependent drag coefficient will be the subject of future work.

At very low stresses satisfying $\hat{\sigma}/\sigma_c \ll (\mathcal{E}/k_B T)^{-1}$ we have $t_r(-\hat{\sigma}) \sim t_r(\hat{\sigma})$. Since the focus of this work is high stress and strain rate loading, where $t_r(\hat{\sigma}) \ll t_r(-\hat{\sigma})$, the contribution to the kinetic equation from reverse dislocation motion can be neglected, i.e. $t_r^{eff}(\hat{\sigma}) \approx t_r(\hat{\sigma})$.

Dislocation drag is negligible at sufficiently low strain rates: $\dot{\epsilon} \leq \dot{\epsilon}_D(\rho_m, \rho_i)$. For example, in copper, with $\dot{\epsilon}_D$ defined as that strain rate for which β/n (see Section 5.2) is less than 1/100, $\dot{\epsilon}_D(10^7 \text{ cm}^{-2}, 10^7 \text{ cm}^{-2}) = 10^3 \text{ s}^{-1}$ and

Figure 4: Flow stress of Cu at 300K and 1000K vs. $\dot{\epsilon}$ for $\rho_m = 10^9 \text{cm}^{-2}$, $\rho_i = 10^{10} \text{cm}^{-2}$, $P = 0$, and $B = 10^{-3} \text{Poise}$. Figure (b) also presents a comparison between the low stress limit for thermal activation (dashed lines), an Arrhenius exponential (Equation 75), and the entire kinetic equation (solid lines). Note that at strain rates of approximately $10^5 - 10^6 \text{s}^{-1}$ the Arrhenius form breaks down.

$\dot{\epsilon}_D(10^9 \text{cm}^{-2}, 10^9 \text{cm}^{-2}) = 10^6 \text{s}^{-1}$; in general, $\dot{\epsilon}_D$ increases as either ρ_m or ρ_i increases. At low strain rates where drag is unimportant we can take $B = 0$, i.e. $x \equiv t_r/t_{T0} \rightarrow \infty$, hence $\zeta = 1$. At stresses above σ_c but not so high that $t_r \approx \tau$, it follows that $x = 2\phi_c/\pi^2 \sim 1/10$ and $\zeta = 0.92 - 0.93$. For $\sigma = \sigma_c$ we find $x \approx \ln[\mathcal{E}(\rho, T)/k_B T]/2\pi^2$, which is at most a few tenths, and ζ is at most a 10–15 % correction. As a reasonable approximation we can take $\zeta = 1$.

Henceforth we take B to be a constant, neglect reverse dislocation glide, and set $\zeta = 1$. Our kinetic equation then assumes the simpler form

$$\dot{\epsilon} = \frac{b\rho_m}{\sqrt{\rho_i} t_r(\hat{\sigma}) + B/b \hat{\sigma}}. \quad (94)$$

The flow stress of copper versus plastic strain rate at two temperatures, $T = 300\text{K}$ and $T = 1000\text{K}$, for fixed mobile and immobile dislocation densities at zero pressure is plotted in Figure 4. Note that the temperature dependence is very weak at stresses above σ_c . Figure 4 is strikingly similar to Figure 11 for the PTW model (Preston et al., 2003).

5.1. Inverse Kinetic Equation: Stress as a Function of Plastic Strain Rate, Dislocation Densities, and Temperature

Our kinetic equation gives the plastic strain rate as a function of the applied stress, mobile and immobile dislocation densities, the material density, and the temperature, but numerical simulations generally require the stress as a function of the strain rate. In this section we approximately solve our kinetic equation for the stress. We do so by constructing a smooth interpolation between the low and high strain rate regimes for which we have simple but accurate analytic approximations, namely Equations 75 and 84.

The first step toward inverting our kinetic equation is constructing a further approximation to our expression for $t_r(\hat{\sigma})$ at low strain rates, Equation 75, which we repeat here for the convenience of the reader:

$$\frac{t_r}{\tau} = 2\sqrt{\pi}A \left(1 - \frac{\hat{\sigma}}{\sigma_c}\right) \exp \left\{ A^2 \left(1 - \frac{\hat{\sigma}}{\sigma_c}\right)^2 \right\}. \quad (95)$$

Equation 95 cannot be inverted analytically, and its numerical inversion poses several difficulties, so we obtain an approximate inverse. We define the variables

$$\chi = \log_{10} \left(\frac{\tau}{t_r} \right), y = \log_{10} \left(\frac{\hat{\sigma}}{\sigma_c} \right). \quad (96)$$

Taking the natural logarithm of Equation 95 yields

$$\begin{aligned}\frac{\chi}{\log_{10} e} &= \ln\left(\frac{1}{2A\sqrt{\pi}}\right) - \{\ln(1 - 10^y) + A^2(1 - 10^y)^2\} \\ &\equiv \ln\left(\frac{1}{2A\sqrt{\pi}}\right) - h(y).\end{aligned}\quad (97)$$

At low strain rates, $y < 0$. The function $h(y) \sim A^2$ for $y \rightarrow -\infty$, and is roughly linear with negative slope for $-1 \leq y < 0$ (h has a logarithmic singularity at $y = 0$), i.e. for $\sigma_c/10 \leq \hat{\sigma} < \sigma_c$. In this linear regime we find that for $A \geq 3$

$$h(y) \approx -A^2 y - 5/2, \quad (98)$$

hence

$$y \approx \frac{1}{A^2} \left\{ \frac{\chi}{\log_{10} e} + \ln(2A\sqrt{\pi}) - \frac{5}{2} \right\} \approx \frac{\chi}{A^2 \log_{10} e} \quad (99)$$

since $|\chi| \gg 1$ at low strain rates. Using the definitions in Equation 96, this equation may be written as

$$\frac{\tau}{t_r} \approx \left(\frac{\hat{\sigma}}{\sigma_c} \right)^{A^2 \log_{10} e}, \quad (100)$$

and using the kinetic equation with $B = 0$ (low strain rates) this becomes

$$\frac{\hat{\sigma}}{\sigma_c} \approx \left(\frac{\dot{\epsilon} \tau \sqrt{\rho_i}}{b \rho_m} \right)^{1/A^2 \log_{10} e}, \quad (101)$$

or equivalently

$$y \approx \frac{1}{A^2 \log_{10} e} \left[x - \log_{10} \left(\frac{b \rho_m}{\sqrt{\rho_i} \tau s^{-1}} \right) \right] \equiv m_- x + b_-, \quad (102)$$

where

$$x = \log_{10} \left(\frac{\dot{\epsilon}}{s^{-1}} \right). \quad (103)$$

At very high rates and stresses, $t_r(\sigma)$ is given by Equation 84

$$\frac{t_r}{\tau} = \frac{t_B}{\tau} \frac{\sigma_c}{\hat{\sigma}} + 1. \quad (104)$$

This can be simplified by dropping the "1", which is a good approximation unless $\hat{\sigma}/\sigma_c \gg 1$. At high stresses the kinetic equation is

$$\frac{\hat{\sigma}}{\sigma_c} \approx \frac{\dot{\epsilon}}{b \rho_m} \left(\sqrt{\rho_i} t_B + \frac{B}{b \sigma_c} \right), \quad (105)$$

or

$$y \approx x + \log_{10} \left[\frac{s^{-1}}{b \rho_m} \left(\sqrt{\rho_i} t_B + \frac{B}{b \sigma_c} \right) \right] \equiv m_+ x + b_+. \quad (106)$$

We now obtain a simple function that interpolates between $y = m_- x + b_-$ at low rates and $y = m_+ x + b_+$ at high strain rates. The slope of the interpolation function smoothly varies from m_- to m_+ over an interval of width $2\Delta x$ around x_c , the intersection point of the low- and high-rate straight lines:

$$\frac{dy}{dx} = \frac{1}{2} \left\{ m_+ + m_- + (m_+ - m_-) \tanh \left[\frac{(x - x_c)}{\Delta x} \right] \right\}, \quad (107)$$

where

$$x_c = \frac{b_- - b_+}{m_+ - m_-} > 0. \quad (108)$$

Figure 5: Mobile and immobile dislocation density (a, b), material density (c), and temperature (d) dependence of $\hat{\sigma}/\sigma_c$ as given by the inverse kinetic equation. Note the smooth transition between low and high strain rate regimes. The immobile and mobile densities, when not being varied, are 10^8 cm^{-2} .

Integrating and choosing the integration constant to ensure that $y(x)$ asymptotes to the low- and high-rate linear approximations we find

$$y(x) = \frac{1}{2} [(m_+ + m_-)x + b_+ + b_-] + (m_+ - m_-) \frac{\Delta x}{2} \ln \left[2 \cosh \left(\frac{x - x_c}{\Delta x} \right) \right]. \quad (109)$$

The width, $2\Delta x$, is roughly the range of x values over which the interpolation Equation 109 is curved, i.e. deviates from the low- and high-rate straight lines. Comparisons of Equation 109 with precise numerical results for dislocation densities from 10^6 cm^{-2} to 10^{12} cm^{-2} show that excellent agreement is realized by setting $\Delta x = 3/4$.

Figure 5 illustrates the dependence of $\hat{\sigma}/\sigma_c$ on strain rate, dislocation densities, mass density, and temperature as given by the inverse kinetic equation. In all four figures, the low-strain-rate and high-strain-rate regimes are clearly distinguished; the inverse kinetic equation provides a smooth transition between these two regimes in all cases. The largest effects can be seen from variations in the mobile and immobile dislocation densities. The inverse kinetic equation exhibits a weak dependency of $\hat{\sigma}/\sigma_c$ on material density, and essentially no dependency on temperature. It is interesting to note that variations in the dislocation densities can drastically change the location of the transition from the low-strain-rate regime to the high-strain-rate regime.

5.2. Summary of Key Equations and Parameters

In this short subsection, we briefly summarize key equations and parameters used in our derivation for the convenience of the reader in Tables 1 and 2, respectively.

Table 1: Key equations derived in preceding sections.

Equation	
Kinetic Equation (Equation 92)	$\dot{\epsilon} = \frac{\zeta b \rho_m}{\sqrt{\rho_i} t_r^{eff}(\hat{\sigma}) + B/b \hat{\sigma}}$
Effective Remobilization Time (Equation 90)	$t_r^{eff}(\hat{\sigma}) = \frac{\tau}{2} \sqrt{\frac{\pi k_B T}{\mathcal{E}}} \exp\left(\frac{\mathcal{E}}{k_B T}\right) \frac{\sigma_c}{\hat{\sigma}}$
Remobilization Time (Equation 73)	$t_r = \frac{1}{2} (1 + \operatorname{erf} A) t_B \int_0^\infty \exp\left[-\frac{t_B}{\tau} \int_0^z \frac{1}{2} \left\{1 - \operatorname{erf}\left[A\left(1 - \frac{\hat{\sigma}}{\sigma_c} (1 - e^{-z'})\right)\right]\right\} dz'\right] dz$
Low Stress Limit (Equation 76)	$t_r^{-1} = \frac{1}{2\tau} \left(\frac{k_B T}{\pi \mathcal{E}}\right)^{\frac{1}{2}} \exp\left\{-\frac{\mathcal{E}}{k_B T} \left(1 - 2 \frac{\hat{\sigma}}{\sigma_c}\right)\right\}$
High Stress Limit (Equation 84)	$\frac{t_r}{\tau} = \frac{t_B}{\tau} \frac{\sigma_c}{\hat{\sigma}} + 1$
Inverse Kinetic Equation (Equation 109)	$\log_{10}\left(\frac{\hat{\sigma}}{\sigma_c}\right) = \frac{1}{2} [(m_+ + m_-) x + b_+ + b_-] + (m_+ - m_-) \frac{\Delta x}{2} \ln\left[2 \cosh\left(\frac{x - x_c}{\Delta x}\right)\right]$
Low Stress Limit (Equation 102)	$\log_{10}\left(\frac{\hat{\sigma}}{\sigma_c}\right) \approx \frac{1}{A^2 \log_{10} e} \left[\log_{10}\left(\frac{\dot{\epsilon}}{s^{-1}}\right) - \log_{10}\left(\frac{b \rho_m}{\sqrt{\rho_i} \tau s^{-1}}\right)\right] \equiv m_- x + b_-$
High Stress Limit (Equation 106)	$\log_{10}\left(\frac{\hat{\sigma}}{\sigma_c}\right) \approx \log_{10}\left(\frac{\dot{\epsilon}}{s^{-1}}\right) + \log_{10}\left[\frac{s^{-1}}{b \rho_m} \left(\sqrt{\rho_i} t_B + \frac{B}{b \sigma_c}\right)\right] \equiv m_+ x + b_+$

Table 2: Model parameters. Material specific parameters are presented for OFE copper.

Model Parameters		
g_b	1/5	
κ	1	
k_B	8.6173×10^{-5}	eV K ⁻¹
$\tau \sim \bar{\nu}^{-1}$	$\sim 10^{-13}$	s
Material Properties		
ϕ_c	0.5	rad
b	0.255	nm
B	$10^{-4} - 10^{-3}$	Poise
ρ_0 (at 0 K)	9.020	g cm ⁻³
T_{melt} (at ρ_0)	1824	K
G (at ρ_0)	52.4	GPa
γ_1	1.87	(g/cc) ^{$\frac{1}{3}$}
γ_2	2.31×10^4	(g/cc) ^{q}
q	4.7	
β	0.20	

5.3. Drag versus Strain Rate

The kinetic equation, Equation 94, can be expressed in the form

$$\frac{b \rho_m}{\dot{\epsilon}} = \sqrt{\rho_i} t_r(\dot{\sigma}) + \frac{B}{b \dot{\sigma}}. \quad (110)$$

The B -dependent term is certainly negligible at sufficiently low strain rates, but how low? To answer this question we approximately solve Equation 110 for $\dot{\sigma}$. Since we are only interested in determining the strain rate at which the drag-limited transit time becomes comparable to the thermally-driven remobilization time, it is sufficient to approximate $t_r(\dot{\sigma})$ in Equation 110 by $t_r(\dot{\sigma})$ from Equation 101 for low strain rates. Substituting Equation 101 in Equation 110 results in the transcendental equation

$$z^n + \beta z = 1, \quad (111)$$

where

$$\begin{aligned} n &= A^2 \log_{10} e \gg 1, \\ z &= \frac{\sigma_c}{\dot{\sigma}} \alpha^{-\frac{1}{n}}, \\ \alpha &= \frac{b \rho_m}{\tau \dot{\epsilon} \sqrt{\rho_i}}, \\ \beta &= \frac{B}{b \tau \sigma_c \sqrt{\rho_i}} \alpha^{\frac{1}{n}-1}. \end{aligned} \quad (112)$$

The value of $\beta \sim B$ at low strain rates ($\leq 10^4 \text{ s}^{-1}$) can vary from $\sim 10^{-10}$ to $\sim 10^2$, hence the series solution to Equation 111

$$z = 1 - \frac{1}{n}\beta - \frac{n-3}{2n^2}\beta^2 - \dots \quad (113)$$

is of limited utility. However, we can approximate the sum of the series with the Padé approximant

$$z \approx \frac{2n + \beta}{2n + 3\beta + \beta^2} \quad (114)$$

whose Taylor series expansion agrees with the first three terms of Equation 113, and for which $z \sim \beta^{-1}$ as $\beta \rightarrow \infty$ (in Equation 111, large β implies $z \ll 1$, thus z^n can be dropped). By definition, drag effects are negligible at strain rates below $\dot{\epsilon}_D(\rho_m, \rho_i)$ which corresponds to $\beta/n = r \ll 1$; in that case, $z \approx 1$ and Equation 101 is recovered. Once again we consider copper and assume $B = 5 \times 10^{-4}$ Poise. We define $\dot{\epsilon}_D$ to be the rate for which $\beta/n = 1/100$ (we find that β/n and β^2/n are equal to $1/100$ at roughly the same strain rate). For $\rho_m = \rho_i = \rho_D$, we have $\dot{\epsilon}_D \approx 10^{-6} \rho_D^{4/3}$; e.g. $\dot{\epsilon}_D = 2 \times 10^3 \text{ s}^{-1}$ at 10^7 cm^{-2} and $\dot{\epsilon}_D = 10^6 \text{ s}^{-1}$ at 10^9 cm^{-2} . If $\rho_{D2} > \rho_{D1}$ then $\dot{\epsilon}_D(\rho_{D1}) \leq \dot{\epsilon}_D(\rho_m, \rho_i) \leq \dot{\epsilon}_D(\rho_{D2})$ for $\rho_{D1} \leq \rho_m, \rho_i \leq \rho_{D2}$.

6. Density and Temperature Dependence

Our kinetic equation, Equation 92, is applicable at the very high plastic strain rates characteristic of explosively driven systems and hypervelocity impacts. However, in addition to high deformation rates, explosive drive and high-velocity impacts also involve high pressures, in some cases exceeding 1000 GPa, and temperatures up to melt. In this section we address the material (mass) density and temperature dependence of the various physical quantities appearing in our kinetic equation. Throughout this section, ρ_0 will denote an arbitrary reference density, and T_m is the melt temperature.

6.1. Parameters, Burgers Vector, and Dislocation Density

The dimensionless parameter κ , and the critical bow-out angle ϕ_c , are assumed to be density and temperature independent. Quantities with dimensions of lengthⁿ – Burgers vector and dislocation density – scale in an obvious way with density, i.e., as $\rho^{-n/3}$. Specifically, the density dependence of the Burgers vector is

$$b(\rho) = b(\rho_0) \left(\frac{\rho_0}{\rho} \right)^{1/3}. \quad (115)$$

The length of dislocation line in a fixed volume decreases as $\rho^{-1/3}$ while the volume decreases as $1/\rho$, hence

$$\rho_{m,i}(\rho) = \rho_{m,i}(\rho_0) \left(\frac{\rho}{\rho_0} \right)^{2/3}. \quad (116)$$

6.2. Shear Modulus, Line Tension, Critical Stress, and Activation Energy

Preston and Wallace (Preston and Wallace, 1992) modeled the temperature- and density-dependent shear modulus as the product of the density-dependent zero-temperature modulus and a linearly decreasing function of the reduced temperature T/T_m

$$G(\rho, T) = G(\rho, 0) \left(1 - \beta \frac{T}{T_m(\rho)} \right). \quad (117)$$

The density-dependent melting temperature can be obtained from the Lindemann melting criterion (Gilvarry's law)

$$\frac{d \ln T_m(\rho)}{d \ln \rho} = 2 \left(\gamma(\rho) - \frac{1}{3} \right), \quad (118)$$

given the density-dependent Grüneisen parameter, $\gamma(\rho)$. An analytic model of $\gamma(\rho)$ has been constructed by Burakovsky and Preston (Burakovsky and Preston, 2004)

$$\gamma(\rho) = \frac{1}{2} + \frac{\gamma_1}{\rho^{1/3}} + \frac{\gamma_2}{\rho^q}, \quad \gamma_1, \gamma_2, q = \text{constant}, q > 1, \quad (119)$$

through consideration of its low- and ultrahigh-pressure limits. This analytic form was obtained under the assumptions: (1) $\gamma \sim 1/2$ as $\rho \rightarrow \infty$, (2) γ is an analytic function of $x \equiv 1/\rho^{1/3}$, essentially the interatomic distance, and (3) the coefficient of x in the Taylor expansion for γ is non-zero. For copper, $\gamma_1 = 1.87 \text{ (g/cc)}^{1/3}$, $\gamma_2 = 2.31 \times 10^4 \text{ (g/cc)}^q$, and $q = 4.7$. Equations 118 and 119 yield a model for the melt temperature as a function of density

$$T_m(\rho) = T_m(\rho_0) \left(\frac{\rho}{\rho_0} \right)^{1/3} \exp \left\{ 6\gamma_1 \left(\frac{1}{\rho_0^{1/3}} - \frac{1}{\rho^{1/3}} \right) + \frac{2\gamma_2}{q} \left(\frac{1}{\rho_0^q} - \frac{1}{\rho^q} \right) \right\}. \quad (120)$$

The melt temperature and the shear modulus along the solidus approximately satisfy the relation

$$\frac{G(\rho, T_m(\rho))}{\rho T_m(\rho)} = \frac{G(\rho_0, T_m(\rho_0))}{\rho_0 T_m(\rho_0)}, \quad (121)$$

which can be justified on the basis of either the theory of dislocation mediated melting or from the theory of the Debye solid (Burakovsky et al., 2003).

Combining Equations 117, 120, and 121 we obtain

$$G(\rho, 0) = G(\rho_0, 0) \left(\frac{\rho}{\rho_0} \right)^{4/3} \exp \left\{ 6\gamma_1 \left(\frac{1}{\rho_0^{1/3}} - \frac{1}{\rho^{1/3}} \right) + \frac{2\gamma_2}{q} \left(\frac{1}{\rho_0^q} - \frac{1}{\rho^q} \right) \right\}, \quad (122)$$

which completes our model for the density- and temperature-dependent shear modulus.

Given $G(\rho, T)$, we also know the density and temperature dependence of the mean dislocation line tension

$$\mathcal{T}(\rho, T) = \mathcal{T}(\rho_0, T) \left(\frac{\rho_0}{\rho} \right)^{2/3} \frac{G(\rho, T)}{G(\rho_0, T)}; \quad (123)$$

Figure 6: Immobile dislocation density, material density, and temperature dependence of the dislocation line tension. In Figure (a) $T = 300\text{K}$ and in Figure (b) $\rho = \rho_0$.

$\mathcal{T}(\rho_0, T)$ is given by Equation 10, which shows that $\mathcal{T} \sim \ln(1/\sqrt{\rho_i})$ at all densities and temperatures. At very high compressions, $\mathcal{T}(\rho, T) \sim \rho^{2/3}$. Figure 6 shows the variation in the dislocation line tension due to changes in the material density, temperature, and network dislocation density. Temperature changes have a minor effect on the line tension. The material density, on the other hand, has a much larger effect, particularly at low immobile dislocation densities. In order to quantify the effects of variations in both the mass density and the network dislocation density on the line tension, we calculate $\mathcal{T}(\rho + \Delta\rho, T = 0) - \mathcal{T}(\rho, T = 0) \equiv \Delta\mathcal{T}$ at fixed ρ_i to lowest order in $\Delta\rho$ using Equation 122 for the density dependence of the shear modulus at $T = 0$:

$$\Delta\mathcal{T} = \frac{5}{32\pi} G'(\rho, 0) b^2 \ln\left(\frac{1}{b^2 \rho_i}\right) \Delta\rho + O(\Delta\rho^2). \quad (124)$$

This result indicates that the change in the line tension for fixed $\Delta\rho$ increases as ρ_i decreases. In addition, since G' increases monotonically with ρ , $\Delta\mathcal{T}$ also increases monotonically with ρ for fixed ρ_i and $\Delta\rho$. Both of these trends are seen in Figure 6.

Equations 10, 117, 122, and 123 provide the density-temperature dependence of the critical stress, $\sigma_c = 2\phi_c \mathcal{T}(\rho, T) \sqrt{\rho_i} / b(\rho)$. Figure 7 shows the effect of variations in material density and temperature on the ρ_i -dependence of σ_c . As for the dislocation line tension, the temperature, which enters σ_c only through the shear modulus, has little effect on the behavior of the critical stress as the immobile dislocation density increases. As the material density increases, the critical stress also noticeably increases; asymptotically, $\sigma_c(\rho) \sim \rho^{4/3}$. The critical stress also significantly increases with increasing immobile dislocation density; Equation 11 shows that the critical stress varies with the immobile dislocation density as $\sqrt{\rho_i} \ln(1/\sqrt{\rho_i})$.

Figure 7: Immobile dislocation density, material density, and temperature dependence of the critical stress. In Figure (a) $T = 300\text{K}$ and in Figure (b) $\rho = \rho_0$.

Figure 8: Immobile dislocation density, material density, and temperature dependence of the activation energy. In Figure (a) $T = 300\text{K}$ and in Figure (b) $\rho = \rho_0$.

Reference to Equation 54 for the activation energy, $\mathcal{E}$, at $\hat{\sigma} = 0$ shows that it is proportional to the product of the force and distance characteristic of intersecting dislocations, namely, the line tension and the length of the Burgers vector: $\mathcal{E} \sim \mathcal{T} b$. This product varies as $G b^3$, which is proportional to the elastic strain energy in length b of a dislocation. As the material is compressed and atoms are pushed closer together, the strain energy, and therefore the activation energy, must increase. Specifically, the density and temperature dependencies of $\mathcal{E}$ are given by

$$\mathcal{E}(\rho, T) = \mathcal{E}(\rho_0, T) \frac{\rho_0}{\rho} \frac{G(\rho, T)}{G(\rho_0, T)}. \quad (125)$$

Asymptotically, $\mathcal{E} \sim \rho^{1/3}$. Figure 8 shows the material density and temperature dependence of $\mathcal{E}$. Once again, temperature variations have little effect, but changes in the material density have a significant impact on the activation energy. The dependence of the activation energy on ρ_i is the same as that of the line tension, $\mathcal{E} \sim \ln(1/\rho_i)$, thus $\mathcal{E}$ decreases linearly with $\ln \rho_i$ at any density, as seen in Figure 8.

6.3. Time Scale of Force Fluctuations

The time scale of the force fluctuations between intersecting dislocations, τ , is of order the inverse mean phonon frequency. Lattice anharmonicity leads to a density dependence of the phonon frequencies, ν_i ; hence, τ is density dependent. We make two approximations in estimating the density dependence of τ . First, we neglect the temperature dependence and employ the following relation which holds at zero temperature:

$$\frac{\partial}{\partial \ln \rho} \langle \ln \nu_i \rangle_{BZ} = \gamma(\rho). \quad (126)$$

The average is over the first Brillouin zone, and $\gamma(\rho)$, the Grüneisen parameter, is given by Equation 119. Our second approximation is

$$\langle \ln v_i \rangle_{BZ} \approx \ln \tau^{-1}. \quad (127)$$

Equations 119, 126, and 127 give

$$-\frac{\partial \ln \tau}{\partial \ln \rho} = \frac{1}{2} + \frac{\gamma_1}{\rho^{1/3}} + \frac{\gamma_2}{\rho^q}, \quad (128)$$

which integrates to

$$\tau(\rho) = \tau(\rho_0) \left(\frac{\rho_0}{\rho} \right)^{1/2} \exp \left\{ 3 \gamma_1 \left(\frac{1}{\rho_0^{1/3}} - \frac{1}{\rho^{1/3}} \right) + \frac{\gamma_2}{q} \left(\frac{1}{\rho_0^{1/3}} - \frac{1}{\rho^{1/3}} \right) \right\}. \quad (129)$$

For copper, $\tau(\rho)/\tau(\rho_0)$ increases to 1.3 at 50% compression, reaches 1.6 at the enormous compression of 5.8, and decreases as $\rho^{-1/2}$ as $\rho \rightarrow \infty$. The uncertainty in the value of $\tau(\rho_0)$ is of order the calculated density dependence, which is weak, so we ignore the dependence of τ on ρ and take it to be a constant.

6.4. Dislocation Drag Coefficient and Bow-out Time

The calculation of the density, temperature, and dislocation velocity dependence of the drag coefficient is beyond the scope of this paper, and the subject of current research. At this time we approximate B as a constant with a value $\sim 10^{-4} - 10^{-3}$ Poise (Al'shitz and Indenbom, 1975). In this approximation, the density dependence of the bow-out time $t_B = B/\pi \mathcal{T} \rho_i$ is due only to $\mathcal{T}$ and ρ_i ; $t_B \sim \rho^{-4/3}$ as $\rho \rightarrow \infty$.

7. Viscous Flow at High Stresses and Strain Rates

For stresses satisfying $\sigma_c < \hat{\sigma} < (t_B/\tau) \sigma_c$, Equation 84 for the node lifetime simplifies to

$$t_r = t_B \frac{\sigma_c}{\hat{\sigma}}. \quad (130)$$

Using Equation 130, the kinetic equation with $\hat{\sigma} \approx \sigma$ may be written

$$\sigma = \frac{1}{b \rho_m} \left(t_B \sigma_c \sqrt{\rho_i} + \frac{B}{b} \right) \dot{\epsilon}, \quad (131)$$

thus, the stress is proportional to the strain rate, as for a Newtonian fluid. In other words, our kinetic equation predicts viscous, fluid-like flow at very high strain rates. The dynamic viscosity, η , is defined by

$$s_{ij} = \eta \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) = 2 \eta \dot{\epsilon}_{ij}, \quad (132)$$

where u_i is the fluid (material) velocity. In terms of $\sigma = (3 s_{ij} s_{ij} / 2)^{1/2}$ and $\dot{\epsilon} = (2 \dot{\epsilon}_{ij} \dot{\epsilon}_{ij} / 3)^{1/2}$, Equation 132 assumes the form

$$\sigma = 3 \eta \dot{\epsilon}. \quad (133)$$

Equations 131 and 133 give the high strain rate dynamic viscosity

$$\eta = \frac{1}{3 b \rho_m} \left(t_B \sigma_c \sqrt{\rho_i} + \frac{B}{b} \right) = \frac{1}{3} \left(1 + \frac{2}{\pi^2} \phi_c \right) \frac{B}{b^2 \rho_m}. \quad (134)$$

In general, the term involving ϕ_c is of order 1/10 (e.g., $\phi_c = 1/2$ for copper), hence

$$\eta \approx \frac{B}{3 b^2 \rho_m}. \quad (135)$$

This result for the shear viscosity is comparable to that obtained by Johnson (Johnson, 1981):

$$\eta \approx \frac{B}{2 b^2 \rho_m}. \quad (136)$$

For $B = 10^{-4} - 10^{-3}$ Poise (Al'shitz and Indenbom, 1975), $\rho_m = 10^6 - 10^{10} \text{ cm}^{-2}$, and $b = 2.55 \times 10^{-8} \text{ cm}$ (copper), Equation 135 gives $\eta = 5 - 5 \times 10^5$ Poise. For comparison, at room temperature, the dynamic viscosity of water is about 100 Poise while that of glycerol is approximately 10^5 Poise.

8. Summary

We have presented a detailed derivation of a kinetic equation that describes the plastic strain rate as a function of mobile and immobile dislocation densities, material density, and temperature. In addition, we have obtained an approximate inverted form of this equation that gives the stress as a function of strain rate, a form that will be useful for numerical implementation. The kinetic equation is applicable to strain rates in excess of 10^{12}s^{-1} because our description of thermal activation is based on MFPT theory rather than the commonly used Van't Hoff Arrhenius equation. The MFPT-based stress-strain response exhibits the sharp, non-Arrhenius upturn without including high-rate phonon drag; in the $\log(\dot{\epsilon}) - \log(\sigma)$ plane our kinetic equation is linear in the low- and high-rate limits with slopes of $(\log_{10} e \cdot \mathcal{E}/k_B T)^{-1} \ll 1$ and unity, respectively (Figure 5).

The current research of the authors includes the formulation of ordinary differential equations for the evolution of the mobile and immobile dislocation densities. The combination of the evolution equations and the kinetic equation developed here will constitute a complete model of dislocation-mediated plastic deformation from quasi-static to very high strain rates, pressures from ambient to around 1000 GPa, and temperatures up to melt.

9. Acknowledgements

AH and DLP gratefully acknowledge support from the Advanced Simulation and Computing (ASC) - Physics and Engineering Models (PEM) Program at Los Alamos National Laboratory (LANL). LANL is operated by Los Alamos National Security, LLC, for the National Nuclear Security Administration of the US Department of Energy.

Appendix A: Comparison of Low-Rate Limit and Van't Hoff-Arrhenius Equation

As shown in the main text, we recovered the usual Van't Hoff-Arrhenius exponential in the low strain rate regime with the exception of an additional prefactor. We mentioned that this prefactor does not result in a significant departure from transition state theory (TST) at low strain rates. In this appendix, we have completed a few simple calculations to prove this. All relevant equations from the main text have been repeated here for the convenience of the reader.

Our exact expression for the remobilization time, t_r is given as (Equation 73 in the main text)

$$t_r = \frac{1}{2} (1 + \text{erf} A) t_B \int_0^\infty \exp \left[-\frac{t_B}{\tau} \int_0^z \frac{1}{2} \left\{ 1 - \text{erf} \left[A \left(1 - \frac{\hat{\sigma}}{\sigma_c} (1 - e^{-z'}) \right) \right] \right\} \right] dz' dz, \quad (\text{A.1})$$

where t_B is the bow-out time (Equation 49 in the main text), τ is the inverse mean phonon frequency, and σ_c is the critical stress (Equation 11 in the main text). The flow stress $\hat{\sigma} = \sigma - \sigma_b$ with σ the true applied stress and σ_b the back stress. Finally, $A = \sqrt{\mathcal{E}/k_B T}$ where $\mathcal{E}$ is the activation energy at zero applied stress, T is the temperature and k_B is the Boltzmann constant. At low stresses, the above equation simplifies to (Equation 76 in the main text)

$$t_r^{-1} = \frac{1}{2\tau} \left(\frac{k_B T}{\pi \mathcal{E}} \right)^{\frac{1}{2}} \exp \left\{ -\frac{\mathcal{E}}{k_B T} \left(1 - 2 \frac{\hat{\sigma}}{\sigma_c} \right) \right\}. \quad (\text{A.2})$$

The corresponding plastic strain rate is (Equation 77 in the main text)

$$\dot{\epsilon} = \rho_m b \mathcal{L}_i t_r^{-1} = \frac{b \rho_m}{2\tau \sqrt{\pi \rho_i}} \left(\frac{k_B T}{\mathcal{E}} \right)^{\frac{1}{2}} \exp \left\{ -\frac{\mathcal{E}}{k_B T} \left(1 - 2 \frac{\hat{\sigma}}{\sigma_c} \right) \right\}. \quad (\text{A.3})$$

As mentioned in the main text, this expression cannot be applied in the limit $\hat{\sigma} \rightarrow 0$ because reverse glide must be included so that $\dot{\epsilon} \rightarrow 0$ in the limit. Although we have obtained the usual Van't Hoff-Arrhenius exponential, which is characteristic of TST, our derivation yields the additional $\sqrt{k_B T/\mathcal{E}}$ prefactor.

First we would like to point out that while TST is a widely accepted approach for modeling the thermal activation aspects of dislocation dynamics, it was not derived specifically for dislocation intersections, but rather chemical reactions. TST is founded on equilibrium thermodynamics, which cannot be rigorously justified for dislocation dynamics.

Figure A.1: Comparison of Equation A.3 (solid lines) and its approximation in which the $\sqrt{k_B T/\mathcal{E}}$ prefactor is eliminated (dashed lines) for 0K, 300K and 800K. We have used $\rho_i = 2 \times 10^{12} \text{cm}^{-2}$ and $\rho_m = 10^8 \text{cm}^{-2}$, which yield close agreement with stress-strain data in copper.

Nevertheless, TST provides an adequate description of the physics of dislocation intersection at low to modest strain rates. Therefore, the low-rate limit, Equation A.3, of our kinetic equation should be essentially equivalent to a TST form. We now explicitly show that this is indeed the case.

We slightly modify Equation A.3 by changing the exponent of the prefactor from $1/2$ to $\alpha/2$; for $\alpha = 1$ we recover Equation A.3 and for $\alpha = 0$ the prefactor is eliminated, as is the case for TST. Solving for σ

$$\sigma = \frac{1}{2} \sigma_c(\rho_i) \left\{ 1 + \frac{k_B T}{\mathcal{E}(\rho_i, T)} \left[\frac{\log_{10} \dot{\epsilon}}{\log_{10} e} - \ln \left(\frac{b \rho_m}{2\tau \sqrt{\pi} \rho_i} \right) + \frac{\alpha}{2} \ln \left(\frac{\mathcal{E}(\rho_i, T)}{k_B T} \right) \right] \right\} + \sigma_b(\rho_i), \quad (\text{A.4})$$

where b is the Burgers vector, ρ_m is the mobile dislocation density, and ρ_i is the immobile dislocation density. In Figure A.1 we compare the flow stress of copper for $\alpha = 1$ (solid lines) with that for $\alpha = 0$ (dashed lines) at strain rates from 1s^{-1} to 10^4s^{-1} at temperatures of 0K, 300K and 800K. There are of course differences due to the prefactor, but we emphasize that the differences are small. For example, at 10^3s^{-1} and 300K, the stresses differ by only 20MPa, which is less than a 4% difference. Even at 800K the difference in stress is only 37MPa. Furthermore, the variations with strain rate or temperature are the same for Equation A.3 and TST.

We now explicitly demonstrate that, to a very good approximation, our Equation A.3 is equivalent to TST. The TST constitutive relation that is most closely related to Equation A.3 is obtained by dropping the prefactor, i.e. setting $\alpha = 0$ in Equation A.4, and rescaling the mobile dislocation density from ρ_m to $\rho_m \langle \sqrt{k_B T/\mathcal{E}} \rangle_T$, where $\langle \dots \rangle_T$ is a thermal average. For $T \in [300\text{K}, T_m]$ and $\rho_i = 2 \times 10^{12} \text{cm}^{-2}$ (as in Figure A.1), we find $\langle \sqrt{k_B T/\mathcal{E}} \rangle_T = 0.41$. In Figure A.2 we compare our Equation A.3 (solid lines) with this TST constitutive relation (dashed lines). The agreement is truly excellent. Hence, the prefactor in Equation A.3 does not induce any significant departures from TST.

Our kinetic equation, which is based on non-equilibrium physics and is specific to dislocation intersection, is indistinguishable from TST at low to modest strain rates. However, in marked contrast to TST, our equation is valid up to the highest plastic strain rates of interest, that is, $\dot{\epsilon} \sim 10^{12} \text{s}^{-1}$.

Appendix B: Mean Dislocation Velocity Correction

Consider a bowing dislocation pinned at $x = 0, \mathcal{L}_i$. For simplicity, we assume $\sigma_b = 0$. Its time-dependent shape, $y(x, t)$, is governed by Equation 47. The solution of Equation 47 subject to $y(0, t) = y(\mathcal{L}_i, t) = 0$ is

$$y(x, t) = \frac{\sigma b}{2\mathcal{T}} x(\mathcal{L}_i - x) - \mathcal{L}_i \sum_{n=1}^{\infty} b_n \sin \left[\frac{(2n-1)\pi x}{\mathcal{L}_i} \right] \exp \left[-(2n-1)^2 \frac{t}{t_B} \right], \quad (\text{B.1})$$

where

$$b_n = \frac{4\sigma b \mathcal{L}_i}{\pi^3 (2n-1)^3 \mathcal{T}}. \quad (\text{B.2})$$

Figure A.2: Comparison of Equation A.3 (solid lines) with TST (dashed lines) for 0K, 300K and 800K. We have used $\rho_i = 2 \times 10^{12} \text{cm}^{-2}$ and $\rho_m = 10^8 \text{cm}^{-2}$ in Equation A.3 and $\rho_m = \langle \sqrt{k_B T / \bar{E}} \rangle_T 10^8 \text{cm}^{-2} = 0.41 \times 10^8 \text{cm}^{-2}$ for TST.

Note that this solution holds only on the interval $[0, \mathcal{L}_i]$. We extend its domain to the entire x -axis by constructing its even periodic extension

$$y(x, t) = \frac{\sigma b \mathcal{L}_i^2}{12\mathcal{T}} - \frac{\mathcal{L}_i}{\pi} \sum_{n=1}^{\infty} \frac{b_n}{n-1/2} \exp\left[-(2n-1)^2 \frac{t}{t_B}\right] - \mathcal{L}_i \sum_{m=1}^{\infty} \left\{ \frac{\sigma b \mathcal{L}_i}{2\pi^2 \mathcal{T} m^2} + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{(n-1/2) b_n}{(n-1/2)^2 - m^2} \exp\left[-(2n-1)^2 \frac{t}{t_B}\right] \right\} \cos\left[\frac{2\pi m x}{\mathcal{L}_i}\right]. \quad (\text{B.3})$$

This solution describes the bowing of a dislocation between obstacles spaced a distance $\mathcal{L}_i$ apart along the entire x -axis. At time t_r (on average) the dislocation passes through the obstacles and glides toward the next row of obstacles. This phase of its motion is described by the following transit solution

$$y_T(x, t) = \frac{\sigma b \mathcal{L}_i^2}{12\mathcal{T}} - \frac{\mathcal{L}_i}{\pi} \sum_{n=1}^{\infty} \frac{b_n}{n-1/2} \exp\left[-(2n-1)^2 \frac{t_r}{t_B}\right] + \frac{\sigma b}{B} (t - t_r) - \mathcal{L}_i \sum_{m=1}^{\infty} \left\{ \frac{\sigma b \mathcal{L}_i}{2\pi^2 \mathcal{T} m^2} + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{(n-1/2) b_n}{(n-1/2)^2 - m^2} \exp\left[-(2n-1)^2 \frac{t_r}{t_B}\right] \right\} \cos\left[\frac{2\pi m x}{\mathcal{L}_i}\right] \exp\left[-4m^2 \frac{t - t_r}{t_B}\right]. \quad (\text{B.4})$$

The transit solution coincides with the bow-out solution, Equation B.3, at $t = t_r$. We define the transit time, t_T , to be the time when y_T at the obstacles equals the inter-obstacle distance:

$$y_T(n\mathcal{L}_i, t_r + t_T) = \mathcal{L}_i, \quad n = 0, \pm 1, \pm 2, \dots \quad (\text{B.5})$$

This condition may be written

$$\frac{\pi^2}{3} - \frac{2}{\pi^2} \sum_{n=1}^{\infty} \frac{\exp\left[-(n-1/2)^2 \beta x\right]}{(n-1/2)^4} + \beta(y-1) - 2 \sum_{m=1}^{\infty} \left\{ \frac{1}{m^2} + \frac{2}{\pi^2} \sum_{n=1}^{\infty} \frac{\exp\left[-(n-1/2)^2 \beta x\right]}{(n-1/2)^2 [(n-1/2)^2 - m^2]} \right\} \exp(-m^2 \beta y) = 0, \quad (\text{B.6})$$

where

$$\begin{aligned} x &= \frac{t_r}{t_{T0}}, \quad y = \frac{t_T}{t_{T0}}, \quad t_{T0} = \frac{B\mathcal{L}_i}{b\sigma}, \\ \beta &= \frac{4\pi^2\mathcal{T}}{b\sigma\mathcal{L}_i} = \frac{5}{4}\pi\frac{G}{\sigma}b\sqrt{\rho_i}\ln\left(\frac{1}{b\sqrt{\rho_i}}\right). \end{aligned} \quad (\text{B.7})$$

The standard expression for the mean dislocation velocity (see Section 5)

$$v = \frac{\mathcal{L}_i}{t_r + t_{T0}}, \quad (\text{B.8})$$

can be corrected by including the factor

$$\zeta = \frac{t_r + t_{T0}}{t_r + t_T} = \frac{x + y}{x + 1}. \quad (\text{B.9})$$

This correction factor was determined by solving Equation B.6 numerically for y for $x \in [0.01, \infty)$ and $\beta \in [0.1, 10]$, which encompasses physically relevant ranges of stress and dislocation density. The correction is largest for $x = 1$ ($t_r = t_{T0}$) and approaches unity for both larger and smaller x . In addition, the correction is only weakly dependent on β . Averaged over β , the correction factor is fit remarkably well by

$$\zeta = \left\{ 1 - \frac{1}{4} \exp \left[-\log_{10}^2 \left(\frac{t_r}{t_{T0}} \right) \right] \right\}^{-1}. \quad (\text{B.10})$$

References

- Al'shitz, V.A., Indenbom, V.L., 1975. Dynamic dragging of dislocations. *Soviet Physics Uspekhi* 18, 1–20.
- Arrhenius, S., 1889. Ueber die reaktionsgeschwindigkeit bei der inversion von rohrzucker durch säuren. *Zeitschrift für Physikalische Chemie* 4, 226–248.
- Ashby, M.F., 1970. Deformation of plastically non-homogeneous materials. *Philosophical Magazine* 21, 399.
- Austin, R.A., McDowell, D.L., 2011. A dislocation-based constitutive model for viscoplastic deformation of fcc metals at very high strain rates. *International Journal of Plasticity* 27, 1–24.
- Austin, R.A., McDowell, D.L., 2012. Parameterization of a rate-dependent model of shock-induced plasticity for copper, nickel, and aluminum. *International Journal of Plasticity* 32–33, 134–154.
- Barton, N.R., Bernier, J.V., Becker, R., Arsenlis, A., Cavallo, R., Marian, J., Rhee, M., Park, H.S., Remington, B.A., Olson, R.T., 2011. A multiscale strength model for extreme loading conditions. *Journal of Applied Physics* 109, 073501.
- Bayley, C.J., Brekelmans, W.A.M., Geers, M.G.D., 2006. A comparison of dislocation induced back stress formulations in strain gradient crystal plasticity. *International Journal of Solids and Structures* 43, 7268–7286.
- Becker, R., 1925. On the plasticity of amorphous and crystalline solids. *Physikalische Zeitschrift* 26, 919–925.
- Bjork, R.L., 1957. Impurity-induced localized modes of lattice vibration in a diatomic chain. *Physical Review* 105, 456–459.
- Bulatov, V.V., Hsiung, L.L., Tang, M., Arsenlis, A., Bartelt, M.C., Cai, W., Florando, J.N., Hiratani, M., Rhee, M., Hommes, G., Pierce, T.G., Diaz de la Rubia, T., 2006. Dislocation multi-junctions and strain hardening. *Nature* 440, 1174–1178.
- Burakovsky, L., Greeff, C.W., Preston, D.L., 2003. Analytic model of the shear modulus at all temperatures and densities. *Physical Review B* 67, 094107.
- Burakovsky, L., Preston, D.L., 2004. Analytic model of the gruneisen parameter all densities. *Journal of Physics and Chemistry of Solids* 65, 1581–1587.
- Burgers, W.G., Burgers, J.M., 1935. Plasticity of rock salt and the Taylor and Becker orowan theories of crystalline plasticity. *Nature* 135, 960.
- Chandrasekhar, S., 1943. Stochastic problems in physics and astronomy. *Reviews of Modern Physics* 15, 1–89.
- Dahlberg, C.F.O., Saito, Y., Öztö, M.S., Kysar, J.W., 2014. Geometrically necessary dislocation density measurements associated with different angles of indentations. *International Journal of Plasticity* 54, 81–95.
- Eyring, H., 1935. The activated complex in chemical reactions. *Journal of Chemical Physics* 3, 107–115.
- Eyring, H., 1936. Viscosity, plasticity, and diffusion as examples of absolute reaction rates. *Journal of Chemical Physics* 4, 283–291.
- Fan, Y., Ossetsky, Y.N., Yip, S., Yildiz, B., 2012. Onset mechanism of strain-rate-induced flow stress upturn. *Physical Review Letters* 109, 135503.
- Follansbee, P.S., Kocks, U.F., 1988. A constitutive description of the deformation of copper based on the use of the mechanical threshold stress as an internal state variable. *Acta Metallurgica* 36, 81–93.
- Friedel, J. (Ed.), 1964. *Dislocations*. Pergamon Press, Oxford.
- Gradshteyn, I.S., Ryzhik, I.M., 1994. *Table of Integrals, Series, and Products*. Fifth ed., Academic Press, San Diego.
- Gröbner, W., Hofreiter, N., 1958. *Integraltafel, Teil II, Bestimmte Integrale*. Springer-Verlag, Wien and Innsbruck.
- Groma, I., Csikor, F.F., Zaiser, M., 2003. Spatial correlations and higher-order gradient terms in a continuum description of dislocation dynamics. *Acta Materialia* 51, 1271–1281.
- Hänggi, P., Talkner, P., Borkovec, M., 1990. Reaction-rate theory: fifty years after Kramers. *Reviews of Modern Physics* 62, 251–341.

- Hirth, J.P., Lothe, J., 1992. Theory of Dislocations. Second ed., Krieger Pub. Co., Florida.
- Hoge, K.G., Mukherjee, A.K., 1977. Temperature and strain rate dependence of flow-stress of tantalum. *Journal of Materials Science* 12, 1666–1672.
- Johnson, J.N., 1981. Dynamic fracture and spallation in ductile solids. *Journal of Applied Physics* 52, 2812–2825.
- Kramers, H.A., 1940. Brownian motion in a field of force and the diffusion model of chemical reactions. *Physica* 7, 284–304.
- Krasnikov, V.S., Kuksin, A.Y., Mayer, A.E., Yanilkin, A.V., 2010. Plastic deformation under high-rate loading: the multiscale approach. *Physics of the Solid State* 52, 1386–1396.
- Krasnikov, V.S., Mayer, A.E., Yalovets, A.P., 2011. Dislocation based high-rate plasticity model and its application to plate-impact and ultra short electron irradiation simulations. *International Journal of Plasticity* 27, 1294–1308.
- Kysar, J.W., Saito, Y., Oztog, M.S., Lee, D., Huh, W.T., 2010. Experimental lower bounds on geometrically necessary dislocation density. *International Journal of Plasticity* 26, 1097–1123.
- Langer, J.S., Bouchbinder, E., Lookman, T., 2010. Thermodynamic theory of dislocation-mediated plasticity. *Acta Materialia* 58, 3718–3732.
- Longuet-Higgins, M.S., 1958. On the intervals between successive zeros of a random function. *Proc. R. Soc. Lond. A* 246, 99–118.
- Madec, R., Devincere, B., Kubin, L.P., 2002a. From dislocation junctions to forest hardening. *Physical Review Letters* 89, 255508.
- Madec, R., Devincere, B., Kubin, L.P., 2002b. On the nature of attractive dislocation crossed states. *Computational Materials Science* 23, 219–224.
- Maradudin, A.A., Mazur, P., Montroll, E.W., Weiss, G.H., 1958. Remarks on the vibrations of diatomic lattices. *Reviews of Modern Physics* 30, 175–196.
- Montroll, E.W., Potts, R.B., 1955. Effect of defects on lattice vibrations. *Physical Review* 100, 525–543.
- Olmsted, D.L., Hector, L.G., Curtin, W.A., Clifton, R.J., 2005. Atomistic simulations of dislocation mobility in al, ni, and al/mg alloys. *Modelling and Simulation in Materials Science and Engineering* 13, 371–388.
- Orowan, E., 1934a. For crystal plasticity. i. *Zeitschrift für Physik* 89, 605–613.
- Orowan, E., 1934b. For crystal plasticity. ii. *Zeitschrift für Physik* 89, 614–633.
- Orowan, E., 1934c. For crystal plasticity. iii. *Zeitschrift für Physik* 89, 634–659.
- Pollak, E., Talkner, P., 2005. Reaction rate theory: What it was, where is it today, and where is it going? *Chaos* 15, 026116.
- Preston, D.L., Tonks, D.L., Wallace, D.C., 2003. Model of plastic deformation for extreme loading conditions. *Journal of Applied Physics* 93, 211–220.
- Preston, D.L., Wallace, D.C., 1992. A model of the shear modulus. *Solid State Communications* 81, 277–281.
- Rosenstock, H.B., Kilck, C.C., 1960. Vibrational modes near impurities. *Physical Review* 119, 1198–1203.
- Schuck, P.C., Marian, J., Adams, J.B., Sadigh, B., 2009. Vibrational properties of straight dislocations in bcc and fcc metals within the harmonic approximation. *Philosophical Magazine* 89, 2861–2882.
- Seeger, A., 1954a. Theorie der kristallplastizität .1. grundzuge der theorie. *Z. Naturforschung* 9, 758–775.
- Seeger, A., 1954b. Theorie der kristallplastizität .2. die grundstruktur der dichtest gepackten metalle und ihr einfluss auf die plastische verformung. *Z. Naturforschung* 9, 856–869.
- Seeger, A., 1954c. Theorie der kristallplastizität .3. die temperatur-abhängigkeit und geschwindigkeitsabhängigkeit der kristallplastizität. *Z. Naturforschung* 9, 870–881.
- Seeger, A., 1955a. Bestrahlungsfehlordnung und diffusionsvorgänge in edelmetallen. *Z. Naturforschung* 10, 251–253.
- Seeger, A., 1955b. The generation of lattice defects by moving dislocations, and its application to the temperature dependence of the flow-stress of fcc crystals. *Philosophical Magazine* 46, 1194–1217.
- Slater, N.B., 1959. Theory of Unimolecular Reactions. Cornell University Press, Ithaca, New York.
- Steinberg, D.J., Lund, C.M., 1989. A constitutive model for strain rates from 10^{-4} to 10^6 s^{-1} . *Journal of Applied Physics* 65, 1528–1533.
- Van't Hoff, J.H., 1896. Studies in Chemical Dynamics. London.
- Vineyard, G.H., 1957. Frequency factors and isotope effects in solid state rate processes. *Journal of Physics and Chemistry of Solids* 3, 121–127.
- Wickham, L.K., Schwarz, K.W., Stölken, J.S., 1999. Rules for forest interactions between dislocations. *Physical Review Letters* 83, 4574–4577.
- Yanilkin, A.V., Krasnikov, V.S., Kuksin, A.Y., Mayer, A.E., 2014. Dynamics and kinetics of dislocations in al and al-cu alloy under dynamic loading. *International Journal of Plasticity* 55, 94–107.
- Yefimov, S., Van der Giessen, E., 2005. Size effects in single crystal thin films: nonlocal crystal plasticity simulations. *European Journal of Mechanics, A/Solids* 24, 183–193.
- Yefimov, S., Groma, I., Van der Giessen, E., 2004. A comparison of a statistical-mechanics based plasticity model with discrete dislocation plasticity calculations. *Journal of the Mechanics and Physics of Solids* 52, 279–300.
- Zerilli, F.J., Armstrong, R.W., 1987. Dislocation-mechanics-based constitutive relations for material dynamics calculations. *Journal of Applied Physics* 61, 1816–1825.

Figure

Figure

Figure

Figure

Figure

Figure

Figure

Figure

Figure

Figure