

Notes on Thermal Activation of Dislocation Glide

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December 04, 2024

Introduction

The plastic deformation of crystalline materials is fundamentally controlled by the thermally-activated motion of dislocations through energy barriers arising from various obstacles [1, 2, 3, 4, 5]. Understanding how these dislocations overcome such barriers under applied stress is crucial for predicting the temperature and strain-rate dependence of mechanical properties. This note explores a comprehensive framework for the activation free energy of dislocation glide, following the seminal work of Kocks and others [6]. We review phenomenological relationships between stress, temperature, and strain rate through the lens of thermally-activated barrier crossing, and demonstrate how these relationships explain experimentally observed yield stress behavior. The treatment bridges microscopic dislocation dynamics with macroscopic mechanical response, providing physical insight into rate-dependent plasticity.

Activation Free Energy of Dislocation Glide

The free energy of activation ΔG for dislocation glide can be expressed as [6],

$$\Delta G = \Delta H - T\Delta S, \quad (1)$$

where ΔH is the activation enthalpy and T is the absolute temperature. While ΔH may exhibit temperature dependence, ΔG is employed here as it represents an equilibrium thermodynamic property. The analysis focuses on the macroscopic behavior of dislocations, characterized through their interaction with energy barriers that manifest as glide resistance on slip planes.

Upon application of an external stress σ , dislocations begin to glide through the crystal lattice. However, interactions between dislocations create obstacles that act as energy barriers, as illustrated in Figure 1a. The applied stress enables the dislocation to advance along the energy landscape toward state A; however, thermal activation is required to surmount the energy barrier and reach state B, thereby continuing the glide process. The activation free energy ΔG can thus be expressed as follows.

$$\Delta G = \int_{\sigma}^{\hat{\tau}} b\Delta a d\tau, \quad (2)$$

where b is the Burgers vector magnitude, Δa is the activation area, $\hat{\tau}$ is the maximum (athermal) stress experienced by the dislocation, often referred to as the Peierls stress, and the integration is performed along the stress ordinate. The corresponding glide resistance diagram, relating the change in swept area to the stress experienced by the dislocation, is shown in Figure 1b.

For short-range obstacles that are sensitive to thermal activation, a generalized phenomenological power-law relationship can be written as,

$$\Delta G = F_0 \left[1 - \left(\frac{\sigma}{\hat{\tau}} \right)^p \right]^q, \quad (3)$$

where F_0 represents the activation free energy in the absence of applied stress, and p and q are positive phenomenological exponents bounded by,

$$0 < p \leq 1; \quad 1 \leq q \leq 2. \quad (4)$$

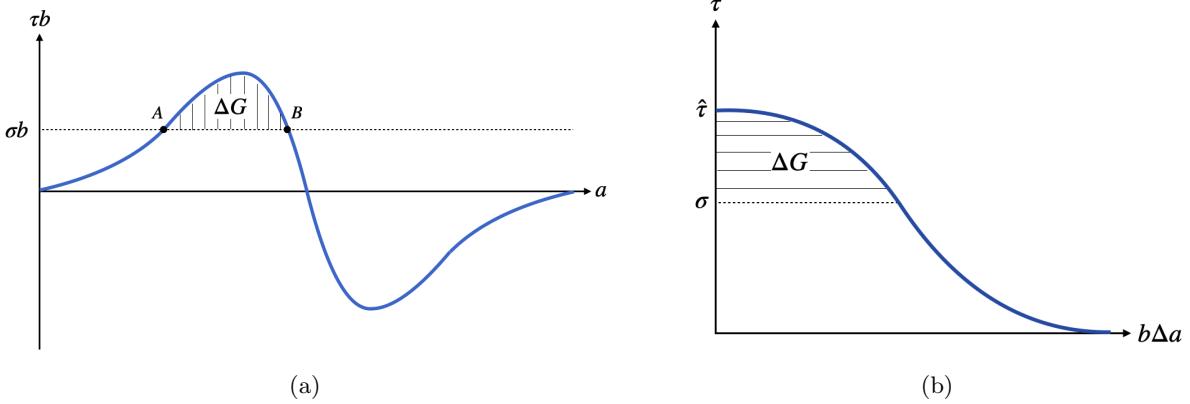


Figure 1: Schematic representation of stress acting on a gliding dislocation: (a) energy landscape as a function of total dislocation swept area a , with the activation free energy ΔG indicated by the shaded region, and (b) glide resistance diagram illustrating the stress τ experienced by the dislocation as a function of the change in swept area (activation area) Δa .

Activation Rate of Dislocation Glide

The general expression for the activation (transition) rate of dislocations across a free energy barrier (obstacle) is derived from the Arrhenius law of activation rates,

$$r = \nu_G e^{-\beta \Delta G} = \nu_H e^{-\beta \Delta H}, \quad (5)$$

where $\beta = 1/(k_B T)$, k_B is the Boltzmann constant, T is the absolute temperature, and ν_G and ν_H are prefactors corresponding to the free energy and enthalpy formulations, respectively. Here, ΔG and ΔH represent the heights of the energy barriers. Using Equation (1), the prefactors can be related as follows.

$$\nu_H = \nu_G \exp\left(\frac{\Delta S}{k_B}\right), \quad (6)$$

The attempt frequency ν_G is generally bounded by,

$$\nu_0 < \nu_G \leq \omega_A, \quad (7)$$

where $\nu_0 \equiv \omega_A b / \lambda$, with ω_A representing the frequency of uncorrelated atomic motions, b the magnitude of the Burgers vector, and λ the wavelength of the dislocation line segment. Analogous to a vibrating string, the dislocation line segment introduces correlation between atomic motions. While numerous approaches have been proposed to determine ν_G , harmonic transition state theory provides a straightforward derivation. Notably, quantum effects become significant at very low temperatures (i.e., below the effective Debye temperature).

The validity of the Arrhenius expression for activation rate (along with the Boltzmann probability distribution) requires certain conditions to be satisfied. First, the activation free energy must satisfy $\Delta G \gg k_B T$. When $\Delta G \approx k_B T$, dynamic effects dominate dislocation velocities, rendering the quasi-static approximation invalid. Conversely, when ΔG substantially exceeds $k_B T$, backward jumps between energy basins become probable, a phenomenon not accounted for in the standard Arrhenius formulation. Second, the Arrhenius expression assumes that dislocation configurations remain predominantly localized near energy minima rather than at saddle points. This implies that the residence time of dislocations within energy basins is significantly larger than the transit time across barriers, ensuring a quasi-equilibrium distribution within each basin.

Temperature Dependence of Strain Rate

The stress dependence of strain rate can be formulated using the activation rate expression. Considering the activation free energy, the strain rate is given by,

$$\dot{\epsilon} = \dot{\epsilon}_0 \nu_G e^{-\beta \Delta G}, \quad (8)$$

where $\dot{\epsilon}_0$ is a reference strain rate. This relationship arises because strain accumulation is directly proportional to the number of dislocations crossing the energy barrier per unit time (i.e., the activation rate).

To examine the stress dependence of strain rate, Equation (8) can be differentiated with respect to stress at constant temperature as follows.

$$\frac{\partial \ln \dot{\epsilon}}{\partial \sigma} \Big|_T = \frac{\partial \ln \dot{\epsilon}_0}{\partial \sigma} \Big|_T + \frac{\partial \ln \nu_G}{\partial \sigma} \Big|_T - \beta \frac{\partial \Delta G}{\partial \sigma} \Big|_T, \quad (9)$$

where it is assumed that the energy barrier structure remains constant during stress variation. The last term in Equation (9) defines the *activation volume*,

$$\Delta V^* = -\frac{\partial \Delta G}{\partial \sigma} \Big|_T, \quad (10)$$

which, from a thermodynamic perspective, relates the change in activation free energy ΔG to the mechanical work performed by the applied stress σ over the activation volume ΔV^* . Analogously, the *activation area* is defined as,

$$\Delta a^* = -\frac{1}{b} \frac{\partial \Delta G}{\partial \sigma} \Big|_T, \quad (11)$$

where b is the magnitude of the Burgers vector. The activation area Δa^* represents the area swept by the dislocation segment during the activation process. It should be noted that Δa^* does not correspond to the total area swept between equilibrium configurations due to the presence of glide resistance along the slip plane (see [6] for further details). As illustrated in Figure 1b, the activation area Δa^* can be geometrically interpreted as the slope of the glide resistance diagram at a given stress level.

Phenomenological Description of Glide Resistance

The phenomenological description of the activation free energy ΔG and its influence on glide resistance profiles is now examined. Historically, many studies have employed box-shaped energy barrier models, assuming constant activation area Δa for $0 < \sigma < \hat{\tau}$. However, experimental observations indicate that in general glide resistance profiles, the stress τ decreases as Δa increases, which can be described by a power law,

$$\tau \propto \frac{1}{(\Delta a)^n}, \quad (12)$$

where $n > 1$ for short-range barriers and $n < 1$ for long-range barriers. This distinction arises because for $n > 1$, the power law decays to zero at large Δa , yielding zero activation energy characteristic of short-range interactions that are thermally activated. Conversely, $n < 1$ corresponds to long-range barriers. The generalized power-law expression for short-range interactions sensitive to thermal activation is given by Equation (3).

As an exercise, one can verify that Equation (3) captures the power-law behavior of Equation (12) at both limits of the glide resistance profile: at the bottom ($\sigma \approx 0$) and at the top ($\sigma \approx \hat{\tau}$). To determine the physically admissible range of the exponents p and q , we impose the constraint that the activation area must increase monotonically with applied stress, requiring,

$$\frac{\partial^2 \Delta G}{\partial \sigma^2} \geq 0. \quad (13)$$

Evaluating the second derivative of Equation (3),

$$\frac{\partial^2 \Delta G}{\partial \sigma^2} = pq F_0 \left(\frac{\sigma}{\hat{\tau}} \right)^{p-2} \left[1 - \left(\frac{\sigma}{\hat{\tau}} \right)^p \right]^{q-2} \left[(q-1)p \left(\frac{\sigma}{\hat{\tau}} \right)^p - (p-1) \left(1 - \left(\frac{\sigma}{\hat{\tau}} \right)^p \right) \right], \quad (14)$$

Examining the limits $\sigma \rightarrow 0$ and $\sigma \rightarrow \hat{\tau}$ yields the constraints $p \leq 1$ and $q \geq 1$, respectively. Additionally, at $\sigma \rightarrow \hat{\tau}$, the resistance profile becomes,

$$\tau = \hat{\tau} \left(1 - (\Delta a)^{1/(q-1)} \right), \quad (15)$$

which requires $q \leq 2$ to ensure a smooth, physically realistic resistance profile. Therefore, the bounds on the phenomenological exponents reads,

$$0 < p \leq 1; \quad 1 \leq q \leq 2. \quad (16)$$

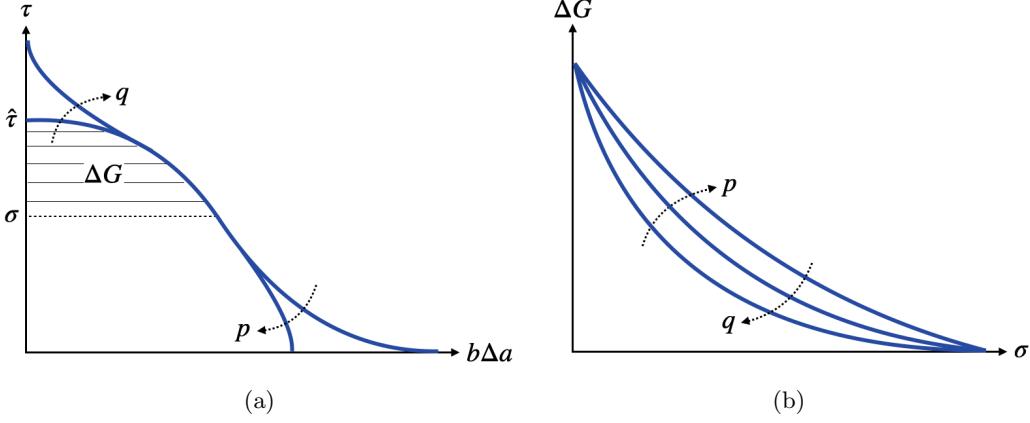


Figure 2: Phenomenological behavior of dislocation glide: (a) glide resistance profile as a function of dislocation swept area, and (b) activation free energy as a function of applied stress for various values of p and q .

Figure 2a illustrates the dislocation glide resistance profile. As p increases, the activation process occurs over a shorter range, whereas decreasing p extends the activation range. Similarly, increasing q sharpens the resistance profile near the peak stress, while decreasing q produces a flatter profile. Figure 2b demonstrates that the activation free energy ΔG decreases more rapidly with applied stress for smaller p and larger q values, and vice versa.

Temperature Dependence of Glide Resistance

The power-law expression for activation free energy (Equation (3)) can be substituted into the Arrhenius relationship for strain rate (Equation (8)) to establish the connection between applied stress and strain rate. This can be written as follows.

$$\dot{\epsilon} = \dot{\epsilon}_0 \nu_G \cdot \exp \left[-\beta F_0 \left\{ 1 - \left(\frac{\sigma}{\hat{\tau}} \right)^p \right\}^q \right], \quad (17)$$

which can be expressed in logarithmic form as,

$$\ln \dot{\epsilon} = \ln \dot{\epsilon}_0 + \ln \nu_G - \beta F_0 \left\{ 1 - \left(\frac{\sigma}{\hat{\tau}} \right)^p \right\}^q, \quad (18)$$

thereby establishing the relationship between the applied stress on dislocation segments σ and the macroscopic strain rate $\dot{\epsilon}$. Equation (18) indicates that strain rate increases monotonically with applied stress. Since the stress acting on dislocations directly contributes to the macroscopic yield stress σ_Y , this framework provides a mechanistic explanation for the well-established experimental observation that materials exhibit higher yield stress under higher strain rates.

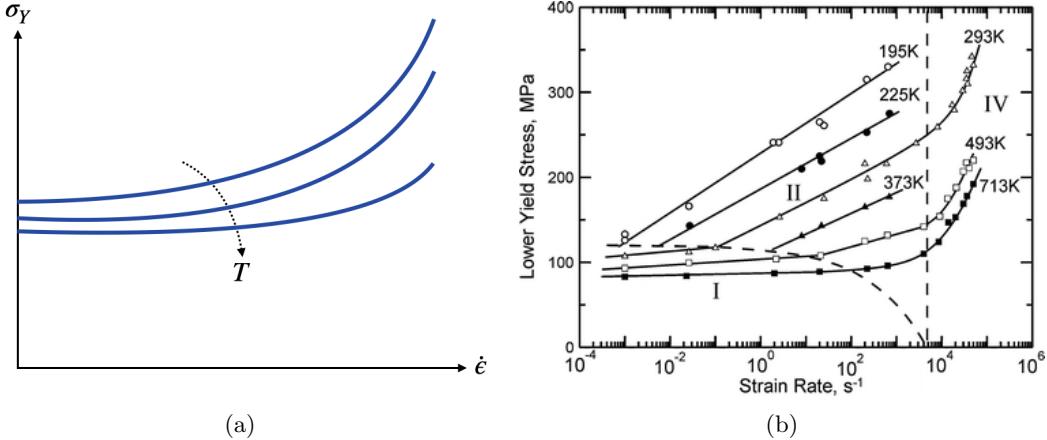


Figure 3: Strain rate dependence of yield stress: (a) theoretical predictions from the Arrhenius-based activation model with stress-dependent activation free energy (Equation (18)), and (b) experimental measurements of lower yield stress as a function of applied strain rate for ferritic stainless steels.

Figure 3 compares the theoretical predictions from Equation (18) with experimental data obtained for ferritic stainless steels. The results demonstrate that the theoretical model successfully captures both the general functional form and the temperature dependence observed in the experiments. Furthermore, the phenomenological parameters p and q can be determined through fitting to experimental data, providing a quantitative link between the microscopic energy landscape and macroscopic mechanical behavior.

Acknowledgement

I thank Hanfeng Zhai and Wurong Jian for their rigorous explanations of dislocation dynamics and their physical interpretations.

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Appendix A: Kramers Rate Expression

In the previous sections, we have assumed that the activation rate of the dislocations crossing the barrier follows the classical Arrhenius law following the equation (8). From the fact that the dislocation dynamics is in the overdamped regime, the corresponding activation rate expression from the Kramers' escape rate expression [7, 8] is given as,

$$r = \frac{\mu_d}{2\pi} \cdot \left[\Delta G''(A) \cdot |\Delta G''(S)| \right]^{1/2} \cdot e^{-\beta \Delta G},$$

where μ_d is the dislocation mobility and A and S corresponds to a basin and the saddle point between the basins of the dislocation activation process. Recall from the equation (3) that ΔG is a function of σ ,

$$r = \frac{\mu_d}{2\pi} \cdot \frac{\partial^2 \Delta G}{\partial \sigma^2} \cdot \left[\sigma''(A) \cdot |\sigma''(S)| \right]^{1/2} \cdot e^{-\beta \Delta G}, \quad (19)$$

where the derivative of the stress is with respect to the spatial domain. Using equation (19), we are able to come up with a more rigorous methodology for characterizing the activation rate. Moreover, we can present a physical interpretation of the equation (19). (1) As the stress field fluctuates more (i.e., σ'' is large), the strain rate becomes larger, which implies that the material exhibits smaller yield stress for a given strain rate. (2) The second order derivative of the activation free energy ΔG with respect to the σ gets larger as σ increases, which implies that yield stress decay is faster for a specific strain rate compared to the case solely considering the exponent term (i.e., $e^{-\beta \Delta G}$). Furthermore, the coefficients and prefactors of the equation (19) can be derived from molecular dynamics simulations related to continuum mechanics dealing with stress and strain.

Appendix B: Perturbation of Stress and Linear Dependence

Since the activation free energy ΔG depends on stress in a nonlinear manner, we can look into a case where there is a small change in the stress. Such cases can be easily linearized since the activation free energy mainly depends on the mean stress level. Suppose we already know the activation free energy ΔG at $\sigma = \sigma_0$. Then, the activation free energy at σ can be expanded as

$$\Delta G(\sigma) = \Delta G(\sigma_0) + (\sigma - \sigma_0) \frac{\partial \Delta G}{\partial \sigma} \Big|_T + O((\sigma - \sigma_0)^2),$$

and using the relation in equation (11) the expansion above reads,

$$\Delta G(\sigma) = \Delta G(\sigma_0) - (\sigma - \sigma_0) b \Delta a^* = \Delta G(\sigma_0) + \sigma_0 b \Delta a^* \Big|_{\sigma_0} - \sigma b \Delta a^* \Big|_{\sigma_0},$$

where the first two terms of the last expression are constant, the activation free energy depends on the stress σ linearly with the prefactor of $b \Delta a^* \Big|_{\sigma_0}$. Recall that the term $b \Delta a^* \Big|_{\sigma_0}$ is often called as *activation volume* V^* . Therefore, the final expression of the activation free energy ΔG at σ can be written as,

$$\Delta G(\sigma) = \Delta G(\sigma_0) - (\sigma - \sigma_0) V^* \Big|_{\sigma_0},$$

which can be interpreted as the work done by the stress acting on the dislocation, decreases the free energy which *activates* the energy barrier crossing behavior of the dislocations. Such linear response relation between the activation free energy and the applied stress to the dislocations is also powerful to use in experiments.