Thermal Activation of Dislocation Glide

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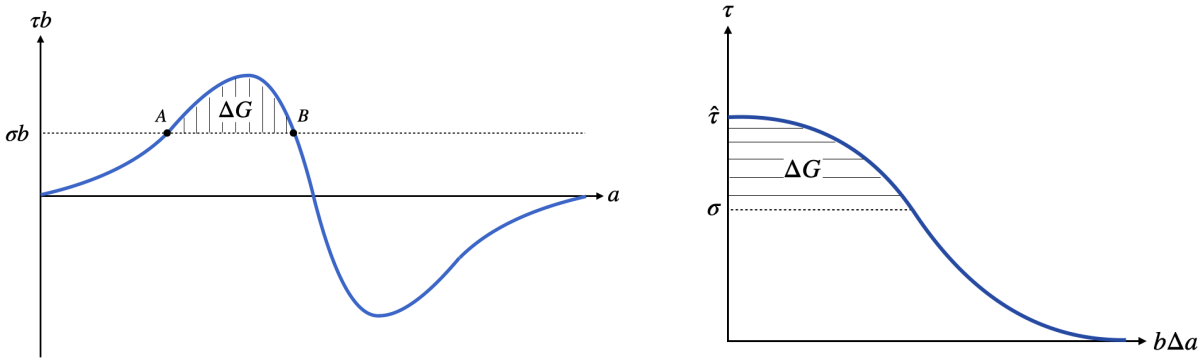
In this paper, we will explore the non-equilibrium behavior of the dislocation glide, which is a primary mechanism of plastic deformations in metals [1, 2, 3, 4, 5]. Concepts of activation free energy and activation rate will relate to the stress and strain rate applied to the dislocations and exhibit their macroscopic behavior. Furthermore, potential research directions will be proposed using more rigorous activation rate expression via Kramers' escape rate expression.

Activation free energy of dislocation glide

Let us deal with the activation energy of the dislocation glide [6]. In this section, We will deal with the free energy of activation ΔG, which can be expressed as,

$$\Delta G = \Delta H - T\Delta S, \tag{1}$$

where ΔH corresponds to activation enthalpy. Since ΔH can be temperature dependent, we will use ΔG instead, which is an equilibrium property (hence no temperature effects). We will focus on the "macroscopic" behavior of dislocations that interact with ΔG and shall describe it by plane glide resistance.



(a) (b)

Figure 1: Stress acting on a dislocation while gliding in two different perspectives where (a) energy landscape diagram respect to the total dislocation swept area a with the activation free energy ΔG inside the shaded region and (b) glide resistance diagram showing the stress τ experienced by the dislocation respect to the change of the swept area (i.e., activation area) Δa.

When stress σ is applied to the dislocation, the dislocation starts to glide. However, due to the dislocations' interactions, the dislocations act as a barrier by themselves, which can be characterized as an energy barrier as shown in the figure 1a. Applied stress helps the dislocation to move along the energy barrier up to state A; however, additional energy is required to cross the energy barrier fully and continue the glide (i.e., to reach state B). Therefore, the activation free energy ΔG can be written as,

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

where $\hat{\tau}$ is the maximum stress experienced by the dislocation and the integration, is along the ordinate instead of the abscissa. Note that $\hat{\tau}$ is often referred to as Peierls stress. Then, the glide resistance diagram that relates swept area change and the corresponding stress experienced by the dislocation can be drawn as figure 1b. A more generalized version of the power law for short-range interactions (sensitive to thermal activation) can be written as

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

where F_0 is the total activation free energy without applied stress σ and p, q are both positive. Note that such a relation is a phenomenological relationship. We also have bounds of the constants as,

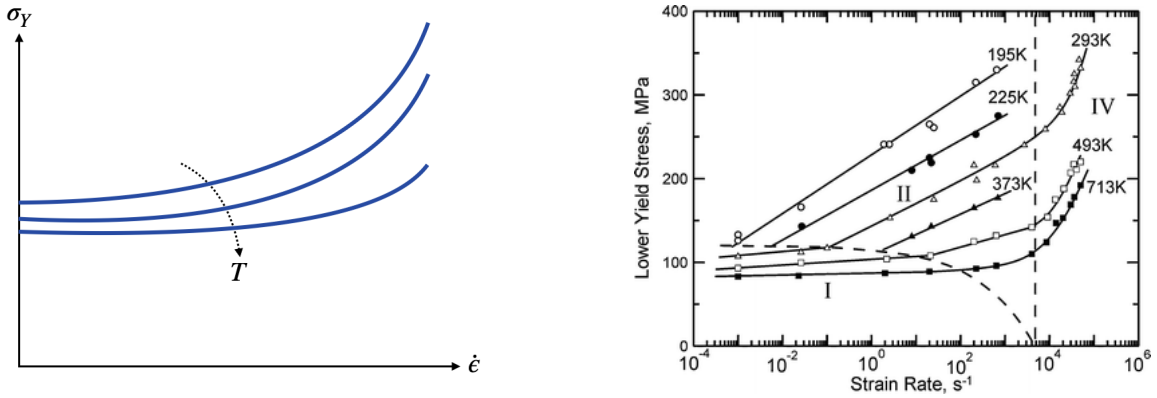
$$0 < p \leq 1; \;\; 1 \leq q \leq 2.$$

Temperature dependence of strain rate

Next, we can formulate stress dependence of strain rate using the activation rate expression. The strain rate expression considering activation free energy reads,

$$\dot{\epsilon} = \dot{\epsilon}_0 \, \nu_G \, e^{-\beta \Delta G}, \tag{3}$$

where $\dot{\epsilon}_0$ is a reference strain rate. This is because the strain increases as more dislocation crosses the energy barrier (activated), and the activation rate is assumed to follow the Arrhenius relation [7]. Hence, the number of activated dislocations per unit time (i.e., activation rate) is proportional to the strain rate.



(a) (b)

Figure 2: (a) Yield stress with respect to the strain rate predicted from the equations relating the activation rate to stress-dependent activation free energy and (b) experimental data of the yield stress with respect to the strain rate for ferritic stainless steels.

We can plug in the power law of the activation free energy from equation (2) into the relationship between the activation rate and the strain rate in equation (3). Then, the equation reads,

$$\dot{\epsilon} = \dot{\epsilon}_0 \, \nu_G \cdot \exp\left[-\beta F_0 \left\{1 - \left(\frac{\sigma}{\hat{\tau}}\right)^p\right\}^q\right] \implies \ln \dot{\epsilon} = \ln \dot{\epsilon}_0 + \ln \nu_G - \beta F_0 \left\{1 - \left(\frac{\sigma}{\hat{\tau}}\right)^p\right\}^q, \tag{4}$$

yields the relationship between applied stress to the dislocation segments σ and the strain rate $\dot{\epsilon}$. Note that the strain rate $\dot{\epsilon}$ increases as stress acting on the dislocation σ increases. By analogy, the stress acting on the dislocations can be considered to contribute to the yield stress σ_Y. Therefore, the well-known relation of the material exhibiting high yield stress under a high strain rate is explained. Figure 2 compares the relationship between the yield stress and the strain rate, predicted from the equation (4) and experimental data obtained on the ferritic stainless steels. The results show that the general shape of the curve predicted from the theory matches the experimental data [8], and its temperature dependence also follows the theoretical prediction.

Sophisticated approach in 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 (3). From the fact that the dislocation dynamics is in the overdamped regime, the corresponding activation rate expression from the Kramers' escape rate expression [9, 10] is given as,

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

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 (2) that ΔG is a function of σ,

$$r = \frac{\mu_d}{2\pi} \cdot \frac{\partial^2 \Delta G}{\partial \sigma^2} \cdot \left[\sigma''(\mathrm{A}) \cdot |\sigma''(\mathrm{S})|\right]^{1/2} \cdot e^{-\beta \Delta G}, \tag{5}$$

where the derivative of the stress is with respect to the spatial domain. Using equation (5), 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 (5). (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 (5) can be derived from molecular dynamics simulations related to continuum mechanics dealing with stress and strain. In conclusion, such rigorous formulation of the activation rate not only provides a more accurate prediction of the behaviors of metals but also paves a way to bridge various research fields of mechanics across microscopic and macroscopic worlds.

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