Acta Materialia 134 (2017) 203–210

Contents lists available at ScienceDirect

Acta Materialia

journal homepage: www.elsevier.com/locate/actamat

Full length article

Modal analysis of dislocation vibration and reaction attempt frequency

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ARTICLE INFO

Article history:
Received 5 July 2016
Received in revised form
31 January 2017
Accepted 2 February 2017
Available online 4 February 2017

Keywords:
Dislocation
Thermal activation
Attempt frequency
Modal analysis

ABSTRACT

Transition state theory is a fundamental approach for temporal coarse-graining. It estimates the reaction rate for a transition processes by quantifying the activation free energy and attempt frequency for the unit process. To calculate the transition rate of a gliding dislocation, the attempt frequency is often obtained from line tension estimates of dislocation vibrations, a highly simplified model of dislocation behavior. This work revisits the calculation of attempt frequency for a dislocation bypassing an obstacle, in this case a self-interstitial atom (SIA) loop. First, a direct calculation of the vibrational characteristics of a finite pinned dislocation segment is compared to line tension estimates before moving to the more complex case of dislocation-obstacle bypass. The entropic factor associated with the attempt frequency is calculated for a finite dislocation segment and for an infinite glide dislocation interacting with an SIA loop. It is found to be dislocation length independent for three cases of dislocation-self interstitial atom (SIA) loop interactions.

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1. Introduction

Dislocations are carriers of plastic deformation whose motion fundamentally influences material behavior. The collective effects of dislocation-mediated unit processes are described and homogenized in higher length and time scale models such as crystal plasticity in both athermal, stress driven and thermally activated regimes. In a strained crystal, dislocations migrate to create permanent deformation, thereby accommodating the applied strain and dissipating energy in the process. Dislocation multiplication and glide necessarily leads to defect interactions which cause strain hardening. Adopting and energy based viewpoint, the interactions between dislocation and obstacles affect the energy required for bypass by virtue of elastic fields (both local and non-local) that interact with the dislocation as well as thermal fluctuations. The rate at which bypass processes occur is ultimately a function of the internal material stress state, temperature, and obstacle configuration. Thermally activated bypass can be one of the key rate controlling processes determining the primary creep response and transition from primary to secondary creep in metals subjected to low stress (with respect to the athermal bypass stress) and moderate temperatures. Such is the case for example of high chromium steels which are readily used in thermal powerplants and are also candidate cladding materials for nuclear applications. A series of experimental studies suggest that in the aforementioned regimes, dislocation obstacle bypass (i.e. remobilization of dislocation lines), potentially mediated by climb, plays a key role in controlling creep in non-irradiated metals [1]. The scenario becomes more complex in the case of irradiated metals. In such case the interaction between glide loops and self-interstitial atom (SIA) cluster condensed in the form of loops is known to largely contribute to the materials strength. A connection with the effective strain rate sensitivity of those materials remains to be established.

To mathematically model such complex processes, numerous constitutive models have been proposed starting with the works of Kocks [2,3], and Mecking and Kocks [4]. More complex constitutive models resolving the fine scale implications of thermal activation in the form of thermally-assisted dislocation glide have been proposed [5–11], but even such modern models assume an attempt frequency with little justification or include the attempt frequency in a reference slip rate, which is also often assumed. These

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http://dx.doi.org/10.1016/j.actamat.2017.02.005
1359-6454/Published by Elsevier Ltd on behalf of Acta Materialia Inc.

dislocation-obstacle bypass attempt frequency estimates can range from 10^{10} 1/s [8] to the order of the Debye frequency [11]. These models do not consider the possible dependence of attempt frequency on defect type, spacing, or any other parameter. The influence of these factors must be quantified before applying a physics-based approach to predicting thermally activated response.

Direct estimation of dislocation-obstacle bypass attempt frequency from first principles was first performed by Friedel [12], who first derived the fundamental frequency of vibration for a dislocation using a line tension model (approximating a dislocation as a string with tension Γ). Granato et al. [13] developed a significantly more advanced analysis for attempt frequencies for dislocation-obstacle bypass events, deriving bounds and estimates for attempt frequency, which are summarized in this work. The adopted methodology of Granato et al. is revisited here, foregoing line tension approximations and instead applying a non-singular dislocation formulation [14] to more realistically describe dislocation dynamics.

This study aims to determine the attempt frequency for a dislocation bypassing a SIA loop using the continuum theory of defects. To this end, the study is divided into three sections. First, the fundamental modes of a finite dislocation segment with pinned ends are characterized and compared to line tension predictions for the fundamental frequency as well as the functional form of the spectrum. Next, the attempt frequency for a finite dislocation segment bowed against an SIA loop is determined and compared to theoretical estimates where possible. A more realistic configuration of an infinite dislocation bowed against an array of SIA loops is then considered and the attempt frequency is determined. The study concludes with discussion of the sensitivity of the numerical calculation of attempt frequency and the possible implications on predictions of the reaction rate.

2. Method

2.1. Summary of theoretical developments

The Arrhenius equation was applied to the case many-body processes in the work of Vineyard [15] by adopting a harmonic approximation in order to extend it to solid state processes. By considering the ratio of configurational partition functions for the normal and activated states for an M-dimensional system and assuming each degree of freedom can be approximated by a harmonic oscillator, the rate of phase points crossing the saddle point can be written as

$$k = \nu_a e^{-\Delta G/k_B T} = \nu_1 e^{\Delta S/k_B} e^{-\Delta H/k_B T} \tag{1}$$

where

$$\nu_a = \nu_1 \prod_{i=2}^{M} (\nu_i/\nu_i'), \tag{2}$$

Here, ν_1 is the fundamental attempt frequency, ν_i is the frequency of the i^{th} mode of the normal state, and ν_i' is the frequency of the i^{th} mode of the activated state. The factor $\prod_{i=2}^{M}(\nu_i/\nu_i')$ is called the entropic factor $e^{\Delta S/k_B}$ as it explicitly accounts for the entropy change during the process.

Granato et al. [13] described a dislocation line using the following partial differential equation

$$\mu y'' + \rho(x)F(y) + b\sigma = \mu\ddot{y}\Big/c^2 \tag{3}$$

where prime symbols represent derivatives with respect to x, dots represent time derivatives, y is the displacement of the dislocation at x in the bypass direction, μ is the line tension, b is the Burgers vector magnitude, $F(y)$ is the anchoring force of the defect, σ is the scalar applied stress, $\rho(x)$ the pinning point density, the mass per unit length is assumed to be μ/c^2 and c is the speed of sound in an isotropic medium. In general, the dislocation mass depends on elastic anisotropy and non-linearities in the dislocation core motion, but is approximated as a function of the isotropic speed of sound for this work. In the absence of obstacles ($\rho(x) = 0$, $F(y) = 0$) and applied stress ($\sigma = 0$), Equation (3) adopts the form of the linear wave equation. At equilibrium, the dislocation takes a configuration $Y(x)$ that minimizes energy about which it makes small oscillatory perturbations, i.e.,

$$y(x,t) = Y(x) + \sum_i z_i(x)\cos(\omega_i t), \tag{4}$$

where $Y(x)$ is the mean equilibrium configuration (accounting for the effect of $b\sigma$ in Equation (3)), i is the mode number, ω_i is an eigenfrequency of the system and $z_i(x)$ represents the spatial dependence of the small oscillations about the mean configuration. Consequently, $z(x)$ will represent shape of each mode of the pinned dislocation. Equation (4) is substituted into Equation (3) for each mode i, resulting in the following equation describing each mode:

$$z_i'' + \left(\omega_i^2\Big/c^2 - [\rho(x)/\mu]f\right)z_i = 0 \tag{5}$$

where $f = -(dF/dy_0)_{y_0=Y_0}$ (representing the rate of change of the pinning force as a function of displacement in y), and the fixed ends of the finite dislocation segment are represented in the boundary conditions as $z_i(-l) = z_i(l) = 0\ \forall\ t$. Granato et al. [13] considered a point defect $\rho(x) = \delta(x)$ as well as a continuously distributed obstacle with density ρ. With the focus of this work on thermally assisted of dislocation-obstacle unpinning, only the case of a single point defect, extended periodically in x, is detailed from the work of Granato. The configuration consists of a single finite dislocation segment of length $2l$ with a point obstacle at dislocation center at $x = 0$. Each modal perturbation of the dislocation $z(x)$ is described by

$$z_i = A\sin((\omega_i/c)(l+x)) \ \text{ for } \ -l < x < 0, \tag{6}$$

$$z_i = \pm A\sin((\omega_i/c)(l-x)) \ \text{ for } \ 0 < x < l. \tag{7}$$

The two solutions are joined with the added conditions

$$\lim_{\varepsilon\to 0} z_i(-\varepsilon) = z_i(\varepsilon)\ \forall\ t \tag{8}$$

$$\lim_{\varepsilon\to 0} z_i'(-\varepsilon) - z_i'(\varepsilon) = z_0 f/\mu\ \forall\ t \tag{9}$$

For even modes $z(0) = 0$ because the center of the dislocation line is a vibrational node, and therefore the even modes are unaffected by the pinning point and do not contribute to the attempt frequency. To derive the odd modes of vibration, Equations (6) and (7) are introduced into Equation (9), and the following transcendental equation results:

$$\tan\theta_i = -(2\mu/fl)\theta_i, \tag{10}$$

where $\theta_i = \omega_i l/c$. When values of θ for each mode in both the relaxed and activated configurations have been obtained numerically, the attempt frequency for the dislocation-obstacle configuration can be obtained by substituting these values into Equation (2) and is then written as