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Depinning transition of a dislocation line in ferritic oxide strengthened steels

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ABSTRACT

The dynamics of an edge dislocation in a medium with random oxide dispersoid particles acting as pinning centres is analysed. The dislocation line undergoes a depinning transition, where the order parameter is the dislocation line velocity v, which increases from zero for driving external resolved shear stresses τ beyond to a threshold value τ_c, known as the critical resolved shear stress. The critical stress is obtained by means of statistical analysis of the motion of a single dislocation in its glide plane, using overdamped, discrete dislocation dynamics simulations.

1. Introduction

Understanding the dynamics of dislocations in a random environment is a long-standing problem dating as far back as the sixties (for a review see for example [1]). Line tension – mainly elastic forces – tend to keep the driven dislocation line straight, while obstacles to dislocation motion (such as dispersoids, precipitates, and impurities) locally promote irregular wandering of the dislocation line. From the competition between obstacles and elastic forces emerges a complicated energy landscape with 'glassy' properties, characterised by many metastable states and energy fluctuations that grow with the linear size L of the system as L^{θ}, where θ is a positive exponent.

Extreme loading conditions (temperatures up to 1300 K, radiation damage up to 100 dpa) necessitate advanced creep resistant alloys for in-core (fasteners, support) and out-of-core (hot gas duct) nuclear applications. Dispersoid strengthening is a particularly important mechanism for these applications. The prediction of microstructure evolution induced by irradiation and by time evolution of dispersoid distributions can be introduced in discrete dislocation dynamics (DDD) computations in order to estimate their effects on the mechanical properties. Determining the response to an externally applied stress in dispersion strengthened materials is an interesting theoretical problem, as the results of the simulations – that are necessarily restricted to finite system sizes – need to be extrapolated to the bulk, often considered to corresponds to an infinite system.

To obtain the critical resolved shear stress (CRSS), which is well defined only for systems with infinite size, many smaller systems with different realisations of the randomness are considered instead of studying a system as large as possible. The depinning is described as a conventional critical phenomenon and the critical stress τ_c is estimated using finite-size scaling arguments [2]. The paper is organised as follows: in Section 3 the model is introduced, Section 5 contains results of our numerical study and the last section is reserved for general conclusions.

2. Material

In this paper the depinning of a dislocation line moving in a glide plane and interacting with random incoherent Y_2O_3 oxide dispersoids (ODS) is investigated in a bcc ferritic PM2000 matrix, a high-resistant Fe–Cr–Al commercial alloy with nominal chemical composition (in wt%) [3] is given in Table 1.

The ferritic ODS alloy PM2000 was supplied by Plansee GmbH in the form of 15 nm thick plates. The alloy was manufactured by mechanically alloying in a high energy mill, with the powder consolidated by hot compaction, followed by a hot and cold rolling procedure and a final thermal treatment [4] giving an uniform dispersion of Y_2O_3.

3. The model

A dislocation is a one-dimensional line defect in the crystal, which is well described within the framework of linear elasticity. In the discrete dislocation dynamics (DDD) models the dislocation line is described by a set of nodes connected by straight segments, which can take any direction between screw and edge orientations in the glide plane [5,6], contrary to the a screw-edge discretisation scheme [7]. The dislocation nodes move under the action of the Peach–Koehler force [8] arising from the self stress due to local curvature and the applied external stress. In the present simula-

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Table 1
Composition of PM2000.

Element	Fe	Cr	Al	Ti	Y_2O_3
wt%	74.5	19	5.5	0.5	0.5

tions, the evolution of the nodal positions is obtained by a simple Euler forward integration scheme [5]. The inertial forces arising from the dislocation acceleration are negligible compared to the drag forces, which are taken to be proportional to the dislocation velocity. The drag coefficient $M(\theta)$ of the dislocation is assumed to depend on the character of the dislocation as [9]

$$M(\theta) = M_s \cos^2 \theta + M_e \sin^2 \theta, \tag{1}$$

where M_s and M_e are the drag coefficients of pure screw and edge dislocation segments, respectively. The angle θ is defined as the angle between the Burgers vector and line direction vector of the segments.

A single edge dislocation gliding through a random obstacle field represented by Y_2O_3 particles modelled as hard core spheres is considered. The size distribution of the Y_2O_3 particles (Fig. 1(b)) is obtained experimentally by means of analysis of several TEM micrographs, taken from thin specimens of the ferritic steel PM2000 [3] with a thickness of approximately 200 nm. The same size distribution was used in previous DDD studies [9,10] to understand the effect of particle hardening on the mechanical properties.

4. Simulation setup

A system of size $L \times L$ is considered, containing an initially straight edge dislocation with Burgers vector, $\mathbf{b} = b\mathbf{i}$, parallel to the x-axis and line direction parallel to the y-axis. Periodic boundary conditions are assumed in the y direction (see Fig. 1(a)). The dislocation, with average edge orientation, travels in the x direction under the action of a constant external resolved shear stress τ_{ext}. The spatial arrangement of particles is random in 3D with uniform distribution and with the constraint that no particles overlap [11]. The radii of the particles are chosen at random from the distribution shown in Fig. 1(b). The fraction of dispersoids is taken as 0.5% to comply with that in PM2000 [3].

The materials parameters used in the simulations for the bcc Fe matrix are: shear modulus μ = 86 GPa, Poisson ratio ν = 0.291, and lattice constant a = 0.287 nm. For the drag coefficients the values for iron single crystals at room temperature measured by Urabe and Weertman [12] are used: 0.66 Pa s for screw, and 0.345 Pa s for edge dislocation segments.

5. Results

To determine the critical stress, an ensemble of 81 statistically equivalent particle configurations was chosen to be created. These particle configurations were used for simulations at different external stresses. In our model only particles intersecting the slip plane of the dislocation play a role in pinning, therefore all particles whose distance from the slip plane, z = 0, is larger than their radii, were discarded.

To calculate the critical stress, simulations for three different system sizes L = 2, 3, and 4.5 μm were performed. At time t = 0 the constant external stress τ_{ext} is switched on, and the initially straight edge dislocation starts to glide in the x direction. For low values of the external stress the gliding dislocation bows out between the spherical obstacles, but is not able to overcome them. At larger external stress, the dislocation might overcome some of the obstacles, leaving Orowan loops [13] around the incoherent, impenetrable dispersoids. When the external stress is further increased, the dislocation is ultimately able to glide from one side (x = 0) to the other (x = L) of the simulation area. This occurs at different stresses for different realisations of the obstacle configuration.

For a constant value of the driving stress and for different realisations of the obstacle configuration a 'transition probability' $P(\tau)$, as the fraction of realisations where the dislocation line travels from one side to another of the simulation area (when it is pulled with constant stress) is defined. Snapshots of a dislocation line moving in the obstacle field, for a typical simulation where the stress is larger, then the threshold value τ_c are presented in Fig. 2. The transition probability is different for different system sizes; generally speaking, the distribution becomes narrower if the system size is increased (Fig. 3(a)).

The critical stress, τ_c, can be determined by finite-size scaling of the transition probability for different system sizes. To this end, the abscissa is rescaled according to $(\tau - \tau_c)L^{1/\nu}$ and the parameters τ_c and ν are adjusted to make distributions corresponding to different system sizes, L, fall on top of each other. To obtain the scaling exponent ν, the model function

$$P(\tau) = \frac{1}{2}\left[1 + \text{erf}\left(\frac{\tau - \tau_c(L)}{\sqrt{2}\sigma(L)}\right)\right] \tag{2}$$

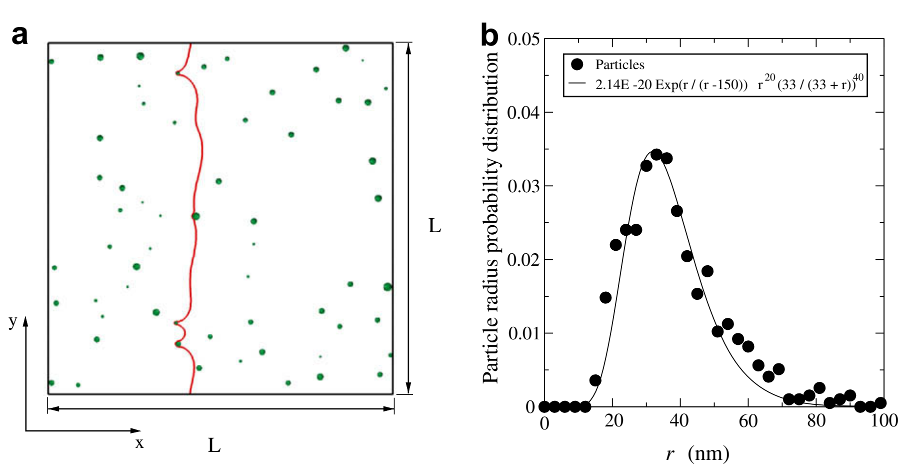

Fig. 1. (Colour online) Simulation setup. A dislocation line travelling in the obstacle field in constant external stress is illustrated. The radius of Y_2O_3 particles is a random variable with probability distribution function shown on the right [10].

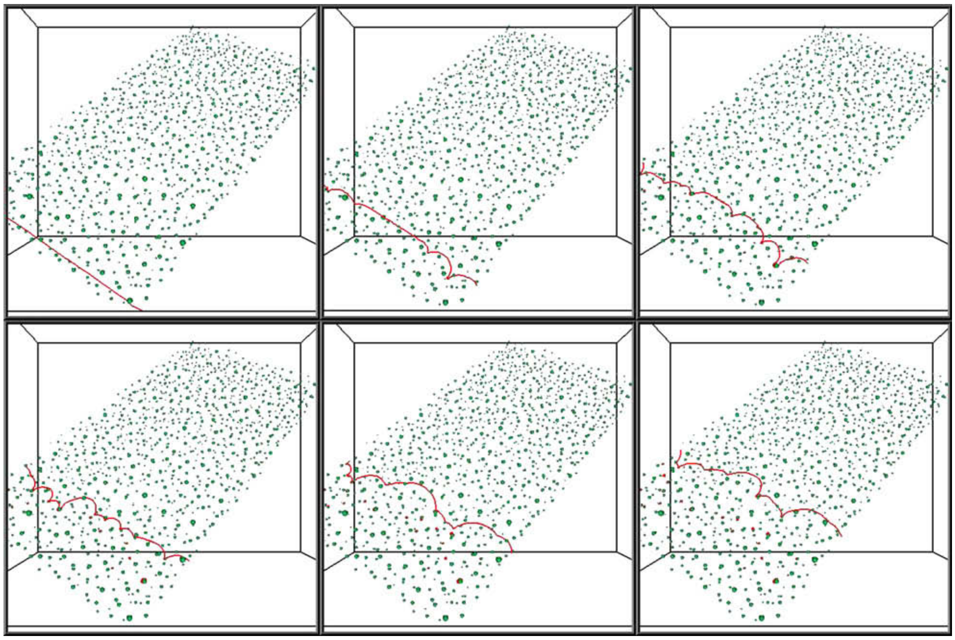

Fig. 2. (Colour online) Snapshots of a dislocation line gliding in a 3 μm × 6 μm box (with periodic boundary conditions) under the influence of a constant external stress.

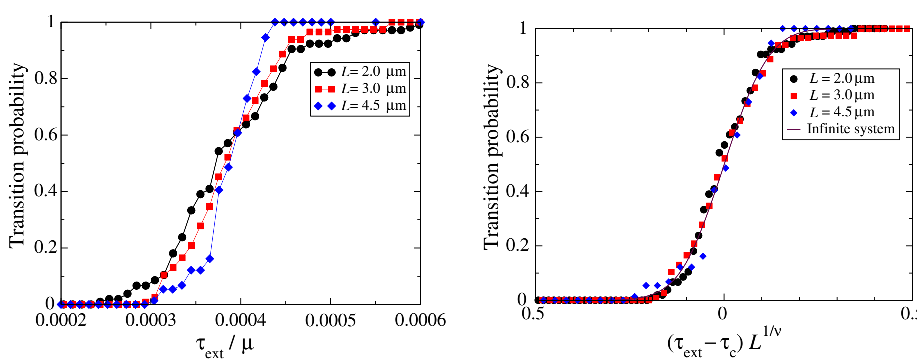

Fig. 3. (Colour online) Left: transition probability *P*. The critical stress can be obtained from the scaling plot (right) of the transition probability for different system sizes. The stresses on the horizontal axis are measured in units of shear modulus μ, and *L* is measured in nm.

was used for the transition probability, implying a surface fit with the model function

$$P(\tau, L) = \frac{1}{2}\left[1 + \mathrm{erf}\left(\frac{(\tau - \tau_c^{\infty})L^{\frac{1}{\nu}}}{\sqrt{2}\sigma_{\infty}}\right)\right], \tag{3}$$

where σ_{∞} is the variance of the cumulative probability density function *P*. Data collapse is obtained for $\tau_c^{\infty} = (384.722 \pm 0.504) \times 10^{-6}\mu$ and exponent $\nu = 1.053 \pm 0.05$ (Fig. 3(b)) (note that an exponent of $\nu \approx 1$ is expected for the depinning of an elastic line [14]). The numerical value of τ_c^{∞} can then be interpreted as the flow stress of the infinite system.

Because our approach only intends to illustrate the technique and does not take into account the interaction of the moving dislocation with the random stress field created by the immobile forest dislocations, the junction formation, and so forth, it is found that the value of the critical stress $\tau_c^{\infty} = 0.000385\mu \approx 33$ MPa is significantly lower than the recently measured experimental single crystal critical resolved shear stress value of 189 MPa for PM2000 single crystals for $\{1\,1\,0\}\langle 1\,1\,1\rangle$ slip systems [15]. Inclusion of the contribution from the forest dislocations to the critical resolved shear stress requires further work and is planned for the near future.

6. Conclusions

A powerful new method for calculating the critical resolved shear stress of technical alloys relevant for nuclear materials, based on techniques from statistical physics has been presented. The technique is illustrated by calculating the critical resolved shear stress τ_c of PM2000 oxide dispersion strengthened commercial ferritic alloy, a possible candidate material for future fusion and fission reactors, by studying the depinning of an edge dislocation gliding in a random field of Y_2O_3 dispersoids. The method presented in this paper allows the extrapolation of the critical resolved shear stress to large (infinite) systems sizes. This value is much less, than the experimentally measured which indicates the necessity to include other hardening mechanisms in the simulations. This approach, however, emerges to be of the possible methods to properly calculate critical resolved shear stress in an infinite system and can be applied also when other hardening mechanisms are present.

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