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Editor's Choice

Bridging time-scales: Grain boundary sliding constitutive law from atomistics

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ABSTRACT

Grain boundary sliding is the key deformation and damage mechanism for high temperature deformation of crystalline materials impacting, thus, applications ranging from nuclear reactors to aircrafts. Despite decades of research—theoretical and experimental—a definitive atomistic understanding of this phenomenon has been elusive. The primary bottleneck is the fact that conventional molecular dynamics can only address pico-to-nano seconds of material physics while the characteristic relaxation times for creep phenomena (including grain boundary sliding) are several orders of magnitude slower. In this letter, we use a fresh approach based on a recently developed potential energy surface sampling method that allows us to bridge long time scales and, for the first time, develop a physically reasonable constitutive law. Our results show a dramatic improvement over what can be gleaned from conventional molecular dynamics and provide insights on the relative merits of existing theories of grain boundary sliding. Our simulations (based on a prototypical metal, Al) answer important questions such as (i) is there a threshold stress for grain boundary sliding?, (ii) what is the form of constitutive law for grain boundary sliding? and others.

At low enough temperatures—low compared to half the homologous temperature—crystalline materials exhibit irrecoverable deformation provided the imposed mechanical stresses exceed the so-called yield threshold [1]. For all practical purposes, this deformation is considered to occur instantaneously. At high temperatures, however, even at stresses below the yield stress, irrecoverable deformation occurs gradually over an extended period of time. At the micro scale, this time-dependent deformation is predicated on several viscous processes such as grain boundary and volume diffusion, grain boundary sliding, dislocation glide-climb, void nucleation, void growth and others [2–5]. These micro mechanisms exhibit characteristic relaxation times that range from seconds to years (depending on the level of applied stress and temperature). This "creeping" deformation behavior is the predominant cause of failure in materials that are subject to high temperature environment: ice glaciers, nuclear reactors, air crafts, electronics among others [6–8]. For example, Sn–Pb alloys (solders) are extensively used in electronics and the melting temperature of this class of alloys is low enough that at even room temperature, creep eventually (in conjunction with other factors) leads to failure [8].

It is now well recognized that grain boundary sliding (GBS) is a key deformation and damage mechanism in creep [9]. Grain boundary sliding is the phenomenon of relative sliding of crystalline interfaces or grains in a slow viscous manner upon application of a macroscopic shear stress. The sliding is accommodated by grain boundary diffusion, volume diffusion and in the case of metals, dislocation glide-climb within the adjacent grains (i.e. grain plasticity).

Although work on grain boundary sliding dates back more than sixty years, some of the first quantitative studies on this are those by Raj and Ashby [11] who presented an analytical study of this phenomenon based on accommodation by grain boundary and volume diffusion. Raj and Ashby's work – the most widely used paradigm of this phenomenon – proposed a linear dependence between the imposed shear stress on the grain boundary and the consequent sliding rate; and an absence of any threshold stress. Extensive theoretical and experimental literature now exists which outline a number of (sometimes) contradictory observations. For example, Chauhan et al. [12] studied the problem from an experimental viewpoint and qualitatively observed a threshold stress for grain boundary sliding in ultra-fine grained Al alloy (300 nm grain

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size). The proposed value of threshold was found to be about 10 MPa (23 times lower than the experimentally determined yield stress). For further details, the reader is referred to the review article by Langdon and references therein [10]. Despite the extensive focus on this phenomenon, several issues still remain open, or at least, relatively unsettled, e.g. (i) in the case of diffusion dominated creep, is the stress-sliding rate relation linear, as predicted by Raj and Ashby [11]? (ii) is there a threshold stress for grain boundary sliding? (iii) what is the qualitative form of the constitutive law for grain boundary sliding?

Given the advent of computational power and the concomitant development in atomistic simulation methods, the latter is a logical route to answer the aforementioned questions and in general to obtain insights into the atomistics of grain boundary sliding. To that end, Qi and Krajewski [13], in a nice work, carried out a molecular dynamics study of a shear test on an Al bicrystal. This study was carried out at 750 K to investigate the effect of applied force and grain boundary mis-orientation on sliding. A linear relationship between constant sliding velocity and applied stress was observed, although the linear fit had positive intercepts indicating a critical value of applied stress below which no sliding was perceived. In other words, their work appears to confirm the linear relation between stress-sliding albeit a sharp threshold stress is predicted—around 0.2 GPa for the material simulated, which is about 10 times lower than the yield strength for the 6 nm grain size used in the simulation [14].

While the work by Qi and Krajewski provided important insights, there is a fundamental limitation of classical molecular dynamics methodology that has prompted us to reexamine this problem with alternative approaches. As is well known, classical molecular dynamics can only handle time-scales of the order of a few pico to nano-seconds. While this is sufficient for several classes of problems, it is a serious deficiency when it comes to the study of creep related phenomena, where the relaxation times are in seconds and sometimes years. In other words, in classical molecular dynamics, the applied strain rate is several orders of magnitude faster than typical grain boundary sliding rates thus preventing conventional molecular dynamics to truly capture the time-dependent nature of the irreversible creep deformation process.

In this communication, we employ a sequence of methods to extract a realistic constitutive law for grain boundary sliding and answer some of the questions raised in the preceding paragraphs. We choose Al bi-crystal as a model material system albeit our approach can be repeated for any material. One motivation for choosing this particular system is that conventional molecular dynamics based results by Qi and Krajewsky [13] are already available, thus facilitating a comparison. Our work is paved by the recent success of the potential energy surface sampling approach (the so-called autonomous basin climbing algorithm [15]). Yip and co-workers have confirmed its applications to several time-dependent problems such as viscosity of supercooled liquids, creep relaxation of metals, and void nucleation rates [16–18]. We note here the recent work by Pattamatta et al. [19] that also shows promise for time-scaling applications.

The simulation layout is as follows (consistent with [13]): An Al bi-crystal was generated by juxtaposing two grains separated initially by a 3 Å gap. The two grains, approximately 60 Å × 40 Å × 20 Å in dimension each, have parallel ⟨1 1 0⟩ axis about which a 25.2° miss-orientation angle is introduced. The simulation cell is periodic along y and z directions to make an infinite grain boundary surface, while non-periodicity in x direction is artificially created by adding a 30 Å vacuum to the two extremes of the bi-crystal (see Fig. 1).

The system was then equilibrated at 300 K under NPT conditions to relax the stresses arising due of the incompatibility of atomic arrangement along the interface. During the course of the simulation, the interfacial gap between the two grains gets filled to form the grain boundary. The correctness of the GB formation was confirmed by calculating the grain boundary energy (0.58 J/m^2), which compares well with Qi et al. [13] (0.548 J/m^2). Our subsequent simulations were carried out at 750 K which is 0.8 homologous temperature; thus well into creep deformation regime. Accordingly, the temperature of the bi-crystal was raised slowly from 300 K to 750 K and subsequently relaxed at 750 K for 50 ps under NPT conditions. The whole structure is subsequently minimized using conjugate gradient iterations. The initial structure of grain boundary interface before commencement of the sliding (computer) experiment is shown in Fig. 2. The GBS can in general be initiated by a strain [17,20] or stress controlled process. Although controlling the strain is a commonly used approach in atomistics, to us it is not the most appropriate to study grain boundary sliding. A strain-controlled simulation would be more appropriate to study creep-stress relaxation, however, sliding (as understood in most creep experiments) appears most clearly via an applied resolved shear stress. Under the application of a shear stress along the grain boundary, we sample the potential energy surface using the Autonomous Basin Climb (ABC) algorithm. This algorithm developed by Kushima and Yip et al. [15,17,16,21] is a modified version of meta-dynamics introduced by Laio and Parinello [22]. The algorithm outputs a list of stable configurations that the system visits successively under given boundary conditions (e.g. an imposed shear stress in the present case). The algorithm moves the system from one energy basin to the other through a series of small activation and relaxation steps. The process starts from a minimum energy configuration, where an activation is introduced by adding a 3 N gaussian penalty function $\Phi_p^k(r)$, centered at the minimum configuration, to the total potential energy of the system:

$$\Phi_p^k(r) = W exp\left[-\frac{(r - r_{min}^k)}{2\sigma^2}\right] \quad (1)$$

where r and r_{min}^k are the atomic configuration at any point and at the kth minimized configuration. The parameters W and σ are constants and determine, respectively, the amplitude (in eV) and width (in ^{2}) of the gaussian penalty function. The choice of these parameters is crucial, and should be carefully adjusted in accordance with the physics of the problem under consideration. For instance, a small W can lead the system to remain in the same well for thousands of iterations, while a large W can lead the system to overcome small barriers without "seeing" them. Once the penalty function is added, the minimum configuration transforms into a saddle point because of the penalty energy (Fig. 3), the system is again relaxed and an activation energy centered at current position is added. This process

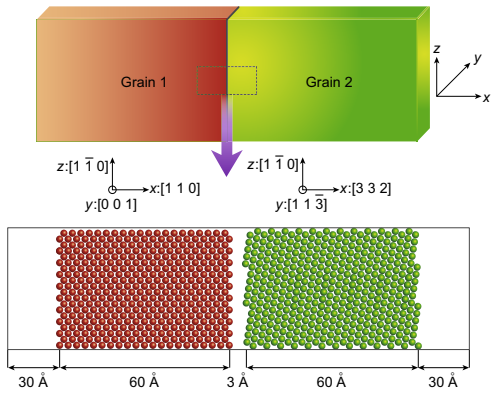

Fig. 1. Orientations of the grains used in the present analysis. Schematics show the convention used to rotate the grain with respect to the other one.