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A simple stochastic model for yielding in specimens with limited number of dislocations

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Abstract

A simple statistical model is developed based on a random distribution and orientation of dislocations in order to explain recent experimental observations of the strength of small specimens containing a limited number of dislocations. Two different types of randomness are introduced, namely, randomness in the spatial location of the dislocations and randomness in the stress needed to activate them. For convenience, the randomness in the activation stress is modeled by assigning a random Schmid factor to the dislocations. In contrast to previous stochastic models, the current model predicts the yield strength not only in the presence of dislocations but also in their absence. Furthermore, the model predicts the scatter in the yield strength in addition to the mean. The model is found to quantitatively explain the yield strength and scatter in micro-compression/tension tests of Mo-alloy fibers using dislocation densities and arrangements measured by transmission electron microscopy. The results of Brenner's classic tensile tests on metallic whiskers are qualitatively reconciled. The model adds credence to the notion that "smaller is stronger" from a purely statistical point of view.

Keywords: Dislocations; Stochastic model; Yield strength; Micromechanics; Size effect

1. Introduction

Over the past decade, there has been significant interest in the mechanical behavior of materials at small length scales due to the unique mechanistic insights offered by testing specimens whose dimensions approach the average dislocation spacing, as well the miniaturization of engineering components to sub-micrometer scales. This has accentuated the need for better characterization tools and pertinent experiments. One such example is the micro-pillar compression test, wherein the initial yield and flow behavior of micrometer size test specimens have been extensively studied, as recently reviewed by Uchic et al. [1]. These experiments offer exciting opportunities to systematically study the effect of specimen size on strength and have given credibility to the popular notion that "smaller is stronger". In small specimens, deformation is often controlled by a limited number of dislocations, and as a result, the yield strength is often very scattered and stochastic as observed by Brenner in his classic tensile tests on metallic whiskers [2]. Brenner had great mechanistic insight, in spite of not having a great deal of supporting microstructural evidence, noting that "the very large scatter in the strength of whiskers as a function of their size indicates that the strengths of the perfect whiskers must be decreased by defects which are distributed statistically in a rather complex manner" [2]. This points not only to the importance of understanding the scatter in strength in such experiments, but also the need for a statistically based approach to model the behavior.

More recently, Johanns et al. [3] have reported results of in situ micro-tensile tests on 10–30 μm long Mo-alloy fibers having nearly square cross-sections with side lengths rang-

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ing from 360 to 550 nm. The fibers were produced by directional solidification of an Mo–NiAl eutectic and were thought to be nearly dislocation free. A large scatter in yield strength was observed in the tensile tests, with strengths ranging from a high near the theoretical strength of ~9.2 GPa down to the bulk strength of ~1 GPa. This was in sharp contrast to micro-pillar compression tests on ~1 μm long specimens of the same material [4], wherein the material yielded consistently at the theoretical strength (~9.2 GPa). An important clue to the difference in behavior came from recent transmission electron microscopy (TEM) observations of the Mo-alloy fibers [5], which revealed that the as-grown fibers were not, in fact, dislocation free, but rather contained a few dislocations with an average linear spacing along the fiber length of about 37 μm. At this spacing, the linear dislocation density (number per unit length) is such that there is a high probability of having a strength-reducing dislocation in a 30 μm tensile specimen, whereas the probability of having one in a 1 μm long compression specimen is very small. Thus, a difference in behavior between the tensile and compression specimens is expected.

In this paper, we use this basic idea to develop a weak-link-based statistical model that numerically describes the behavior. Most of the prior statistical modeling work has been based on molecular dynamics [6,7] or dislocation dynamics [8] assuming a Weibull distribution of strengths. In addition, most statistical models for deformation in small specimens have been based on the nucleation of dislocations [6,7] or the activation of pre-existing dislocations [9–11], but not both. Here, both are considered since they may act simultaneously to produce scatter in the observed strengths. In this context, the approach taken here provides an estimate of not only the mean value of the yield strength, but also an estimate of the scatter in strength and how it may be distributed. We begin by providing a physical description of the model along with a statistically based mathematical development that describes it, and then move onto applying the model to the Mo-fiber experiments and Brenner's observations for copper whiskers.

2. Modeling approach

Fig. 1 shows a schematic overview of the proposed weak-link one-dimensional (1-D) model, wherein random test sections of length ℓ are drawn from a large sample space of length L and subjected to compression or tensile testing. If the randomly drawn test sections are dislocation free, then dislocations must first be nucleated and the specimen yields at the theoretical strength. However, if the specimen contains dislocations, then yielding is determined by the dislocation that needs the lowest stress for activation and movement. Hence, the yield strength depends both on the spatial distribution of dislocations and the distribution of their activation strengths. In this way, the dislocation distribution in the test section of length ℓ can be considered to be comprised of two types of randomness, namely, randomness in the spatial distribution of the dislocations and randomness in the strength of the dislocations, i.e. the stress needed to activate them. While the randomness in the spatial distribution is fairly straightforward to describe, the randomness in the activation stress can be modeled in several different ways, e.g. a random Schmid factor, variable source length, solute distribution, crystal orientation, etc. For simplicity, the randomness in the activation stress is modeled here by assigning a random Schmid factor to the dislocations, although other types of randomness could also be included in the basic modeling framework. A mathematical description for the model is developed in closed form by simple statistical methods and independently verified using Monte Carlo techniques. The Monte Carlo simulations help not only in validating the analytical model but also in visualizing the scatter in strength expected when only a limited number of tests are conducted.

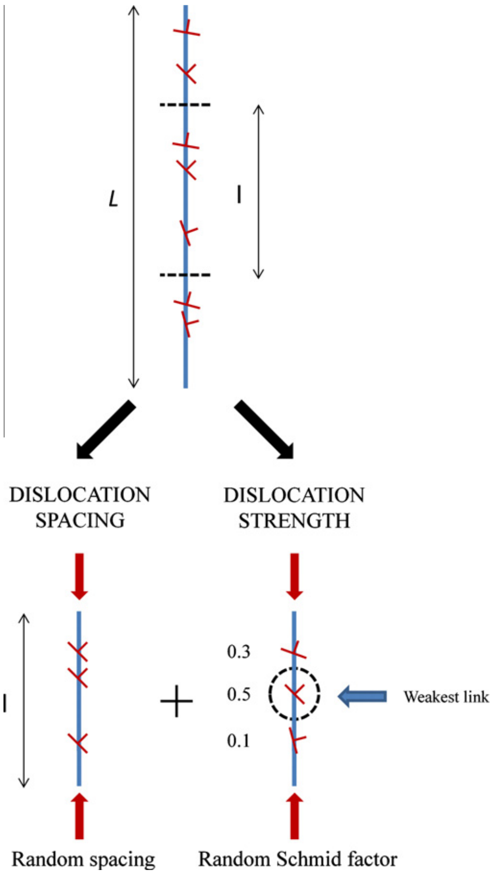

Fig. 1. Generic framework to model the yield strength of small one-dimensional specimens with a limited number of dislocations.

The model development is presented in four parts. First, a simple model for yielding based on randomness in the spatial distribution of the dislocations is developed in Section 2.1. This model is then extended in Section 2.2 to include randomness in the activation stress by assigning a random Schmid factor to the dislocations. A mathematical description for the scatter in the yield strength is presented in Section 2.3, and finally, the model is extended to two-dimensional (2-D) dislocation structures in Section 2.4.