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Section 4. Mechanical behavior of irradiated materials

On the relationship between uniaxial yield strength and resolved shear stress in polycrystalline materials

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Abstract

Attempts to correlate radiation-induced microstructural changes with changes in mechanical properties rely on a well-established theory to compute the resolved shear stress required to move dislocations through a field of obstacles. However, this microstructure-based shear stress must be converted to an equivalent uniaxial tensile stress in order to make comparisons with mechanical property measurements. A review of the radiation effects literature indicates that there is some confusion regarding the choice of this conversion factor for polycrystalline specimens. Some authors have used values of 1.73 and 2.0, based on an inappropriate application of the von Mises and Tresca yield criteria, respectively. The basic models pertinent to this area of research are reviewed, and it is concluded that the Taylor factor with a value of 3.06 is the correct parameter to apply in such work.

1. Introduction

The relationship between radiation-induced microstructural evolution and changes in mechanical properties has been the subject of considerable research for many years. Much of this work has been carried out under the auspices of various national research programs on fusion reactor materials, and can be found in the proceedings of the US Topical Meetings on Fusion Reactor Materials and the International Conferences on Fusion Reactor Materials [1]. While only incremental improvements have been made in measuring hardness or tensile properties during this period, continuing advances in transmission electron microscopy (TEM), atom probe field ion microscopy, and various X-ray and neutron scattering techniques have provided a much more detailed description of the irradiated microstructure. Since the theory needed to compute the increment in matrix hardening from a given distribution of dislocation obstacles is well established [2–9], this improved microstructural characterization should lead to good agreement between observed microstructural and mechanical property changes and enable better estimates of parameters in the hardening theory to be obtained. However, an examination of the radiation effects literature published over the last 30 years is not uniformly encouraging.

The purpose of this short paper is to point out a particular error that has frequently been made when microstructural measurements are used to predict mechanical property changes in irradiated materials. This process involves calculating the increase in shear strength required to move dislocations through a field of obstacles of a given type, and then converting that shear strength to an equivalent uniaxial yield strength. The Taylor factor (3.06) is the most appropriate parameter to use in this conversion. Values of 1.73 and 2.0 have also been used, apparently as a result of a misunderstanding about the proper application of the von Mises and Tresca yield criteria.

2. Hardening due to radiation-induced defect structures

The initial model used to compute matrix hardening by barriers to dislocation motion was developed by Orowan [2] for impenetrable obstacles, those which are hard enough that the dislocation is unable to cut through them and can only pass through the field of

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obstacles by bowing around them. For simplicity, the following discussion considers the case of only a single type of obstacle. Based on Orowan's model, the most commonly used expression for the change in shear stress, $\Delta\tau_s$, induced in the dislocation glide plane by a regular array of defects is shown in the following equation:

$$\Delta\tau_s = \alpha G b (Nd)^{0.5}, \tag{1}$$

where G is the shear modulus of the matrix, b the magnitude of the dislocation Burgers vector, N the defect number density, d the defect diameter, and the square-root factor is the reciprocal of the average distance between obstacles. In principle, the α factor in Eq. (1) is determined by the angle between adjacent dislocation segments at the point where the dislocation breaks free of the obstacle [8]; if the critical angle is $\Phi, \alpha = \cos(\Phi/2)$. This factor is typically referred to as the 'barrier strength', and accounts for the fact that some obstacles may be partially cut or sheared by the dislocation as it bows out. This reduces the amount of energy required for a dislocation to glide through the field of obstacles, and the barrier strength is intended to provide a relative measure of the defect's ability to impede dislocation glide. For impenetrable Orowan obstacles, $(\Phi/2) = 0$ and $\alpha = 1.0$. In practice, relatively few measurements of the critical angle have been made for radiation-induced defects. Rather, a comparison of microstructural observations and mechanical property measurements has been used to infer values of α for different types of defects [1].

Various corrections to the Orowan equation have been proposed [7–9], and one of the updated versions is given by Kelly [8]:

$$\Delta\tau_s = \alpha \frac{0.83\, Gb}{[(Nd)^{-0.5} - d]} \frac{\ln(d/r_0)}{2\pi(1-\nu)^{0.5}}, \tag{2}$$

where ν is Poisson's ratio and r_0 is the dislocation core radius. The factor 0.83 in Eq. (2) accounts for a random distribution of particles, the denominator in the second factor corrects the particle spacing for finite particle size, and the final factor provides an improved estimate of the dislocation line tension and the interaction between line segments when the dislocation is bowing around an obstacle. The α factor has been included in Eq. (2) to indicate its correspondence with Eq. (1). The overall result of these corrections lowers the predicted shear stress, and quite different values of α will be obtained if Eq. (1) is used rather than Eq. (2).

3. Yield criteria and compatibility criteria

In order to compare the shear stress value obtained from Eqs. (1) or (2) with a measured uniaxial yield strength, a conversion factor must be applied. It is evident from the literature in this area that some confusion exists regarding the selection of this conversion factor. It appears that the errors in the literature may have arisen because the distinction between two different, but related problems was misunderstood. The first problem is that of relating multi-axial yield behavior to uniaxial yield behavior. There are two commonly applied solutions to this problem, one by von Mises which is referred to as the von Mises yield criterion [10]. The other is the Tresca yield criterion [11]. The second problem relates yield in polycrystalline materials to that in single crystals. Work of von Mises, the von Mises compatibility criterion, was also applied in developing a solution to this problem [12].

3.1. Yield criteria

Most engineering tensile data are obtained from uniaxial tensile tests, while engineering structures are typically used in multi-axial stress states. The von Mises yield criterion states that yielding under multi-axial conditions initiates when the elastic distortion energy reaches a critical value. In the case of pure shear, the yield strength is reduced relative to uniaxial tension: $\sigma_y(\text{shear}) = \sigma_y(\text{tension})/(3)^{0.5}$. The Tresca yield criterion assumes that yield occurs when the maximum resolved shear stress on any plane reaches some critical value. In the case of pure shear, the yield strength is reduced relative to uniaxial tension: $\sigma_y(\text{shear}) = \sigma_y(\text{tension})/2$. There are many examples in the radiation effects literature in which either the von Mises or Tresca yield criteria is quoted as the reason for using a conversion factor of $(3)^{0.5}$ or 2.0 to obtain a uniaxial tensile strength from the shear stress computed with Eqs. (1) or (2). However, this is a misapplication of the concept of yield criteria since the problem at hand is not that of comparing uniaxial and multiaxial stress conditions.

3.2. Compatibility criteria

One of the basic elements of elasticity theory is that deformation must occur in such a way as to maintain the continuity of the material. This requirement can be expressed mathematically as a set of compatibility equations. The von Mises compatibility criterion arose from his demonstration that five independent slip systems were required for a material to undergo plastic deformation by slip [12]. In the absence of sufficient slip systems, phenomena such as grain boundary sliding, pore formation, cracking, or fracture will occur to accommodate the deformation. His compatibility criterion essentially states that all the grains in a polycrystalline material must undergo the same deformation (strain) as the overall specimen deformation. The von Mises compatibility criterion is relevant to the problem of obtaining the correct factor for converting shear stress to tensile stress in polycrystalline samples.

4. Yielding in a uniaxial tensile test: role of resolved shear stress

When a single crystal specimen is loaded in uniaxial tension, the applied stress, σ_u, is resolved on the slip planes in the material as illustrated in Fig. 1. The resolved shear stress, τ_s on any given plane is determined by the angle between the plane normal and the applied stress: $\tau_s = \sigma_u \cos(\phi) . \cos(\theta)$. Yielding occurs by dislocation slip when the resolved shear stress on one of the planes exceeds a critical value. The Schmid factor, m, is defined as the ratio of the resolved shear stress to the axial stress, $m = \cos(\phi)\cos(\theta)$, or $\sigma_u = \tau_s/m$ [13]. The maximum value of m occurs when the shear plane is at a 45° angle to the applied stress and $m_{max} = \cos(45) \cos(45) = 0.5$. Alternately, the minimum value of σ_u(single crystal) $= 2\tau_s$.

The relationship between σ_u and τ_s is of course the same in polycrystalline specimens, but is complicated by the fact that maximum resolved shear stress will vary from one grain to another. In addition, material compatibility and continuity act to limit the deformation of any one grain that may be favorably oriented for slip. By applying a simple compatibility criterion and assuming that all the grains in the material deformed uniformly,

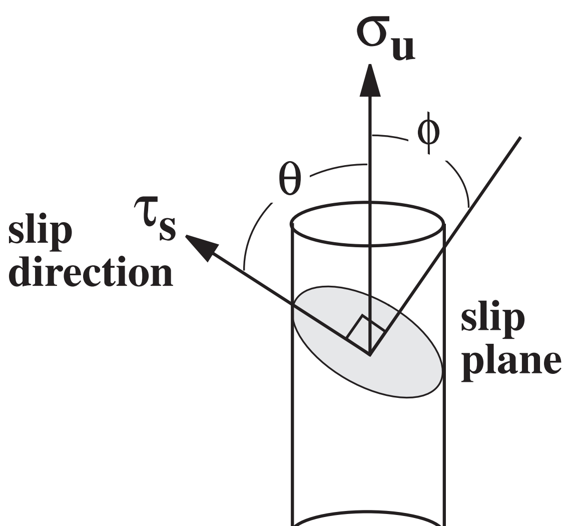

Fig. 1. Illustration of resolved shear stress in tensile test with a single crystal specimen.

Taylor [3,4] derived a relationship between uniaxial yield strength and the resolved shear stress in a polycrystal. Such an analysis amounts to determining an effective average reciprocal Schmid factor for the polycrystalline material. The average value obtained by Taylor for fcc aluminum was about 3.06 and has since been termed the Taylor factor. Subsequently, Bishop and Hill [5] performed a more general analysis for fcc materials and found the same value of 3.06. Further work by Kocks [6] led to the same value, and indicated that the average Taylor factor for bcc materials that slip on $\{1\,1\,0\}$ planes is also 3.06. Thus, for most of the engineering materials of interest to the fusion reactor community, the Taylor factor, $T = 3.06$, and $\Delta\sigma_u$(polycrystal) $= T\Delta\tau_s$.

Taylor's value of 3.06 is actually an upper limit for the ratio of uniaxial yield strength to resolved shear stress [3,4,6]. However, his research indicated that this value provided good agreement with experimental data on aluminum. Kocks' more detailed analysis [6] demonstrated that this upper limit should be close to the actual solution. Although slightly lower values may be obtained for specific slip systems or due to material texture [6], it seems sensible to recommend that the value of 3.06 be used to provide a standard basis of comparison when publishing results of microstructure-mechanical property correlations.

5. Summary

Confusion between the von Mises (and Tresca) yield criteria and analysis based on the von Mises compatibility criterion has led to the use of incorrect parameters when calculated resolved shear strengths (based on microstructural measurements) are converted to equivalent uniaxial yield strengths (for comparison with measured tensile data). The use of these varied and incorrect conversion factors has limited our ability to correlate data from different research groups and to arrive at consistent estimates of dislocation barrier strengths. In the case of most polycrystalline bcc and fcc materials, the Taylor factor of 3.06 is the most appropriate parameter to use.

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