DEFORMATION AT THE LIMIT OF ELASTIC STABILITY

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ABSTRACT

We describe mechanical behavior in a defect-free world and find many familiar features. Among them: (1) In a world governed by elastic stability, the common bcc metals would exhibit "pencil glide" in $\langle 111 \rangle$ and would cleave on $\{100\}$. They would be "conditionally brittle" at low temperature. (2) The common fcc metals would glide on $\{111\}$ and would not cleave under simple tensile loads. They would be ductile at low temperature. (3) The maximum values of the nanohardness of simple metals would be very nearly what they are.

1. INTRODUCTION

We think it appropriate that a conference devoted to the status of the dislocation theory contains at least one paper that ruminates on what the world would be like if there were no such thing: if the world were a theorist's dream (though a metallurgist's nightmare) in which all solids were perfect crystals undisturbed by defects of any kind. In such a world solids would shear, and they would break in tension, but their strengths would be governed by the elastic stability of the lattice rather than the critical resolved shear stress.

There are, in fact, several practical reasons to be interested in behavior at the limit of elastic stability [1]. First, elastic instability defines the ideal limit of strength [2-4], and it is sometimes useful to know the highest strength a particular material can possibly have. Second, the elastic limit is actually reached, or, at least, closely approached in a number of experimental situations. The most common case is deformation via stress-induced phase transformations, as in certain austenitic steels and in Si in indentation. However, even normal, ductile metals seem to approach the limit of strength in nanoindentation experiments, and stronger alloys may also do so in the region of stress concentration ahead of a crack. Finally, elastic instability is one of the few problems in solid mechanics that can actually be solved *ab initio*. Existing pseudopotential codes are capable of following elastic deformation to the point of instability with reasonable accuracy, and a number of calculations have been done [1,5-8].

The authors have been studying the limits of strength for some years now. In the course of that investigation we have often been surprised both by the simplicity and the

familiarity of behavior at the limit of strength. A surprising variety of mechanical behaviors that are ordinarily attributed to the peculiarities of dislocations would also be found in a defect-free world at low temperatures at which thermal activation is unimportant. In the limited space available here we discuss three examples. (1) In a defect-free world, the common bcc metals would exhibit "pencil glide" in $\langle 111 \rangle$ and would cleave on $\{100\}$. They would be "conditionally brittle". (2) The common fcc metals would glide on $\{111\}$ and would not cleave under simple tensile loads. They would be ductile. (3) The maximum values of the nanohardness of simple metals would be very nearly what they are.

2. BCC METALS

Computations of the ideal tensile strengths of unconstrained bcc metals show that they are weakest when pulled in a $\langle 100 \rangle$ direction, and would, therefore, be expected to cleave on $\{100\}$ planes. *Ab initio* calculations [1,9,10] give an ideal tensile strength of about 30 GPa for W ($0.07E_{100}$), and an approximate value around 10.5 GPa for Fe ($0.08E_{100}$) where E_{100} is the tensile modulus in the $\langle 100 \rangle$ direction.

There is a simple crystallographic argument that explains both the cleavage plane and the ideal tensile strength (Fig. 1). Applying a uniaxial tensile stress along $\langle 100 \rangle$ carries the bcc structure into an fcc structure with the same volume at a tensile strain of 0.26 (the "Bain strain"). By symmetry, both structures are unstressed, so the tensile stress must pass through at least one maximum along the transformation path, at a critical strain much less than 0.26. If we assume a single maximum (that is, if fcc symmetry produces an energy maximum along the strain path) and fit the stress-strain curve with a sinusoid that has the correct modulus at low strain, the tensile strength in $\langle 100 \rangle$ is given by

$$\sigma_m \approx 0.08E_{100} \quad (1)$$

in agreement with the *ab initio* calculations.

The ideal shear strength of a bcc metal also reflects its symmetry. In our study of tungsten [9], we calculated the ideal strengths of all of the experimentally observed slip systems in bcc metals. The strength for slip in a $\langle 110 \rangle$ direction on a $\{110\}$ plane was 19.3 GPa. The strengths for relaxed shear (uniaxial stress) in the $\langle 111 \rangle$ direction on the

Fig. 1: The Bain strain connecting the bcc and fcc structures. If bcc is pulled in tension on $[001]$ while contracting along $[100]$ and $[010]$ it generates an fcc crystal as shown.

$\{110\}$, $\{112\}$ and $\{123\}$ planes were almost identical: $\tau_m \approx 17.7 \text{ GPa} \approx 0.11G_{111}$, where G_{111} is the shear modulus for shear in the $\langle 111 \rangle$ direction. While we did not check all possible slip systems, it seems very probable that the minimum should involve shear in a close packed direction, and it is likely that the minimum strength for any slip system in bcc will be $\approx 0.11G_{111}$. In all three cases the shear strain at instability is about 0.17. A calculation for Mo gives similar results, with $\tau_m \approx 15.6 \text{ GPa} \approx 0.12G_{111}$. The symmetry rule that governs this case is illustrated in Fig. 2. Essentially, a shear in the $\langle 111 \rangle$ direction tilts planes that are perpendicular to the $\langle 111 \rangle$ axis. If we allow relaxation of the atom positions in these planes, they come into an atomic registry that changes the crystal symmetry at a shear strain of ≈ 0.34 , irrespective of the plane of tilt (the shear plane). There is, hence, a maximum in the shear strength at about half this shear, 0.17. If we fit the stress-strain relation with a sinusoid that gives the correct modulus in the elastic limit, we obtain

$$\tau_m \approx 0.11G \quad (2)$$

in good agreement with the *ab initio* calculations.

A number of bcc metals have similar strengths for slip in the $\langle 111 \rangle$ direction on various planes, a phenomenon that is known as “pencil glide” and is attributed to the peculiarities of dislocation glide in bcc. These calculations show that defect-free crystals would behave in a very similar way.

The balance between the shear and tensile strengths suggested by eqs. (1) and (2) is such that, in a defect-free world, the common bcc metals would cleave if loaded along $\langle 100 \rangle$, but not if loaded in other directions. Taking W as an example, a uniaxial load along $\langle 100 \rangle$ would reach the ideal cleavage strength, $\approx 30 \text{ GPa}$, when the shear stress in the most favorable slip system was only around 14 GPa, below the ideal shear strength. However, a uniaxial load along $\langle 111 \rangle$ or $\langle 110 \rangle$ would cause the shear strength to be exceeded before the tensile stress in $\langle 100 \rangle$ reached the ideal value. A single crystal would be ductile or brittle, depending on the direction of the load.

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2. FCC METALS

The tensile strength of defect-free fcc crystals could, in theory, also be governed by the Bain strain. As illustrated in Fig. 3, an fcc crystal can be converted into bcc by straining in tension in the $[110]$ direction. The tensile strain required to reach bcc is, in fact, relatively small, so the estimated strength would be small as well. However, reaching bcc from fcc with a $[110]$ pull requires very substantial relaxations in the perpendicular directions. The crystal must expand equally along $[1-10]$, and contract to an even greater degree along $[001]$. These large relaxations are inconsistent with the Poisson contractions of typical fcc metals in the linear elastic limit. Fcc metals do not start out along this deformation path when pulled along $[110]$ and, apparently, never find it.

Nonetheless, the $[110]$ direction does seem to be the weak direction for tension in fcc. Defect-free fcc metals have very high tensile strengths when pulled along $[100]$ or $[111]$, but are relatively weak when pulled along $[110]$. Our own recent (unpublished) *ab initio* calculations of Al and Cu give $[110]$ tensile strengths of 5.2 GPa ($0.07E_{110}$) and 6.5 GPa ($0.05E_{110}$) respectively. (These numbers are reasonably close to those Milstein and Chantasiriwan [11] found from an “embedded atom” model, but the Cu value is very different from that published by Sob, et al. [10]. The latter authors apparently did not allow asymmetric relaxation in the plane perpendicular to $[110]$.) The common weakness in the $\langle 110 \rangle$ directions suggests an extremum dictated by symmetry, but we have not yet identified it.

By contrast, the shear behavior of defect-free fcc crystals is conventional. The weak directions in shear are $\langle 112 \rangle$ directions in $\{111\}$ planes, as one would expect from a rigid-ball model of the close-packed fcc structure. There is significant relaxation in the plane as the shear approaches instability, which is significantly different in character for Al and Cu [12]. However, in both cases [8] the ideal shear strength is about $0.08G_{111}$: 1.85 GPa ($0.084G_{111}$) for Al, 2.65 GPa ($0.088G_{111}$) for Cu.

The shear strengths of Al and Cu are low enough to insure that defect-free material will be ductile under normal conditions. Even though the ideal tensile strengths of these crystals are not very high when they are pulled along $\langle 110 \rangle$, the shear stresses on

Fig. 3: Bain strain of an fcc lattice through tension along $[110]$. The crystal must expand equally along $[1-10]$, and contract dramatically along $[001]$.

the most favorably oriented slip systems are exceeded well before the ideal tensile strength is reached.

3. NANOINDENTATION

A nanoindentation test is, essentially, a microhardness test done with a nanotipped indenter. Until the substrate yields, the deformation field of the indenter should be approximately Hertzian, which makes it possible to use the data to infer the stresses and strains at which yielding occurred. Moreover, since the maximum shear in a Hertzian strain field is well beneath the surface, nanoindentation tests can sample defect-free volumes, and may, therefore, test the ideal strength.

Surprisingly, the shear strengths inferred from recent nanoindentation tests substantially exceed the computed ideal strengths. Thus, Bahr, et al. [13] report data showing shear stresses as high as 28 GPa in W prior to yielding, well beyond the value (18 GPa) that corresponds to the ideal strength on any of the common slip planes. Nix [14] reported preliminary Mo data giving a maximum strength of 23 GPa, compared to the theoretical shear strength of 15.6 GPa.

The discrepancy between these values is largely removed if one recognizes that the Hertzian stress field is modified by non-linearity as the ideal strength is approached. If we assume (on geometric grounds) that the Hertzian solution gives a reasonable approximation to the strain field, but, because of the softened moduli, mis-estimates the stress at the instability, and use sinusoidal stress-strain dependence, we obtain the maximum shear stress

$$\tau_m = \left[\frac{2}{\pi} \right] \tau_H = 0.64 \tau_H \quad (3)$$

where τ_m is the ideal shear strength and τ_H is the instability stress inferred from the linear elastic Hertzian stress field. A preliminary finite-element calculation using a sinusoidal stress-strain relation confirms the small perturbation of the Hertzian strain field, but

Fig. 4: Maximum τ under a rigid indenter, with linear and sinusoidal stress-strain relations. When the shear stress of the sinusoidal material hits maximum, it is about $0.69 \tau_{\text{linear}}$.

shows the large effect on the stress field (Fig. 4). In this case, $\tau_m \approx 0.69 \tau_H$, in reasonable agreement with eq. 3. Using eq. (3), the measured shear strength of W drops to 17.8 GPa while that of Mo drops to 14.6 GPa, in good agreement with the theoretical estimates.

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