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Elastic Stability and the Limits of Strength

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Abstract. The upper limit of strength (the "theoretical strength") has been an active subject of research and speculation for the better part of a century. The subject has recently become important, for two reasons. First, given recent advances in *ab initio* techniques and computing machines, the limits of strength can be calculated with considerable accuracy, making this one of the very few problems in mechanical behavior that can actually be solved. Second, given recent advances in materials engineering, the limits of strength are being approached in some systems, such as hardened or defect-free films, and their relevance is becoming recognized in others. The present paper discusses some interesting results from recent research on the limits of strength, with an intermixture of speculations based on those results. Topics include the inherent nature of {100} cleavage and "pencil slip" in bcc metals, the inherent ductility of fcc metals, the anomalous properties of Al, and the possibility of measuring ideal strength with nanoindentation.

Introduction

It is, perhaps, appropriate that a conference devoted to the thermal processing of materials contain at least one paper that considers what the world would be like if processing were unnecessary and irrelevant; 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 the forces required to deform or fracture solids would be determined solely by the elastic stability of the parent crystal lattice.

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 strength [2-4], and it is useful to know the highest strength a particular material could possibly have. Second, the elastic limit is reached, or, at least, closely approached in a number of experimental situations. A familiar example is deformation via stress-induced phase transformations, as in certain austenitic steels. 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. Third, 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 were done through the 1990's [1,5-8].

In the course of a continuing study of elastic instability, the authors have been impressed by the simplicity and the familiarity of behavior at the limit of strength. A surprising variety of mechanical phenomena that are ordinarily attributed to the peculiarities of dislocations would also be found in a defect-free world. In the limited space available here we discuss three examples. (1) In a defect-free world, the common bcc metals would would cleave on {100} and exhibit "pencil glide" in <111>. Most would be brittle at low temperature. (2) The common fcc metals would glide in {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.

BCC Metals

Ideal strength in tension. Computations of the ideal tensile strengths of unconstrained bcc metals show that they are weakest when pulled in a <100> direction. The majority of those we have investigated fail in tension (cleave) on {100} planes. *Ab initio* calculations [1,9-13] give an ideal tensile strength of about 30 GPa for W ($0.07E_{100}$), 29 GPa for Mo ($0.\ 078E_{100}$) and 13 GPa for Fe ($0.087E_{100}$) where E_{100} is the tensile modulus in the <100> direction, and the stresses are computed at 0K.

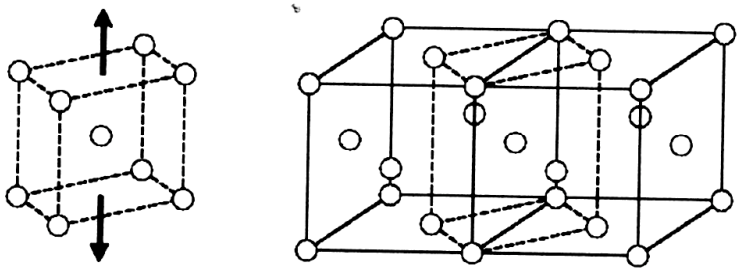

Fig. 1: The Bain strain connecting the bcc and fcc structures. If bcc is pulled in tension on [001] while contracting along [100] and [010] it generates an fcc crystal as shown.

There is a simple crystallographic argument that explains both the cleavage plane and the ideal tensile strength (Fig. 1). A relaxed tensile strain along <100> 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 stain much less than 0.26. If we fit the stress-strain curve to a sinusoid that has the correct modulus at low strain, the tensile strength in <100> is given by

$$\sigma_m \sim [e_B/\pi]E_{100} = 0.08E_{100} \qquad (1)$$

where e_B is the Bain strain and E_{100} is Young's modulus for <100> tension.

The same reasoning explains why the ideal strength increases when the normal tension is supplemented by a hydrostatic tension, as it is, for example, near the tip of a crack. Hydrostatic tension expands the unit cell, which increases the Bain strain and raises the stress at instability. *Ab initio* calculations for Fe [14] show that the ideal tensile strength increases by almost 50% when the tensile stress is supplemented by a hydrostatic tension that is equal in magnitude.

The element Nb is anomalous among the bcc metals we have studied [10,15]. While the ideal tensile strength of Nb is lowest for <100> loading, as in the other bcc's, the failure mode is not in tension across the {100} planes, but in shear on the <111>{112} system. After some significant

tensile strain, Nb deviates from the tetragonal, Bain strain path onto an orthorhombic strain path that is characterized by unequal contractions in the <100> directions perpendicular to the axis of load. The eventual failure is in shear, rather than tension. This preference for shear failure is preserved, though with a smaller margin, when hydrostatic tension is superiomposed. The results suggest that Nb may not exhibit the ductile-brittle transition that is typical of bcc metals. The experimental evidence is unclear [10].

Ideal strength in shear. The ideal shear strengths of bcc metals also reflects their symmetry. Calculations of the ideal strength of bcc W [19, 15] in relaxed shear in the <111> direction on the {110}, {112} and {123} planes give almost identical values, $\tau_m \sim 17.7$ GPa $\sim 0.11G_{111}$, where G_{111} is the shear modulus for shear in the <111> direction. In all three cases the shear strain at instability is about 0.17. Calculations for Fe [13] and Mo [10] give very similar results, with $\tau_m \sim 7.2$ GPa ($0.11G_{111}$) for Fe, ~15.8 GPa ($0.12G_{111}$ for Mo). Nb is, again, unusual; the ideal shear strength in the <111>{112} system is anomonously large, 6.4 GPa ($0.15G_{111}$), and is still larger for the common alternative systems [10].

The symmetry rule that governs the shear strength of typical bcc's is illustrated in Fig. 2 [10,15]. Essentially, a shear in the <111> direction tilts planes that are perpendicular to the <111> 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. This common stress-free, saddle-point structure is body-centered tetragonal. There is a maximum in the shear strength at about half the saddle-point shear, at e ~ 0.17. If we fit the stress-strain relation with a sinusoid that gives the correct modulus in the elastic limit, we obtain

$$\tau_m \sim 0.11G_{111} \qquad (2)$$

in good agreement with the *ab initio* calculations.

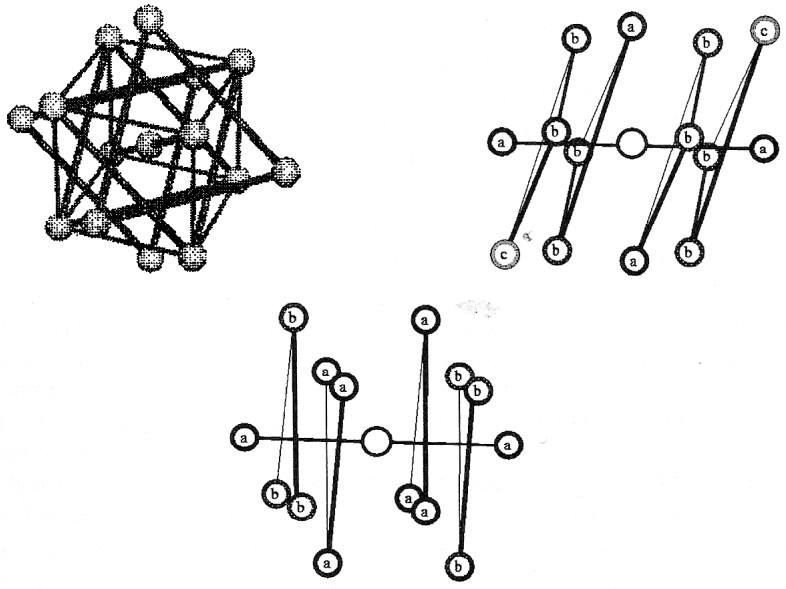

Fig. 2: Instability in shear in [111]. [111] shear tilts planes of atoms (equilateral triangles perpendicular to [111]) until they come into registry, as at right, creating a new symmetry.

A number of bcc metals have similar strengths for slip in the <111> 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 bcc crystals would tend to 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 <100>, but not if loaded in other directions. Taking W as an example, a uniaxial load along <100> would reach the ideal cleavage strength, ~ 30 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 <111> or <110> would cause the shear strength to be exceeded before the tensile stress in <100> reached the ideal value. A single crystal would be ductile or brittle, depending on the direction of the load.

FCC Metals

Ideal strength in tension. The tensile strength of defect-free fcc crystals could, in theory, also be governed by the Bain strain [16]. 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 along $[\bar{1}10]$, 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.

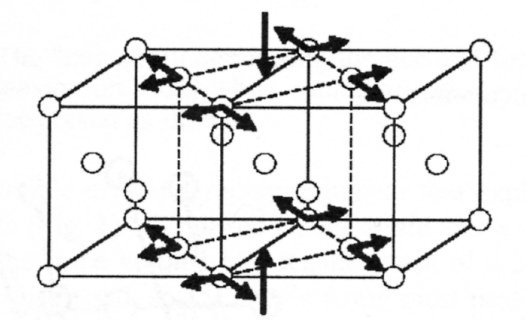

Fig. 3: Bain strain of an fcc lattice through tension along [110]. The crystal must expand equally along $[\bar{1}10]$ and contract dramatically along [001].

Nonetheless, the <110> directions are the weak directions for tension in all of the fcc metals that have been studied to date: Al, Cu, Ir and Pd [17]. If the fcc crystal is pulled quasistatically to failure under uniaxial tension, the failure mode at the elastic limit is not a tensile failure across the perpendicular {110} plane, but rather a shear failure (the "flip strain"). In this deformation mode the <110> tensile direction is stretched while the perpendicular <100> direction contracts, with the ultimate consequence that the two directions are interchanged. It can be shown that the failure mode is, in fact, a failure in shear in the <112>{111} system, which is the normal mode of shear failure in an fcc crystal.

This result suggests a simple explanation for the fact that fcc crystals do not exhibit a conventional ductile-brittle transition on cooling; the inherent failure mechanism is in shear. Those fcc metals that do become brittle at low temperature, such as Ir and nitrided austenitic steels, do so only after significant plastic deformation; their "cleavage" is by decohesion on slip or twin planes.

If we assume deformation at constant volume with a sinusoidal stress-strain curve, the "flip" instability occurs at an engineering strain of 0.08 and a stress of $\sigma_m = 0.05E_{110}$, where E_{110} is Young's modulus for tension in the <110> direction. The most recent *ab initio* calculations of the ideal tensile strengths of fcc metals under quasistatic loading give the following values: for Al, σ_m = 5.2 GPa = $0.07E_{110}$, for Cu, σ_m = 6.2 GPa = $0.05E_{110}$, for Pd, σ_m = 5.2 GPa = $0.06\ E_{110}$, and for Ir, σ_m = 36 GPa = $0.06E_{110}$ [17]. Note that the exceptional strength of Ir is a consequence of its large elastic modulus, and is in no way anomalous. The anomaly is the high dimensionless strength of Al. However, recent research has shown that the actual strength of Al is determined by a phonon instability that intrudes slightly before the elastic instability, decreasing the ideal strength. No similar instability has been found in other fcc's.

The ideal strength in shear. The mode of failure of fcc crystals in shear is conventional, though the behavior of at least some fcc's, Al in particular, is not. The weak directions in shear are <112> directions in {111} planes, as one would expect from a rigid-ball model of the close-packed fcc structure. A sinusoidal model of that failure mode predicts a shear strength, $\tau_m \sim 0.085G_{111}$.

The ideal shear behavior of Al and Cu [17,18] make an interesting comparison. While the deformation of Cu remains nearly planar in the {111} shear plane as the instability is approached, Al expands significantly perpendicular to the shear plane. The consequence is that while Cu has an ideal strength near the estimate, τ_m = 2.7 GPa ~ $0.11G_{111}$, the calculated shear strength of Al is much larger, both in absolute magnitude and in dimensionless terms: $\tau_m \sim 3.4$ GPa = $0.15\ G_{111}$. (This number is a bit of an overestimate, since Al experiences a phonon instability before reaching peak strength [19], but is qualitatively correct. It is significantly higher than the number reported in earlier work [8], which used a less accurate pseudopotential.)

Comparing the ideal tensile and shear strengths of Al and Cu leads to a curious result: at the limit of strength, Cu is stronger than Al in tension, though weaker in shear. This is true despite the fact that the failure mode is precisely the same in the two cases: a shear instability in the system <112>{111}. The reason is the perpendicular expansion of Al during shear. Tension in the <110> direction imposes a tension across the {111} shear plane, assisting the normal displacement of {111}planes and lowering the stress required for Al to fail in shear.

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. [20] 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 [21] 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 almost entirely removed if one makes two corrections [22]. First, the Hertzian stress field is modified by non-linearity as the ideal strength is approached. Finite-element calculations using a sinusoidal stress-strain relation show that the Hertzian stress field is correct except in the immediate vicinity of the maximum shear stress, even when the maximum shear stress approaches the ideal strength. However, the value of the maximum shear stress is significantly decreased, to $\tau_m \sim 0.69\ \tau_H$, where τ_H is the Hertzian value. Second, the

triaxiality of the stress field near the point of maximum shear increases the ideal shear strength. When these (and a couple of other, minor corrections) are made the maximum shear strengths that can be inferred from nanoindentation experiments on W (22.8-24.0 GPa) and Mo (16.0-16.8 GPa) are very close to the theoretical values of the ideal strength (W = 22.1-23.3 GPa; Mo = 17.6-18.8 GPa), as they should be. This result suggests that nanoindentation may provide a viable means for measuring ideal strength.

Acknowledgements

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