Ideal Shear Strengths of fcc Aluminum and Copper

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The ideal shear strength is the minimum stress needed to plastically deform an infinite dislocation-free crystal and is an upper bound to the strength of a real crystal. We calculate the ideal shear strengths of Al and Cu at zero temperature using pseudopotential density functional theory within the local density approximation. These calculations allow for structural relaxation of all five strain components other than the imposed shear strain and result in strengths on $\{111\}$ planes of 1.85 and 2.65 GPa for Al and Cu, respectively (8%–9% of the shear moduli). In both Al and Cu, the structural relaxations reduce the ideal shear strengths by 35% to 45%, but the directions of relaxation strain in each are qualitatively different. [S0031-9007(99)08769-4]

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The mechanical strength of a typical structural material is a complex, microstructure-sensitive property that has not been successfully attacked with *ab initio* models. The reason is that any realistic model must treat a large number of interacting dislocations for long periods of time, which requires calculations of a size and duration well beyond even the projected capabilities of known computing machines. However, the mechanical strength of a material is bounded from both above and below. The upper limit is the lesser of two critical stresses: the ideal shear strength, at which the material becomes unstable with respect to spontaneous plastic deformation in shear; and the cleavage stress, at which the material becomes unstable with respect to fracture by the spontaneous separation of atomic planes.

The upper limit of strength is of obvious interest in the science of strong solids, and theorists have attempted to compute it from atomic models since at least the 1920s [1,2]. Relevant work through the mid-1980s is summarized by Kelly and Macmillan [3]. The bulk of this work relies on the use of semiempirical bonding functions that have simple mathematical form. More sophisticated bonding models have been used in recent years [4–8]; some of which employ first-principles methods. Much of the recent work [5,8] on the shear strength follows Frenkel [2] in confining the shear to a displacement between two adjacent atomic planes. Other researchers permit uniform shear but constrain the deformation to be rigid in the shear plane [4,6,7]. These constraints are often unphysical, will always increase the predicted shear strength, and may produce significant overestimates [5,8]. To our knowledge, the work presented here is the first to accurately explore the very significant effects of full atomic relaxation.

Recent advances in theory and computational capability have made it possible to do *ab initio* calculations of the ideal shear and cleavage strength by deforming unconstrained crystals to failure. This paper specifically computes the ideal shear strengths of Al and Cu in the fully unconstrained case. The shear strength is calculated as the stress required to induce instability in a homogeneous, quasistatic shear in a $\langle 112\rangle$ direction in a $\{111\}$ plane, which is the weak direction for shear in these fcc crystals. Both constrained and fully unconstrained shears are treated. Since the calculation is quasistatic, it does miss possible phonon-induced instabilities near the critical state and may, therefore, overestimate the ideal shear strength. The influence of lattice vibrations is currently under study.

The total energies of Al and Cu are computed as a function of strain using the local density approximation pseudopotential total-energy scheme with a plane-wave basis set [9–12]. The pseudopotential for Cu was generated including semirelativistic corrections [13], while the pseudopotential for Al was constructed without relativistic corrections [14]. We used a cutoff energy of 40 Ry for Al and 70 Ry for Cu. These choices ensure convergence to less than 1 mRy (0.013 eV) per atom.

A large number of wave vectors (k points) is needed to sample the Brillouin zone in these calculations. This is true for two reasons. First, shearing reduces the symmetry of the crystal and, hence, increases the size of the irreducible wedge of the Brillouin zone. Second, the shape of the Brillouin zone changes under shear. The grid of k points deforms along with it, so the individual k points move relative to the Fermi surface. This causes spurious changes in the energy if the k-point grid is too coarse. We determined the number of k points needed by increasing the number until the results did not change. A grid of 2400 k points was needed in the irreducible wedge of the Brillouin zone to adequately describe the energy of Al under shear. A grid of 1300 k points was needed for Cu.

The shear stress is found by straining the crystal in a series of incremental simple shears, calculating the energy E and relaxed volume V as a function of the strain, and taking the derivative of the energy with respect to the strain; the ideal shear strength is the maximum value of

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this derivative. Using a Cartesian coordinate system with unit vectors $\boldsymbol{e}_3$ perpendicular to the plane of shear and $\boldsymbol{e}_1$ in the direction of displacement, the associated strain increment is, in dyadic form,

$$\delta\boldsymbol{\epsilon} = \epsilon_{13}(\boldsymbol{e}_1\boldsymbol{e}_3 + \boldsymbol{e}_3\boldsymbol{e}_1). \tag{1}$$

To accomplish this strain under fully relaxed conditions, we fix ϵ_{13} $(= \epsilon_{31})$ and adjust the other five independent components of the strain tensor until their associated stresses vanish. This is done with a quasi-Newton method [15] that increments the free strains to relax the calculated stresses to less than 0.05 GPa.

There is no unique definition of finite strain [16]. However, the three lattice parameters, $\boldsymbol{a}^\alpha$, are defined at each step of the deformation and can be described by the three functions, $\boldsymbol{a}^\alpha(n)$, where n is the number of incremental strain steps in the simulation. Let $\boldsymbol{D}(m,n)$ be the Cartesian tensor that describes the deformation between steps m and n. Then

$$a_i^\alpha(n) = a_i^\alpha(m) + D_{ij}(n,m)a_j^\alpha(m). \tag{2}$$

We use the deformation tensor, $\boldsymbol{D}(m,n)$, to define the true strain as

$$\epsilon_{ij}(n) = \sum_{m=2}^{n} \frac{D_{ij}(m,m-1) + D_{ji}(m,m-1)}{2}, \tag{3}$$

and the engineering strain as

$$\epsilon_{ij}^E(n) = \frac{D_{ij}(n,0) + D_{ji}(n,0)}{2}. \tag{4}$$

The derivatives of the energy with respect to the true strain are the stresses that drive incremental deformation, and therefore the true strain is used to calculate the stress. The engineering strains are more convenient to directly describe lattice distortions at instability.

The energy density is a unique function of the strain, ϵ_{13}, when either (1) the crystal is unrelaxed, so that ϵ_{13} is the only nonzero strain or (2) the crystal is fully relaxed, so that there is only one nonzero stress, and the value of ϵ_{13} fixes all other strains. In either case, the conjugate shear stress is

$$\tau = \sigma_{13} = \frac{1}{V}\frac{\partial E}{\partial \epsilon_{13}} = \frac{1}{V}\frac{\partial E}{\partial \gamma_{13}}, \tag{5}$$

where $\gamma_{ij} = \epsilon_{ij} + \epsilon_{ji} = 2\epsilon_{ij}$ is the shear.

The relevant shear modulus, G', is determined by the second derivative, $\partial^2 E/\partial\gamma^2$, evaluated at zero strain. For shear on a $\{111\}$ plane of a cubic crystal,

$$G_u' = \frac{1}{3}(C_{11} + C_{44} - C_{12}), \tag{6}$$

and

$$G_r' = \frac{3C_{44}(C_{11} - C_{12})}{4C_{44} + C_{11} + C_{12}}, \tag{7}$$

where G_u' governs the unrelaxed case ($\epsilon_{ij} = 0$, unless $ij = 13$ or 31), G_r' governs the relaxed case ($\sigma_{ij} = 0$, unless $ij = 13$ or 31), and the C_{ij} are the Voigt elastic constants for the cubic crystal.

A homogeneous shear in a $\langle 112\rangle$ direction on a $\{111\}$ plane of fcc regenerates the fcc structure when the relative displacement of atoms in adjacent planes is $b/\sqrt{3}$, where b is the nearest neighbor distance. It is sufficient to calculate the energy to the midpoint of this shear. The energy is calculated at a sequence of values in this range and then fit to a cosine series to facilitate the computation of the derivatives that determine the stresses and shear moduli. As a rough check, we also calculate the stresses directly from the Hellman-Feynman theorem [17]; however, these stresses are significantly less accurate than those determined from the energy, provided that the fit to the energy curve is good.

The essential results are summarized in Figs. 1–3 and Tables I–III. Figures 1 and 2 show the energy of Al and Cu as a function of the shear strain, $E(\gamma)$, computed both with and without relaxation, and Fig. 3 plots the stress-strain curves, $\tau(\gamma)$, for the two materials studied in the fully relaxed case. Table I lists the calculated values of the lattice constants and the elastic moduli and compares them to experiment, Table II includes the calculated values of the ideal shear strength, and Table III includes the strain components at the point of instability in the fully relaxed case, where ϵ_{22} and ϵ_{33} are the elongations perpendicular to the direction of shear, and $\Delta V/V$ is the dilation. (The shears γ_{12} and γ_{23} are zero because the $\langle 112\rangle$ shear direction lies in a mirror plane.)

Table I shows that the equilibrium value of the lattice constant is calculated to within a few percent in this paper. The elastic moduli are calculated to an accuracy of about ±10%; the experimental values fall within this range. The imprecision in the shear moduli is due largely to the difficulty of calculating the curvature (second derivative)

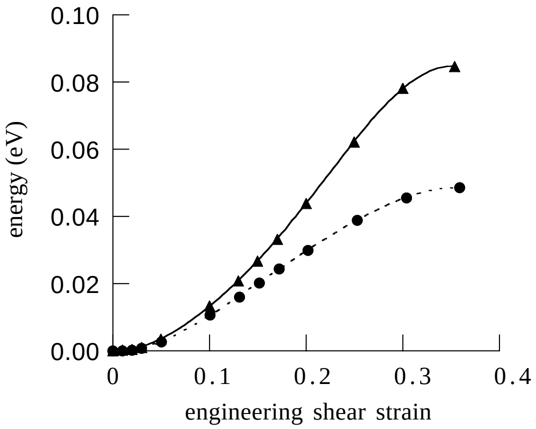

FIG. 1. Aluminum energy vs engineering strain for both the unrelaxed (▲'s and smooth fit) and relaxed (●'s and dashed fit) cases.

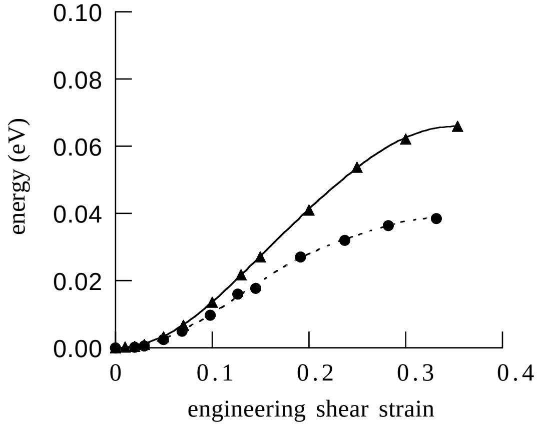

FIG. 2. Copper energy vs engineering strain for both the unrelaxed (▲'s and smooth fit) and relaxed (●'s and dashed fit) cases.

TABLE I. Calculated and experimental lattice parameters and elastic moduli.

	Al		Cu	
	calc	expt.	calc.	expt.
Lattice constant (Å)[a]	4.12	4.05	3.57	3.61
G_r' (GPa)[b]	22 ± 3	24.5	30 ± 4	30.5
G_u' (GPa)[b]	27 ± 3	24.8	40 ± 4	40.8

[a] Experimental values from Ref. [19].

[b] Shear moduli are defined by Eqs. (6) and (7). Experimental Voigt elastic constants are from Ref. [20].

of the energy function, since the differences in energy at small applied strains are at the limits of our current numerical resolution. The local density approximation is a second source of imprecision.

Figures 1 and 2 show the importance of stress relaxation to the energy function. The remaining results (Fig. 3 and Tables II and III) have several other features that are physically interesting. First, while the calculated values of $\tau_r/G_r' \approx 0.085$ are significantly lower than other recent estimates which range from 0.12 to 0.17 [4,6], the critical shear strengths remain closer to the original estimate of Frenkel [2], $\tau_r \approx 0.11G_r'$, than to more recent and more widely accepted values [3], $\tau_r \approx 0.033G_r'$. Second, full structural relaxation is obviously important. The reason these calculated values are significantly lower than other recent estimates is because previous researchers have neglected the possibility of any uniform volume change or relaxation within the slip plane. We find strains of 3% in the slip plane in both Al and Cu, and a volume change of 1.4% in Al. Structural relaxation also affects the critical strain at shear instability, which is significantly smaller than the value, $\gamma_c = 17.8\%$, that classical models would suggest. Third, Al and Cu respond quite differently at large strains, as shown by the values of the critical strains. In Al, the relaxation strain is an expansion perpendicular to the $\{111\}$ plane of shear ($\epsilon_{33} > 0$), partly compensated by a perpendicular contraction in the plane ($\epsilon_{22} < 0$), but causing a significant volume increase. In Cu, ϵ_{33} is small, the relaxation strain is in the plane ($\epsilon_{22} > 0, \epsilon_{11} < 0$), and the volume change is small. Fourth, despite the fact that Al does not form extended stacking faults, the $\langle 112 \rangle$ directions in $\{111\}$ planes remain the weak directions. The calculations show that when a shear strain is applied in a different direction lattice relaxation rotates the shear into a $\langle 112 \rangle$ direction.

Finally, how accurate are the calculated values of the ideal shear strength? This is a difficult question to answer since there are no directly comparable experimental data known to us. The calculations relate, strictly, to perfect crystals in the limit of zero temperature. There are no data known to us on dislocation-free Al, but Brenner [18] did measure the strength of nominally dislocation-free Cu whiskers. He found a tensile yield strength of 2.9 GPa for tension along $\langle 111 \rangle$, which translates into a critical resolved shear stress, τ_c, of 0.82 GPa ($0.027G_r'$) for slip on the $\{111\}$ plane in the $\langle 112 \rangle$ direction. Brenner's measurements were done at room temperature, so the strength must be corrected to 0 K. While there is no exact way to do this, a crude model described by Kelly and Macmillan [3] suggests that $\tau_c(0) \approx 2.5\tau_c(273)$ is not a bad estimate. Using this approximation, we project $\tau_c \approx 1.1$ GPa at 273 K, which is not unreasonable in light of the Brenner result. A better test can be made

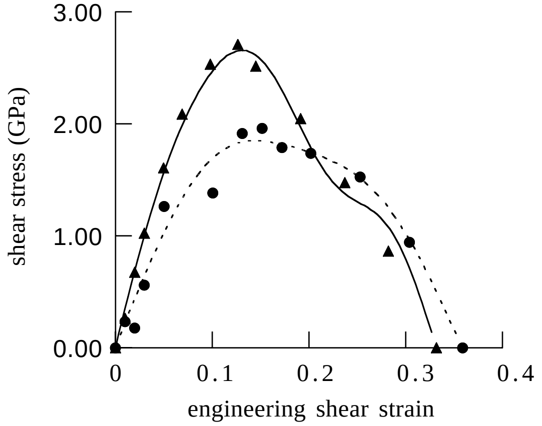

FIG. 3. Stress vs engineering strain for Cu (▲'s and smooth fit) and Al (●'s and dashed fit). The data points are the calculated Hellman-Feynman stresses, and the smooth curves are the derivatives of the smooth fits to the energies.

TABLE II. Ideal shear strengths with and without structural relaxations.

	Failure stress		
	τ_r (GPa)	τ_r/G_r'	τ_u (GPa)
Al	1.85 ± 0.1	0.084	3.4 ± 0.1
Cu	2.65 ± 0.2	0.088	4.0 ± 0.1

TABLE III. Engineering strains at shear instability.

	Failure strain (%)				
	γ_{13}^E	ϵ_{11}^E	ϵ_{22}^E	ϵ_{33}^E	$\Delta V/V$
Al	14.5	1	−3	3	1.4
Cu	13	−3	3	0.2	0.4

by computing the strength of high-melting-point materials, which should show a much smaller thermal effect. Studies of W and Ti(C,N) are now underway.

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