A simple prediction of the theoretical tensile strength of cubic crystals based on the shear strength calculations

M. Černý[a] and J. Pokluda[b]

Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic

[a]cerny.m@fme.vutbr.cz, [b]pokluda@fme.vutbr.cz

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Abstract. This work presents a simple way how to estimate the uniaxial tensile strength on the basis of the theoretical shear strength calculations taking its dependence on superimposed normal stress into account. The atomistic simulations of the shear and tensile deformations in cubic crystals are performed using first principles computational code based on pseudo-potentials and plane wave basis set. Six fcc crystals are subjected to shear deformations in convenient slip systems and a special relaxation procedure controls the stress tensor. Obtained dependence of the ideal shear strength on normal tensile stress seems to be almost linearly decreasing for all investigated crystals. Taking these results into account, the uniaxial tensile strength values in $\langle 110 \rangle$ and $\langle 111 \rangle$ directions were evaluated for selected fcc crystals.

Introduction

Uniaxial tensile tests belong to the easiest experimental strength measurements. Results of such experiments yield usually values orders of magnitude lower than theoretical predictions. The first attempts to calculate the theoretical tensile strength assumed that the crystal breaks by a brittle fracture along a plane perpendicular to the loading axis (tearing stress) [1-3]. Even in many later studies based on semiempirical [4] or first-principles [5,6] atomistic approaches was the tensile strength calculated as a tearing stress. Later on, Born's criteria for stability of solid crystals were modified to predict the first onset of instability [7]. However, this approach is computationally very time-consuming. Recent theoretical studies based on atomistic modelling as well as experiments on whiskers [3] suggested that rupture of many perfect crystals is related to reaching the shear strength in some convenient shear system rather than approaching the maximum tensile stress that leads to tearing. An illustration of such shear system is in Fig.1.

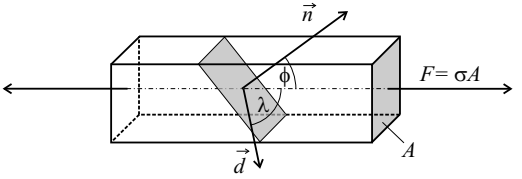

Fig.1 Illustration of shear system in a crystal sample under tensile stress. The angles ϕ and λ are measured between crystal axis and normal vector $\boldsymbol{n}$ and shear direction $\boldsymbol{d}$, respectively.

When the crystal is subjected to tensile stress σ, certain slip systems can be exposed to a combination of shear and tensile (normal to the shear plane) stresses. The displayed vectors $\boldsymbol{n}$ and $\boldsymbol{d}$ determine the vertical to the shear plane and the shear direction, respectively. The angles ϕ and λ in

Fig.1 are measured between the vectors and the crystal axis. The normal stress σ_n can be expressed by means of the tensile stress σ and the angle ϕ as

$$\sigma_n = \sigma \cos^2 \phi \,. \tag{1}$$

Assuming that some shear instability can precede the onset of tearing, the tensile strength $\sigma_{\max}$ can be estimated from the corresponding theoretical shear strength $\tau_{\max}$ using the relation

$$\sigma_{\max} = \frac{\tau_{\max}}{\cos\phi \cos\lambda}, \tag{2}$$

where $\sigma_{\max}$ represents a tensile stress value at which the shear stress in a convenient shear system reaches its maximum ($\tau_{\max}$). The relation is similar to the well known Schmid's law

$$\tau_c = \sigma_y \cos\phi \cos\lambda \,, \tag{3}$$

that expresses the relation between the critical resolved shear stress τ_c required to move dislocations across the slip plane and the yield stress σ_y in crystals with defects. However, the equation (2) holds only for a perfect single crystal. Another significant difference lies in the influence of a normal stress on the shear stress. Whilst, in the Schmid's law, τ_c is considered to be independent on the normal stress, at least in fcc crystals, the influence of tensile (as well as compressive) σ_n on the shear strength has been reported recently for fcc and bcc metals [8-10] and for diamond ceramics [11]. In this paper, the influence of normal stress is studied particularly in the region of tensile stresses and the obtained results are used for a simple estimate of $\sigma_{\max}$.

Computational procedure

Six fcc crystals (Al, Ni, Cu, Ir, Pt and Au) were subjected to homogeneous shear deformations in $\langle \bar{1}\,\bar{1}\,2 \rangle \{111\}$ slip system in two distinct ways. In the first approach (from now on called rigid-planes approach) we keep the shear planes undistorted during the whole shear process. Only the interplanar distance is allowed to change in order to set the normal stress to a prescribed value. This approach is consistent with previous calculations of Kelly et al. [12] as well as with our recent study [8]. However, the present work utilizes calculated stress tensor, whereas the study in Ref. [8] was based on calculation of the total energy.

The other approach (relaxed-planes) lies in a full relaxation of the stress tensor (including possible in-plane stresses) and the computational procedure goes the same way as described in Ref. [9]. In both approaches, the main attention was paid to the tensile region of normal stresses. The homogeneous shear was simulated using a single atom in the simulation cell.

The studied shear system is illustrated in Fig. 2. For the sake of clearness, only two adjacent planes are displayed. When the upper plane A moves to the right ($[\bar{1}\,\bar{1}\,2]$ direction) their atoms must overcome a high energy barrier related to over-passing the atoms in the B plane. The final position of the selected atom in plane A is marked by the dashed circle in Fig. 2. The corresponding structure has fcc symmetry of an opposite stacking order (with respect to the original state). The same state can be reached moving the A plane to the left. In this case, the corresponding energy barriers as well as the related stresses are substantially lower. Although the plane shift then cannot continue the same way (because of the consequent higher energy barrier), the instant of

approaching the shear strength is the first onset of instability. Thus, the computed σ_{max} values can be considered to be the theoretical tensile strengths.

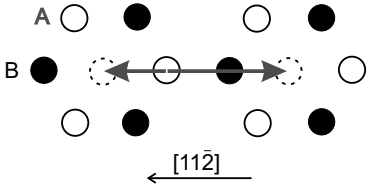

Figure 2: Two adjacent {111} A (open circles) and B (solid circles) planes in fcc crystals for illustration of the $\langle 112 \rangle \{111\}$ shear system.

For the calculations of Hellman-Feynman stress tensor, we utilized the Vienna Ab initio Simulation Package (VASP) [12]. This code uses plane wave basis set and ultra-soft pseudo-potentials of Vanderbilt type [14]. In case of Ni, the projector augmented-wave potential [14] was used instead along with the spin-polarized calculations (to take the ferromagnetic ordering in Ni into account). The exchange-correlation energy was evaluated using either the local density approximation (Pt, Au) or the generalized-gradient approximation (Al, Ni, Cu, Ir). The 18x18x18 *k*-points mesh was used in all our calculations with the exception of Al, where a finer mesh 31x31x31 was used. The solution was considered to be self-consistent when the energy difference of two consequent iterations was smaller than 10 μeV.

Results and discussions

The computed $\tau_{max}(\sigma_n)$ functions from the rigid-planes approach are displayed in Fig. 3 for the region of tensile normal stresses up to 20 GPa. In order to fit conveniently all the data points into one diagram, the τ_{max} values for Ir are divided by 3.

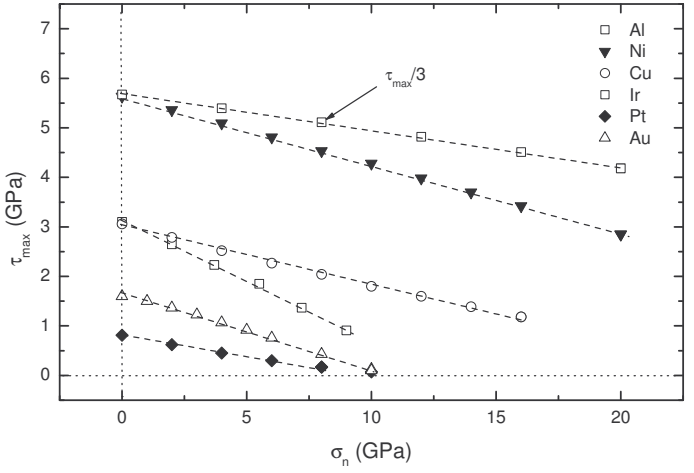

Figure 3: Theoretical shear strength τ_{max} as a function of normal stress σ_n in the rigid-planes approach. Dashed lines represent linear regressions of the displayed data points.

As can be seen from the regression lines, the functions are almost linearly decreasing and can be expressed as

$$\tau_{\max} = \tau_r - k\sigma_n, \tag{4}$$

where k expresses slope of the regression lines and τ_r can be considered to be the theoretical shear strength in the absence of normal stress [8]. The regression parameters are collected in Table 1.

Table 1: Regression parameters for $[11\bar{2}]\{111\}$ shear strength in both, the rigid-planes and the relaxed-planes approaches.

Element	rigid-planes		relaxed-planes		
	τ_r (GPa)	k	τ_r (GPa)	k	TSS* (GPa)
Al	3.12	0.238	3.07	0.319	2.84
Ni	5.64	0.139	5.05	0.123	5.05
Cu	3.01	0.117	2.43	0.080	2.16
Ir	17.1	0.223	17.3	0.249	
Pt	2.75	0.138	2.05	0.177	
Au	1.66	0.152	1.05	0.171	0.85

* Ref. [16]

Comparing the computed data with previous results [8] one can see a good agreement in the τ_r values while more remarkable differences can be found in k values. They are probably caused not only by different assessment but also by the different selected range of interpolated data (with respect to normal stresses). The most remarkable disagreement in τ_r can be found for Pt (11%) and Au (19%). All the other values match the previous results within 5%. It should be noted, however, that a significant deviation from the linear trend was found formerly in the range of higher tensile stresses in the case of Ir [8].

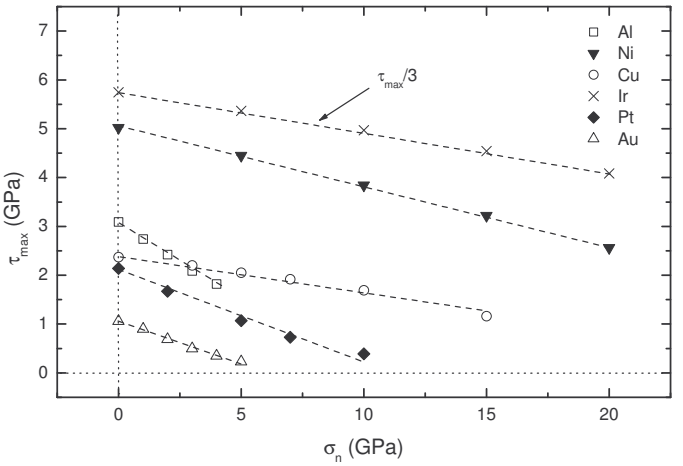

Figure 4: Theoretical shear strength as a function of normal stress in relaxed-planes approach. Dashed lines represent linear regressions of the displayed data points.

The results of relaxed-planes calculations are displayed in Fig. 4. Again, within the limited range of normal stresses, the $\tau_{\max}(\sigma_n)$ functions can be approximated by linear functions and their regression parameters were also added to Table 1. Comparing both approaches one can see that the full relaxation of stresses remarkably lowers the shear strength of Au, Cu and Pt.

In order to estimate the theoretical tensile strength $\sigma_{\max}$, the relations (1), (2) and (4) can be combined to the final form

$$\sigma_{\max} = \frac{\tau_r}{\cos\phi(\cos\lambda + k\cos\phi)}. \tag{5}$$

The obtained $\sigma_{\max}$ values (from both approaches) for uniaxial tension in $[110]$ and $[11\bar{1}]$ directions are listed in Table 2. Uniaxial tension was applied to the crystal in the most favorable representative of the family of symmetry-equivalent directions $\langle 110\rangle$ and $\langle 111\rangle$. The σ_t values, that were collected from available literature, represent corresponding values of tearing stress.

Table 2: The estimated theoretical tensile strengths $\sigma_{\max}$ in $\langle 110\rangle$ and $\langle 111\rangle$ directions (in GPa) along with the available literature data for tearing stress σ_t.

Element	$\sigma_{\max}$: rigid-planes		$\sigma_{\max}$: relaxed-planes		σ_t from literature	
	$[110]$	$[11\bar{1}]$	$[110]$	$[11\bar{1}]$	$[110]$	$[111]$
Al	5.0	9.2	4.5	8.8	4.2 [a]	14.8 [a]
Ni	10.0	17.1	9.1	15.4	11.7 [a]	39.3 [a]
Cu	5.5	9.2	4.6	7.5	5.5 [a]	26.5 [a]
Ir	27.6	50.4	27.1	50.6	26.5 [b]	43.5 [b]
Pt	4.9	8.3	3.5	6.1		30.0 [b]
Au	2.9	5.0	1.8	3.2	2.8 [a]	13.6 [a]

[a] Ref. [4]
[b] unpublished results

It can be seen, that the predicted $\sigma_{\max}$ values for $[11\bar{1}]$ direction (obtained from both approaches) are substantially lower than the tearing stresses for all studied fcc crystals with the exception of Ir. On the other hand, the tearing stresses in [110] direction were computed so low that the predicted $\sigma_{\max}$ values are of a comparable magnitude.

Table 3: The estimated tensile strength $\sigma_{k=0}$ without the correction by the normal stress (in GPa).

Element	rigid-planes		relaxed-planes	
	$[110]$	$[11\bar{1}]$	$[110]$	$[11\bar{1}]$
Al	6.6	9.9	6.5	9.8
Ni	12.0	18.0	10.7	16.1
Cu	6.4	9.6	5.2	7.7
Ir	36.3	54.4	36.7	55.1
Pt	5.8	8.8	4.4	6.1
Au	3.5	5.3	2.2	3.2

In the case of $k = 0$, σ_{max} would be calculated simply as the shear strength divided by the Schmid factor $\cos\phi\cos\lambda$. To evaluate the impact of the normal stress influence, results for $k = 0$ were listed in Table 3. The corresponding values $\sigma_{k=0}$ are higher than σ_{max} in all cases. The correction by the normal stress reduces the predicted tensile strength mostly by 5–10% in case of $\langle 111 \rangle$ tension whereas a more remarkable reduction (mostly by 20–30%) can be found for $\langle 110 \rangle$ tensile direction.

Summary

The theoretical tensile strength was estimated from the theoretical shear strength and its dependence on normal stress in a selected shear system. The dependence was calculated from first principles as a linearly decreasing function of tensile normal stress for all studied fcc crystals. The estimated tensile strength values in $[11\bar{1}]$ direction were found lower than the stresses necessary for tearing in most of the studied elements (except in Ir). On the other hand, the tensile stresses in [110] directions are well comparable to the corresponding tearing stresses. Considering the influence of normal stress on the shear strength reduces the tensile strength by 5–10% in case of $\langle 111 \rangle$ tension and by 20–30% for $\langle 110 \rangle$ tensile direction.

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