Intrinsic Strength Asymmetry Between Tension and Compression of Perfect Face-Centered-Cubic Crystals

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Abstract The strength asymmetry between tension and compression is a typical case of mechanical response of materials. Here we achieve the intrinsic strength asymmetry of six face-centered-cubic perfect crystals (Cu, Au, Ni, Pt, Al and Ir) through calculating the ideal tensile and compressive strength with considering the normal stress effect and the competition between different crystallographic planes. The results show that both the intrinsic factors (the ideal shear strength and cleavage strength of low-index planes) and the orientation could affect the strength asymmetry, which may provide insights into understanding the strength of ultra-strong materials.

KEY WORDS: Perfect crystal; Strength asymmetry; Tension; Compression

1 Introduction

Usually, materials display different mechanical responses under various loading conditions [1]. Specifically, for some materials, their strength and fracture mode strongly rely on the loading direction, showing an asymmetry between tension and compression (the *t/c* asymmetry). Materials exhibiting *t/c* asymmetry include single crystals or polycrystalline materials of face-centered-cubic (fcc) [2–8], body-centered-cubic (bcc) [8, 9] and hexagonal-close-packed (hcp) [10, 11] structures with different scales of sample or grain size and diverse constituents, metallic glasses [12–15] and its composites [16], ceramics [1], intermetallics [3, 17, 18], superalloys [19], biological materials [20], graphene [21] and so on. Although such a wide range of material kind, the origin of the *t/c* asymmetry

usually is owing to the pressure dependence of various kinds of defects (dislocations, interfaces, cracks, etc.), the phase transformation [11], and the normal stress or non-Schmid effect [7, 12, 22].

For perfect crystals, *t/c* asymmetry also exists because the normal stress on the shear plane strongly affects the shear strength. Through first-principle method, Černý et al. [23–25] calculated the normal stress (including both the positive and negative directions) effect on the shear strength along a specific shear plane of some perfect crystals. However, the tensile or compressive process, which simulates the experimental loading along an arbitrary crystallographic direction, has not been taken into account. While Tschopp and McDowell [2, 22] calculated the *t/c* asymmetry of the critical stresses for the occurrence of homogeneous dislocation nucleation in Cu perfect crystal with molecular dynamic (MD) method, the fracture of perfect crystal that homogeneously deforms without the aid of dislocations and other defects has not been considered. And neither of the two studies mentioned above is paid attention to the competition between different crystallographic planes, such as the shear of {111} plane and the cleavage of {100} plane, which could lower the tensile strength along some specific loading orientations [26].

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In this study, firstly we applied the raw data of ideal cleavage strength and shear strength of six fcc crystals (Cu, Au, Ni, Pt, Al and Ir) with the fracture criterion [27–29] to calculate the ideal compressive strength along an arbitrary direction. Then, the t/c asymmetry was achieved with the presently obtained ideal compressive strength and the previous results of ideal tensile strength [26]. Finally, the orientation-dependent t/c asymmetries of the studied six crystals are analyzed.

2 Analysis

Supposing that a uniaxial stress σ_A , tension or compression is performed on a perfect single-crystal specimen [26], then the corresponding normal stress σ and shear stress τ along a certain crystallographic plane could be denoted as

$$\sigma = \sigma_A \cos^2 \phi, \quad (1)$$

$$\tau = \sigma_A \cos \phi \cos \lambda, \quad (2)$$

where ϕ and λ are the angles between the loading axis and the normal stress direction and the shear stress direction, respectively. When σ_A equals the ideal tensile strength σ_T or the ideal compressive strength σ_C , fracture happens. In order to calculate the ideal strength for loading along an arbitrary crystallographic direction, a universal fracture criterion for high-strength materials, in which both the tensile and compressive normal stress effect are considered, can be employed [26, 29]. According to this criterion, the fracture occurs along a specific plane if satisfying

$$\beta \left(\frac{\sigma}{\sigma_0} \right)^2 + \left(\frac{\tau}{\tau_0} \right)^2 = 1, \quad (3)$$

where σ_0 and τ_0 are the ideal cleavage strength of this plane and the ideal shear strength along the shear direction of this plane, respectively, and β is an extrinsic parameter associated with the loading direction. Generally, for compressive loading, β equals $-1/2$ (the effect of the value of β would be discussed later), while for tensile loading, β equals 1, and Eq. (3) changes into

$$\left(\frac{\sigma}{\sigma_0} \right)^2 + \left(\frac{\tau}{\tau_0} \right)^2 = 1, \quad (4)$$

which is the unified tensile fracture criterion [27] and had been used in our previous work [26]. Combining Eqs. (1–3), the ideal tensile strength can be expressed as,

$$\sigma_T = \frac{1}{\cos \phi_T \sqrt{\frac{\cos^2 \lambda_T}{\tau_0^2} + \frac{\cos^2 \phi_T}{\sigma_0^2}}}, \quad (5)$$

and correspondingly, the ideal compressive strength can be expressed as,

$$\sigma_C = \frac{1}{\cos \phi_C \sqrt{\frac{\cos^2 \lambda_C}{\tau_0^2} - \frac{1}{2} \frac{\cos^2 \phi_C}{\sigma_0^2}}}. \quad (6)$$

Equations (5) and (6) are the general formulas for calculating the ideal tensile strength or compressive strength of perfect crystal with an arbitrary orientation, respectively. Under tensile stress states, both shear fracture and cleavage fracture could happen, which means that the fracture could be mode I or a mixed mode I and mode II, which has been discussed in detail in our previous work [26]. While for compressive stress states, only the shear fracture along $\{111\}\langle 112 \rangle$ (the twinning direction for fcc crystals) or mode II fracture could happen. Correspondingly, the ideal cleavage strength σ_0 and the ideal shear strength τ_0 of the six fcc crystals are $\sigma_{0\{111\}}$ and $\tau_{0\{111\}\langle 112 \rangle}$, respectively, which is collected from the literature [26].

The Mohr's stress circle diagram, as shown in Fig. 1, qualitatively describes the fracture strength and the fracture angle under both tensile and compressive stress states. Due to the anisotropy, the fracture angle, which is the angle between loading axis and the normal direction of the weakest fracture plane, is given and not tangent to the failure line. Under compressive stress states, cleavage fracture cannot happen and the normal stress only displays a negative effect on the shear fracture, while under tensile stress state, the normal stress facilitates the shear process. Besides the different effects of normal stress, another difference in the computing process between tensile strength and compressive strength is the selection of fracture systems of $\{111\}\langle 112 \rangle$. Fracture could only happen when λ , the angle between the loading direction and the shear direction, is less than $\pi/2$. Consequently, for a certain loading direction, tension and compression cannot share the same fracture system. According to Eq. (6), the ideal compressive strength of the perfect fcc crystals under an

Fig. 1 Qualitative representation of the tensile strength and compressive strength through the Mohr's stress circles and fracture criterion lines. The diameters of the two Mohr's circles denote the fracture strength of tension and compression, respectively

arbitrary loading orientation can be gained, and hence, the *t/c* asymmetry can also be achieved. MTEX3.5.0 [30] was used to calculate the minimum compressive strength under the consideration of the competition between the different systems of $\{111\}\langle 112\rangle$, and to draw the stereographic contour plots of the ideal compressive strength and the strength asymmetry.

3 Results and Discussion

3.1 Ideal Compressive Strength

The ideal compressive strength values of the six fcc perfect crystals can be calculated according to Eq. (6), in a similar manner as the calculation of the ideal tensile strength [26]. The fracture under uniaxial compression is totally undertaken by $\{111\}\langle 112\rangle$ along any loading orientation, and thus, σ_0 and τ_0 here are the ideal cleavage strength of $\{111\}$ planes and the ideal shear strength of $\{111\}\langle 112\rangle$, respectively. The compressive strength along $\langle 100\rangle$, $\langle 110\rangle$ and $\langle 111\rangle$ loading orientations and the tensile results [26] are listed in Table 1. Unlike the tensile strength, the compressive strength along the three simple orientations for nearly all metals obeys the same sequence of $\sigma_{C\langle 100\rangle} < \sigma_{C\langle 110\rangle} < \sigma_{C\langle 111\rangle}$.

When $\tau_{0\{111\}\langle 112\rangle}/\sigma_{0\{111\}} \approx 0$, Eq. (6) could be changed into:

$$\sigma_C \approx \frac{\tau_{0\{111\}\langle 112\rangle}}{\cos \lambda_C \cos \phi_C}, \quad (7)$$

where $\cos \phi \cos \lambda$ equals $\sqrt{2}/3$ and $2\sqrt{2}/9$ for $\langle 100\rangle$ and $\langle 111\rangle$ orientations, respectively. Correspondingly, the difference in the compressive strength between the two orientations is $(\sigma_{C\langle 111\rangle} - \sigma_{C\langle 100\rangle})/\sigma_{C\langle 100\rangle} = 0.5$ for $\tau_{0\{111\}\langle 112\rangle}/\sigma_{0\{111\}} \approx 0$ and becomes smaller according to Eq. (6) with increasing value of $\tau_{0\{111\}\langle 112\rangle}/\sigma_{0\{111\}}$, as shown in Fig. 2a, while for both $\langle 100\rangle$ and $\langle 110\rangle$

Fig. 2 Variation of compressive strength of **a** $\langle 110\rangle$, **b** $\langle 111\rangle$ orientations against $\langle 100\rangle$ orientation with the variation of $\tau_{0\{111\}\langle 112\rangle}/\sigma_{0\{111\}}$ of six fcc crystals

orientations, $\cos \phi \cos \lambda$ equals $\sqrt{2}/3$; thus, correspondingly the compressive strength of these two orientations is the same, i.e., $\sigma_{C\langle 100\rangle} = \sigma_{C\langle 110\rangle}$ and the difference in the compressive strength between the two orientations becomes larger according to Eq. (6) with increasing value of $\tau_{0\{111\}\langle 112\rangle}/\sigma_{0\{111\}}$, as shown in Fig. 2b.

The results of the ideal compressive strength as the function of loading orientation of the six single crystals are

Table 1 Tensile and compressive strength of the six fcc single crystals along $\langle 100\rangle$, $\langle 110\rangle$ and $\langle 111\rangle$ loading orientations

Crystals	Tensile strength (GPa) [26]			Compressive strength (GPa)		
	$\langle 100\rangle$	$\langle 110\rangle$	$\langle 111\rangle$	$\langle 100\rangle$	$\langle 110\rangle$	$\langle 111\rangle$
Cu	4.57	4.53	6.87	4.59	4.61	6.87
Au	1.80	1.80	2.70	1.80	1.80	2.70
Ni	10.65	9.5	14.25	10.74	10.84	16.07
Pt	4.68	3.5	5.25	4.69	4.70	7.03
Al	5.88	4.89	7.34	6.10	6.35	9.06
Ir	35.13	26.3	39.45	37.22	39.74	54.96

plotted in Fig. 3. Clearly, all the plots of the six crystals show nearly the same distribution with the changes of loading orientation. The details about the maximum and minimum compressive strength and the corresponding loading orientations of the six fcc crystals are listed in Table 2. Specifically, for all crystals, the maximum happens at the same $\langle 111 \rangle$ direction, where the angles between $[111]$ direction and three of the four $\{111\}$ planes, i.e., $(11\bar{1})$, $(\bar{1}11)$ and $(\bar{1}\bar{1}1)$ planes, are the largest, or the highest resolved shear strength happens in this case. There are two loading directions along which the minimum compressive strength happens for each crystal. However, the loading orientations along which the minimum of the compressive strength happens are almost the same, which is due to the slight effect

of normal stress. If $\sigma_{0\{111\}} \gg \tau_{0\{111\}\langle 112 \rangle}$ or $\beta = 0$, the normal stress effect would be none and the corresponding orientations where the minimum compressive strength happens are $\langle 0.169, 1, 1 \rangle$ and $\langle 0.171, 0.171, 1 \rangle$, where $\cos\phi \cos\lambda$ of the two orientations are the same. Since $|\beta|$ equals 1/2 for uniaxial compression, smaller than that for uniaxial tension ($|\beta| = 1$), the normal stress effect under compression is smaller than that for the tensile condition. The minor difference in the orientation along which the lowest compressive strength happens for the six fcc crystals, as shown in Table 2, is due to the value of $\tau_{0\{111\}\langle 112 \rangle} / \sigma_{0\{111\}}$: the orientations toward to $\langle 111 \rangle$ and $\langle 110 \rangle$ along the loading orientation line of $\langle 100 \rangle$ – $\langle 111 \rangle$ and $\langle 110 \rangle$ – $\langle 111 \rangle$, respectively, with decreasing value of $\tau_{0\{111\}\langle 112 \rangle} / \sigma_{0\{111\}}$.

Fig. 3 Stereographic contour plots of compressive strength of **a** Cu, **b** Au, **c** Ni, **d** Pt, **e** Al, **f** Ir. Black spots are denoted as the loading orientations where the maximum or minimum compressive strength appears

Table 2 The maximum compressive strength (σ_{Cmax}) and the minimum compressive strength (σ_{Cmin}) as well as the corresponding loading orientation(s) of the six fcc crystals

Elements	σ_{Cmax} (GPa)	Orientation	σ_{Cmin} (GPa)	Orientations
Cu	6.87	$\langle 111 \rangle$	4.33	$\langle 0.167, 1, 1 \rangle$, $\langle 0.175, 0.175, 1 \rangle$
Au	2.70	$\langle 111 \rangle$	1.70	$\langle 0.168, 1, 1 \rangle$, $\langle 0.173, 0.173, 1 \rangle$
Ni	16.07	$\langle 111 \rangle$	10.16	$\langle 0.163, 1, 1 \rangle$, $\langle 0.178, 0.178, 1 \rangle$
Pt	7.03	$\langle 111 \rangle$	4.43	$\langle 0.168, 1, 1 \rangle$, $\langle 0.173, 0.173, 1 \rangle$
Al	9.06	$\langle 111 \rangle$	5.82	$\langle 0.146, 1, 1 \rangle$, $\langle 0.201, 0.201, 1 \rangle$
Ir	54.96	$\langle 111 \rangle$	35.73	$\langle 0.134, 1, 1 \rangle$, $\langle 0.210, 0.210, 1 \rangle$

3.2 Asymmetry Between Tensile and Compressive Strength

From the results of the previously calculated ideal tensile strength [26] and the present ideal compressive strength, the asymmetry between tensile and compressive strength, κ , along an arbitrary loading orientation can be calculated by Eq. (8):

$$\kappa = \frac{\sigma_C}{\sigma_T} = \frac{\cos^2 \phi_T \sqrt{(\cos \lambda_T / \cos \phi_T)^2 + (\tau_{0\{111\}\langle 112 \rangle} / \sigma_{0\{111\}})^2}}{\cos^2 \phi_C \sqrt{(\cos \lambda_C / \cos \phi_C)^2 - \frac{1}{2} (\tau_{0\{111\}\langle 112 \rangle} / \sigma_{0\{111\}})^2}}, \quad (8)$$

when the tensile fracture is undertaken by the shear of $\{111\}\langle 112 \rangle$; otherwise, when the tensile fracture occurs with the cleavage of $\{110\}$ plane, the asymmetry can be calculated by Eq. (9):

$$\kappa = \frac{\sigma_C}{\sigma_T} = \frac{\cos^2 \phi_T \tau_{0\{111\}\langle 112 \rangle} / \sigma_{0\{110\}}}{\cos^2 \phi_C \sqrt{(\cos \lambda_C / \cos \phi_C)^2 - \frac{1}{2} (\tau_{0\{111\}\langle 112 \rangle} / \sigma_{0\{111\}})^2}}. \quad (9)$$

The results of the asymmetry of the six fcc crystals along $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$ loading orientations are listed in Table 3. For $\langle 100 \rangle$ orientation in all crystals, shear fracture of $\{111\}\langle 112 \rangle$ always happens under either tensile or compressive loading. Consequently, $\kappa_{\langle 100 \rangle}$ is the only function of $\tau_{0\{111\}\langle 112 \rangle} / \sigma_{0\{111\}}$, as shown in Fig. 4a. While for $\langle 110 \rangle$ and $\langle 111 \rangle$ orientations of Ni, Pt, Al and Ir, the cleavage of $\{110\}$ plane dominates the tensile fracture. Hence, the tensile strength is significantly lowered through the competition between shear of $\{111\}\langle 112 \rangle$ and cleavage of $\{110\}$ planes, and correspondingly, they exhibit higher values of κ , as shown in Fig. 4b and Table 3. Meanwhile, the ratio of $\tau_{0\{111\}\langle 112 \rangle} / \sigma_{0\{110\}}$ also dramatically influences $\kappa_{\langle 110 \rangle}$ and $\kappa_{\langle 111 \rangle}$, as shown in Fig. 4b. For example, for Cu and Au with very small values of $\tau_{0\{111\}\langle 112 \rangle} / \sigma_{0\{111\}}$, the shear fracture of $\{111\}\langle 112 \rangle$ dominates the tensile fracture along the three orientations.

Table 3 Asymmetry between tensile and compressive strength of the six fcc single crystals along $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$ loading orientations

κ	Cu	Au	Ni	Pt	Al	Ir
$\langle 100 \rangle$	1.0042	1.0006	1.0087	1.0020	1.0380	1.0595
$\langle 110 \rangle$	1.0170	1.0024	1.1410	1.3431	1.2992	1.5111
$\langle 111 \rangle$	1.0011	1.0001	1.1281	1.3393	1.2355	1.3937

Fig. 4 Variation of asymmetries between tensile and compressive strength of **a** $\langle 100 \rangle$ orientation ($\kappa_{\langle 100 \rangle}$) with the variation of $\tau_{0\{111\}\langle 112 \rangle} / \sigma_{0\{111\}}$ and **b** $\langle 110 \rangle$, $\langle 111 \rangle$ orientations ($\kappa_{\langle 110 \rangle}$ and $\kappa_{\langle 111 \rangle}$) with the variation of $\tau_{0\{111\}\langle 112 \rangle} / \sigma_{0\{110\}}$ of six fcc crystals

As a result, the difference between tensile and compressive strength is too small to be distinguished, as shown in Fig. 4 and Table 3. Therefore, the tensile fracture mode could be the main factor dominating the strength asymmetry and the ratio of $\tau_{0\{111\}\langle 112 \rangle} / \sigma_{0\{111\}}$ also slightly influences the asymmetry.

Furthermore, the asymmetry as the function of loading orientation for the six single crystals is plotted in Fig. 5. For the studied six perfect crystals (Cu, Au, Ni, Pt, Al and Ir), all the maximum of the asymmetry happens at the same loading orientations represented by the line $\sim \langle 0,0.5,1 \rangle - \langle 0,1,1 \rangle$. The maximum κ values for six perfect crystals are listed in Table 4. However, the specific orientations for the minimum of the strength asymmetry are different for different crystals. For Cu and Au, the minimum values of κ are 0.784 and 0.565, occurring at the line $\langle 0.386,0.566,1 \rangle - \langle 0.503,1,1 \rangle$ and $\langle 0.483,0.879,1 \rangle - \langle 0.511,1,1 \rangle$ loading orientations, respectively, while as listed in Table 4, for Ni, Pt, Al and Ir, the minimum values of κ are 0.904, 0.894, 0.952 and 0.986, happening at the line $\langle 0.227,0.227,1 \rangle - \langle 0.239,0.239,1 \rangle$, $\langle 0.222,0.222,1 \rangle$, $\langle 0.187,0.187,1 \rangle - \langle 0.195,0.195,1 \rangle$ and $\langle 0.165,0.165,1 \rangle - \langle 0.170,0.170,1 \rangle$.

Fig. 5 Stereographic contour plots of the asymmetry between tensile strength and compressive strength of **a** Cu, **b** Au, **c** Ni, **d** Pt, **e** Al, **f** Ir. Black spots and lines are denoted as the loading orientations where the maximum and minimum t/c asymmetries happen. For further analysis, the orientations where cleavage would happen under tension [26] are encircled with white dashed lines and marked with C (cleavage) inside the circles

Table 4 The maximum t/c asymmetry ($\kappa_{\max}$) and the minimum asymmetry ($\kappa_{\min}$) as well as their corresponding loading orientation(s) of the six fcc crystals

Elements	$\kappa_{\max}$	Orientations	$\kappa_{\min}$	Orientation(s)
Cu	1.017	$\langle 0,0.499,1 \rangle - \langle 011 \rangle$	0.784	$\langle 0.386,0.566,1 \rangle - \langle 0.503,1,1 \rangle$
Au	1.002	$\langle 0,0.499,1 \rangle - \langle 011 \rangle$	0.565	$\langle 0.483,0.879,1 \rangle - \langle 0.511,1,1 \rangle$
Ni	1.141	$\langle 0,0.501,1 \rangle - \langle 011 \rangle$	0.904	$\langle 0.227,0.227,1 \rangle - \langle 0.239,0.239,1 \rangle$
Pt	1.343	$\langle 0,0.501,1 \rangle - \langle 011 \rangle$	0.894	$\langle 0.222,0.222,1 \rangle$
Al	1.299	$\langle 0,0.501,1 \rangle - \langle 011 \rangle$	0.952	$\langle 0.187,0.187,1 \rangle - \langle 0.195,0.195,1 \rangle$
Ir	1.511	$\langle 0,0.501,1 \rangle - \langle 011 \rangle$	0.986	$\langle 0.165,0.165,1 \rangle - \langle 0.170,0.170,1 \rangle$

loading orientations, respectively. The reason for the difference in the critical orientation for the minimum κ between Cu, Au and the remained four crystals is that the tensile strength of Cu or Au is undertaken by the cleavage of the plane along the corresponding orientation, near which the tensile strength is the maximum [26]. The difference between Cu, Au and the remained Ni, Pt, Al and Ir for the minimum κ roots from the difference of ideal strength data (the ideal shear strength of $\{111\}\langle 112 \rangle$ and the ideal cleavage strengths of $\{111\}$ and $\{110\}$ as listed in [26]) of the six fcc crystals. On one hand, the higher $\tau_{0\{111\}\langle 112 \rangle} / \sigma_{0\{110\}}$ leads to the easier cleavage of $\{110\}$ plane, which could reduce the tensile strength of some specific orientation; on the other hand, the lower $\tau_{0\{111\}\langle 112 \rangle} / \sigma_{0\{111\}}$ could lead to the more significant

normal stress effect, which would reduce the tensile strength and increase the compressive strength and finally obtain a higher t/c asymmetry. Through further manipulation of the results of the t/c asymmetry for the six fcc crystals in Fig. 5, the percentages of orientations for $\kappa > 1$ and $\kappa \leq 1$ in all the orientations of the spatial space were obtained and are displayed in Fig. 6a. Obviously, for the possibility to occur $\kappa > 1$, the six crystals can be sequenced as Au < Cu < Ni < Pt < Al < Ir, as shown in Fig. 6a. Furthermore, the average strength asymmetry $\bar{\kappa}$ of the six perfect crystals exhibits a sequence of Au < Cu < Ni < Al < Pt < Ir, as shown in Fig. 6b. These results suggest that Au is the metal which is the most difficult to show large strength asymmetry, while for Ir nearly along all orientations the compressive strength is

Fig. 6 **a** Percentages of orientations for $\kappa > 1$ and $\kappa \leq 1$ among all the orientations of the spatial space **b** average strength asymmetry ($\bar{\kappa}$) of the six fcc crystals

higher than the tensile one, and certain strength asymmetry always exists. The obtained sequence here is grossly consistent with the sequence for cleavage [26], which thus may imply that the perfect crystal which is easy to cleave tends to show large strength asymmetry.

By comparing with the results simulated by the MD method, it is found that the corresponding orientation of the maximum asymmetry calculated in this study is well consistent with the previous results of Cu [2, 7, 22]. On the other hand, although for Ni, Pt, Al and Ir, the MD simulated results of the orientations corresponding to the minimum strength asymmetries are consistent with our results, for Cu and Au a discrepancy exists. This is mainly due to the transition of different tensile fracture mechanisms that happens near the orientation of the minimum t/c asymmetry, i.e., the highest tensile strength results in the minimum strength asymmetry [26]. Another reason is that the tensile or compressive strength calculated by the MD method is the stress for the homogenous nucleation of dislocations, which is different from the ideal fracture of a specific crystallographic plane. Interestingly, both the results here and the MD results [2, 7, 22] of the asymmetry sometimes are smaller than 1, i.e., the compressive strength is lower than the tensile strength, which is not consistent with the results in the high-strength isotropic materials [29]. The reason is

that both the ideal shear fracture and the nucleation of dislocations of single crystals are definitely orientation dependent, while for the polycrystalline materials the orientation dependence is eliminated through the equalization of the spatial space of the multi-crystalline grains.

Above results show that the strength asymmetry may depend upon the loading orientation (λ_T , ϕ_T , λ_C and ϕ_C). Besides the extrinsic factor, both the tensile fracture mode and the normal stress could also affect the asymmetry. Concerning the effect of tensile fracture mode, if the shear of $\{111\}\langle 112 \rangle$ dominates the fracture under tension, the asymmetry can be expressed as Eq. (8), while, if the cleavage of $\{110\}$ planes dominates the fracture along certain orientation, the asymmetry can be expressed as Eq. (9). Whether to choose Eq. (8) or Eq. (9) mainly depends on the value of $\tau_{0\{111\}\langle 112 \rangle}/\sigma_{0\{110\}}$ [26]. For the normal stress effect, according to Eqs. (8) and (9), higher $\tau_{0\{111\}\langle 112 \rangle}/\sigma_{0\{111\}}$ would lead to a higher asymmetry and higher $\tau_{0\{111\}\langle 112 \rangle}/\sigma_{0\{110\}}$ would also result in a higher asymmetry, which could be expressed by Eq. (9). Consequently, both $\tau_{0\{111\}\langle 112 \rangle}/\sigma_{0\{111\}}$ and $\tau_{0\{111\}\langle 112 \rangle}/\sigma_{0\{110\}}$ are the intrinsic factors to influence the asymmetry. However, only the value of $\tau_{0\{111\}\langle 112 \rangle}/\sigma_{0\{111\}}$ was considered [21, 22], which is because only the shear fracture is undertaken by the dislocations under tensile loading. Furthermore, the value of β , which affects the tensile/compressive asymmetry as the coefficient of $\tau_{0\{111\}\langle 112 \rangle}/\sigma_{0\{111\}}$, also plays an important role. In fact, the exact coupling function between the normal stress and shear stress, i.e., the exact value of β , needs the help of ab initio method. Here we make β equals 1 and $-1/2$ for tensile and compressive loading, respectively, which is more simple and time saving but clear enough to reveal the loading axial direction effect on the asymmetry.

3.3 Correlation with Isotropic Materials

For the isotropic materials, $\lambda = \theta = 90^\circ - \phi$ (θ denotes as the fracture angle [27, 29]) and both $\tau_{0\{111\}\langle 112 \rangle}/\sigma_{0\{111\}}$ and $\tau_{0\{111\}\langle 112 \rangle}/\sigma_{0\{110\}}$ can be changed into the isotropic form $\alpha = \tau_0/\sigma_0$. With the relationship between ϕ and α [29],

$$\tan \phi_T = \sqrt{1 - 2\alpha^2}, \quad (10)$$

$$\tan \phi_C = \sqrt{1 + \alpha^2}. \quad (11)$$

Combining with Eqs. (10) and (11), Eq. (8) could be changed into,

$$\kappa = \frac{\sigma_C}{\sigma_T} = \sqrt{\frac{1 + \alpha^2/2}{1 - \alpha^2}}, \quad (12)$$

which is consistent with the result of the asymmetry of isotropic materials with $0 \leq \alpha \leq \sqrt{2}/2$ [29], while for the case of the cleavage of $\{110\}$ plane under uniaxial tension,

$$\tan \phi_T = 0. \quad (13)$$

Combining with Eqs. (11) and (12), Eq. (8) could be changed into the form

$$\kappa = \frac{\sigma_C}{\sigma_T} = 2\alpha\sqrt{1 + \alpha^2/2}, \quad (14)$$

which is also consistent with the result of the asymmetry of isotropic with $\alpha \geq \sqrt{2}/2$. The results of isotropic counterpart made from our anisotropic model are consistent with the results directly derived from the isotropic materials, which indirectly proves our demonstration. Besides, most of the tension–compression asymmetry of polycrystalline materials stems from deformation history [31] or the texture effect [32], which is not considered here.

4 Conclusions

1. The compressive strength of the six fcc crystals along $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$ orientations obeys the same sequence of $\sigma_{C\langle 100 \rangle} < \sigma_{C\langle 110 \rangle} < \sigma_{C\langle 111 \rangle}$. With decreasing value of $\tau_{0\{111\}\langle 112 \rangle}/\sigma_{0\{111\}}$, the difference between $\sigma_{C\langle 100 \rangle}$ and $\sigma_{C\langle 111 \rangle}$ becomes larger, while the difference between $\sigma_{C\langle 100 \rangle}$ and $\sigma_{C\langle 110 \rangle}$ is getting smaller. When $\tau_{0\{111\}\langle 112 \rangle}/\sigma_{0\{111\}} = 0$, $\sigma_{C\langle 100 \rangle} = \sigma_{C\langle 110 \rangle} = 2\sigma_{C\langle 111 \rangle}/3$, the maximum of compressive strength happens along $\langle 111 \rangle$ orientation, while the minimum of the compressive strength depends on the value of $\tau_{0\{111\}\langle 112 \rangle}/\sigma_{0\{111\}}$. When $\tau_{0\{111\}\langle 112 \rangle}/\sigma_{0\{111\}} = 0$, the corresponding orientations of the minimum compressive strength are $\langle 0.169, 1, 1 \rangle$ and $\langle 0.171, 0.171, 1 \rangle$.
2. The maximum asymmetries of the six fcc crystals all happen along $\sim \langle 0, 0.5, 1 \rangle$ – $\langle 0, 1, 1 \rangle$. The minimum asymmetries of Cu and Au possess the similar distribution under different loading orientations, while the corresponding orientations of minimum asymmetries for Ni, Pt, Al and Ir locate at the line of $\langle 100 \rangle$ – $\langle 111 \rangle$ and the higher value of $\tau_{0\{111\}\langle 112 \rangle}/\sigma_{0\{110\}}$, the nearer to $\langle 100 \rangle$ orientation. The higher value of $\tau_{0\{111\}\langle 112 \rangle}/\sigma_{0\{110\}}$ and $\tau_{0\{111\}\langle 112 \rangle}/\sigma_{0\{111\}}$ will cause more tendency to cleavage under tensile stress, which results in lower tensile strength and higher asymmetry. Otherwise, higher value of $\tau_{0\{111\}\langle 112 \rangle}/\sigma_{0\{111\}}$ and $|b|$ will lead to a higher normal stress effect and in succession the higher compressive strength and lower tensile strength and higher asymmetry.
3. This mechanical behavior of ideal crystals under different stress states could not only give guidance to the materials selection for high-strength materials, but also shed lights on better understanding of the elastic strain engineering of ultra-strength materials and the

deformation and fracture mechanisms of anisotropy materials under different stress states.

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