Elastic Constants and Plastic Deformation

Hassel Ledbetter**
**Mechanical Engineering
University of Colorado, Boulder, Colorado 80309, USA
E-mail:Hassel.Ledbetter@colorado.edu

Contrary to the usual view that solid-state elastic and plastic properties fail to correlate, we show many such correlations, mainly with the elastic shear modulus $G$. These correlations occur because plastic-deformation properties involve dislocation motion, dislocations moving under applied force in an elastic continuum where forces between dislocations and dislocation-lattice interactions are controlled by $G$. We find that many strength properties vary linearly with $G$, thus simply to one another. We give a new expression for hardness in terms of atomic properties and the Debye temperature.

Key words: Creep, Elastic constants, Elongation, Fatigue strength, Hardness, Plastic-deformation properties, Shear modulus, Theoretical strength, Ultimate strength, Yield strength.

1. Introduction

Many respected scientists would consider the above title oxymoronic, that no connections exist between elastic constants such as the shear modulus and plastic-deformation properties such as hardness and yield strength. Their reasoning usually follows from the fact that elastic constants are nearly structure insensitive while plastic-deformation properties can depend strongly on structure. By structure, we mean variables such as crystal structure, impurity level, inclusion content, temperature, pressure, dislocation density and arrangement, other defect content, prior mechanical and thermal treatment, and many more. Here, we show the error of this view, especially when we consider similar-structure materials. Advantages of connecting elastic—plastic properties are many. First, elastic constants have been measured accurately on a very wide material variety, both polycrystals and monocrystals.1,2 Second, elastic constants relate to many mechanical—physical properties.3 Third, elastic constants connect directly to a solid’s most basic properties: for example volume, cohesive energy, Debye characteristic temperature, melting point.3 Largely, plastic-deformation properties remain to be connected explicitly to these basic properties. Fourth, elastic-constant theory stands in an advanced state,4 even quantum-mechanical ab initio calculations can be made that agree well with measurement.5

2. Approach

Mainly, we establish elastic—plastic correlations by reviewing previous measurement studies. In some cases, we inject some more-basic solid-state physics.

3. Results

We can summarize our main results with the following interrelationships:

\[ H \sim YS \sim US \sim TS \sim FS \sim G \]

Here $H =$ hardness, $YS =$ yield strength, $US =$ ultimate strength, $TS =$ theoretical strength, $FS =$ fatigue strength, $G =$ elastic shear modulus. At first, this relationship seems odd, that so many different plastic-deformation properties vary linearly with a single elastic constant, the isotropic shear modulus $G$. However, further thought brings credibility; and below we give the measurement support.
4. Hardness and shear modulus

For many years, scientists associated hardness with the bulk modulus $B$, the resistance to volume change. However, recent studies reversed this view, associating hardness with the shear modulus $G$, the resistance to shape change. Figure 1a confirms the correlation.

In Fig. 1a, “superhard” materials lie above the dashed line at 40 GPa. For obvious reasons, the upper region shows few points. Scatter in points below the line probably results mainly from different crystal structures and different electronic structures. A more accurate correlation should result from considering monocrystals with the same crystal structure and similar electronic structures. Figure 1b confirms the improved correlation. $C_{44}$ denotes (100)[010] shear resistance. That $C_{44}$, not $G$, is the appropriate shear modulus for this case suggests that in the alkali halides the mobile dislocations possess Burgers’s vectors in {100} planes. Many more linear $H—G$ correlations could be shown. Indeed, fundamental theory predicts this correlation.

Fig 1 Hardness versus shear modulus. Upper shows results for many compounds and for diamond. Lower shows results for monocrystal compounds with the same crystal structure and, in principle, identical interatomic bonding (electron distribution). This figure shows clearly a linear $H—G$ proportionality. For brevity, we omit similar diagrams that we found for several other material sets. Thus, following Teter, searches for superhard materials should use high shear modulus as a predictor. As shown below, high $G$ also predicts higher general plastic-deformation resistance.
5. Hardness and theoretical (ideal) strength

This key, venerable topic deserves a review by itself, especially because of recent-year improvements in basic theory and in computer speed. We shall simply cite a few results. Frenkel made one of the earliest theoretical-strength estimates in 1926 (before the dislocation concept emerged), finding \( \sigma(\text{max}) = \frac{b}{2\pi a}G \). \(^{12}\) MacKenzie\(^{13}\), Krenn and colleagues\(^{14}\), and others provided improved estimates. (Here \( b \) denotes the spacing between atoms in the slip direction and \( a \) denotes spacing between atomic planes.) But all these theories take the same simple general form: \( \sigma(\text{max}) = cG \). From this result, we assume that other plastic-deformation properties take the same form. Below, we confirm this supposition.

6. Hardness and yield strength

Yield strength represents the stress at which significant numbers of dislocations break away from pinning points and move through the lattice, the onset of plastic (irreversible) deformation. Figure 2, for a huge number (more than 150) of hypoeutectoid ferritic steels, shows the variation of yield strength with hardness.\(^{15}\) A clear trend appears: yield strength increases linearly with increasing hardness. For the two properties, the dislocation movements must be similar, even though the first corresponds to uniaxial extension and the second to indentation.

![Diamond Pyramid Hardness vs. Yield Strength](image)

Fig. 2 Yield strength versus hardness for hypoeutectoid ferritic steels. Solid line represents linear least-squares fit. Dashed lines represent \( \pm 1 \) standard error. Courtesy of C. Van Tyne (Colorado School of Mines).

7. Hardness and ultimate strength

Ultimate strength corresponds to that applied force where “necking” begins and strain appears to increase with lower applied force, that is, to the maximum in the stress—strain curve. Figure 3 shows high-temperature ultimate strength versus hardness for several metals.\(^{16}\)
Proceedings of
ATEM'11

8. Creep

Creep refers to plastic flow at constant stress, usually at low stresses and high temperatures. Creep, steady-state increase of strain with time, occurs according to the following relationship, or a similar alternative:

$$\frac{d\varepsilon}{dt} = \frac{K D \sigma^{4.5}}{T M^{0.5} b^{0.5} G^{3.5}}$$

Here, epsilon denotes strain, $t$ time, $K$ a universal constant, $D$ atomic diffusivity (strongly temperature dependent), $\sigma$ stress, $T$ temperature, $M$ number of dislocation sources, $b$ Burgers-vector magnitude, $G$ shear modulus. Clearly the shear modulus enters prominently. Many theories and correlations predict a $G$ exponent much higher than 3.5. (Higher exponents seem inconsistent with our other findings that strength properties vary as $G^1$. Thus, creep seems to be a basically different deformation process. Perhaps the difference lies simply in dislocation climb rather than dislocation glide.) Connecting creep rate with hardness is difficult because it requires creep measurements at constant diffusivity. So we shall avoid this issue, except to note $G$'s key role in creep.

9. Ductility

So far, we considered strength properties. Now we touch on a compliance property: ductility or malleability. Ductility must relate reciprocally to hardness. But fundamental studies seem lacking. Figure 4 helps us understand ductility in terms of the elastic constants; the diagram plots the $C_{44}/C_{12}$ ratio versus the shear-modulus/bulk-modulus ratio $G/B$. The condition $C_{12} = C_{44}$ represents the Cauchy relationship, proposed in the mid-1800s and believed by many elasticians then to apply to all solids. Soon after, many materials were found to possess lower ratios. In recent years, many higher-ratio materials were found: and many studies focused on trying to explain this unusual behavior, referred to as negative Cauchy pressure. For our purposes, we note that the most malleable metal, gold, occurs at the lower left and that the brittle metals rhodium and iridium occur near the Cauchy condition. Several brittle elements, notably three with diamond-cubic crystal structure occur above the Cauchy line. No theory yet emerged to explain this ductility trend. Indeed, neither has an empirical correlation. In Fig. 4, the straight line represents a
least-squares fit; the dashed curve represents results predicted from simple elastic-constant theory.\footnote{\textsuperscript{18}}

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{plot.png}
\caption{Cauchy ratio versus shear-modulus/bulk-modulus ratio. Ductile materials occur at the lower left, brittle at the upper right. Most materials near or above the line $C_{12} = C_{44}$ show brittleness.}
\end{figure}

\section{10. Stress—strain curve}

If one could calculate a material’s stress—strain curve, several plastic-deformation properties described above would accompany the calculation. Considerable efforts in this direction emerged from the Krenn-and-colleague group at LLNL.\footnote{\textsuperscript{19}} Figure 5 shows some of their results.

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{stress_strain.png}
\caption{Normalized stress—strain curves for Mo and W. Calculated by ab initio methods for $\{110\}<110>$ slip. Results shown for both simple shear and a shear path that allows for triaxial stress states that occur in indentation measurements. The solid line represents a nonlinear elastic—plastic finite-element-model calculation. Indentation was considered perpendicular to $\{100\}$ surfaces, the strongest direction for a b.c.c. lattice. Courtesy of C. Krenn (Lawrence Livermore National Laboratory).}
\end{figure}
11. Atomistic expression for hardness

We consider an atomistic (nearly \textit{ab initio}) expression for hardness for four reasons: (1) among all plastic-deformation properties, hardness may be the most familiar, (2) hardness can be measured relatively accurately, (3) hardness can be calculated from \textit{ab initio} quantum-mechanical theories, (4) hardness interrelates with a wide variety of plastic-deformation properties. Details will appear elsewhere, but the basic relationship derived from lattice dynamics is the following:\(^\text{20}\)

\[ H = K m \theta^2 / V^{1/3} \]

Here, \(K\) denotes a material-independent constant containing Planck’s constant, Boltzmann’s constant, and Avogadro’s number; \(m\) denotes atomic number, \(\theta\) denotes Debye characteristic temperature, \(V\) denotes atomic volume. Figure 6 shows hardness plotted versus the above atomic parameter and we see a nearly perfect linear relationship. Similar diagrams result for other sets of materials. By connecting hardness with the Debye temperature, we can now connect hardness with a very wide assortment of mechanical—physical properties;\(^\text{21}\) a wide assortment indeed as shown for example in a review by Herbstein.\(^\text{22}\)

Fig. 6 Hardness versus a near-\textit{ab-initio} atomic parameter that includes atomic mass, atomic volume, and the Debye characteristic temperature. Through the Debye temperature, this parameter connects hardness with many physical properties that include melting temperature, specific heat, entropy, and many more.

12. Conclusions

1. Plastic-deformation properties correlate with elastic constants.
2. Especially, they correlate with the elastic shear modulus \(G\).
3. They correlate simply, nearly linearly, when deformation proceeds by dislocation glide.
4. Thus, various plastic-deformation properties interrelate among themselves; here hardness is particularly useful.
5. A new atomistic expression for hardness provides insight into its fundamental aspects. This expression applies to a wide material variety, even metals where the
dislocation arrangement is more complicated than in nonmetals.

6. The task remains to develop fundamental theories connecting the various plastic-deformation properties.

Acknowledgments

In preparing this review, I profited enormously from three sources: (1) publications by C. Krenn and colleagues at LLNL, (2) discussions with and publications by J. Gilman (now deceased) at UCLA, (3) interactions with J. Rodgers at Innovative Materials, Quebec.

References

(19) Krenn, C., Roundy, D., Cohen, M., Chrzan, D., Morris, J., Connecting

(20) Ledbetter, H., A new atomistic expression for hardness, to be published.

(21) Table 1.13 in Ref. 3. Compiled for elastic constants, this table applies also to Debye temperatures, which one can calculate simply and accurately from the elastic constants.