Materials selection in micro- or nano-mechanical design: Towards new Ashby plots for small-sized materials

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Abstract

Conventional Ashby plots for material selection may not appropriately describe material properties at small-length scales, new plots taking account of size effects are urgently needed for micro- or nano-mechanical design. Here, I show strength–modulus, strength–density, and size effect–Peierls stress plots for various solid materials at small scales.

Keywords: Size effect; Plastic deformation; Micro-compression; Focused ion beam; Small scales; Ashby plots

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1. Introduction

For decades, Ashby plots for material selection have provided a qualitative guide for choosing appropriate materials for engineering applications [1], such as strength–density and strength–modulus charts [2]. The conventional Ashby plots were established based on the properties of coarse-grained or single-crystalline materials in their bulk forms. At micrometer or nanometer length scales, the material properties, however, may not be identical to those of the bulk ones. Size dependence of strength in metals presents a good example of this multiscale complexity [3]: at the nanometer scale ($< \sim 100$ nm), the activities of an individual dislocation and material surfaces may dominate the material strength; at sub-micrometer scales (~ 100 nm– 1 μ m) – a length scale of mean dislocation spacing, dislocation segments may control the strength; at micrometer scales (~ 1 μ m– 100 μ m), one may observe a transition between small-scale strength to macroscopic strength, where the latter represents the strength used in conventional Ashby plots. Consequently, conventional Ashby plots may not appropriately describe material properties when the length scale of a material is reduced into micrometer and nanometer regimes.

Micro- or nanoelectromechanical systems (MEMS or NEMS) generally consist of many components in the dimension from a few micrometers to a few nanometers. Appropriate selection of materials with desired properties is critical to overall functionality and reliability of the systems. Therefore, to create new Ashby-type plots that take account of the size dependence of material properties is highly desirable to meet the challenge of rapid development of microelectronics and nanotechnology sectors.

In 2004, Uchic and his co-workers first reported size-dependent strength of micrometer-sized metal pillars, in which Ni micro-pillars were fabricated using the focused ion beam (FIB) milling technique and compressed by a nanoindenter with a flat-punch tip [4]. Over a decade, significant advances have been made in applying this methodology to study mechanical properties of materials in small dimensions – usually between a few microns down to 100 nanometers. A large number of materials reveal strong size dependence of strength when their sample dimensions are reduced into the micro- and nanoscales. Meanwhile, the yield strengths of these micro/nano-pillars can attain a significant fraction of their theoretical ones. Dou and Derby [5] quantify the micro-compression data using a power-law fit, as:

$$\frac{\sigma}{G} = A \left(\frac{D}{b} \right)^{-m} \quad (1)$$

where σ is yield strength or flow stress, G is the shear modulus of a corresponding slip system, A is a constant, D is the pillar diameter, b is the Burgers vector, and m is so-called size-effect exponent. Since the Uchic's work was published, over a thousand related studies have been reported, which covers a broad range of materials (see reviews [6-8]). Table 1 presents a summary of some representative materials: pure metals (e.g., face-centered-cubic (fcc) Au [9, 10], Al [11, 12], Ni [13], and Cu [14, 15]; body-centered-cubic (bcc) Nb, Ta, Mo, and W [16, 17]; and hexagonal close packed (hcp) Ti [18, 19] and Mg [20]), ionic crystals (e.g., NaCl [21], KCl [22], LiF [23, 24], and MgO [25]), covalent crystals (e.g., Si [26] and GaAs [27]), ordered intermetallics (e.g., TiAl [28]), disordered intermetallics (e.g., high-entropy alloys (HEAs) [29, 30]), complex metallic alloys (CMAs, e.g., $\text{Al}_{13}\text{Co}_4$ [31]), quasicrystals (QCs, e.g., icosahedral Al-Pd-Mn [32] and decagonal Al-Ni-Co [33]) and metallic glasses (MGs, e.g., Cu- and Zn-based ones [34]). The measured m values in fcc metals all fall in the range of ~0.6-0.7. Such value is

nearly identical to all FIB-milled fcc micro-pillars. Later investigations reveal that bcc metal pillars (Nb, Mo, Ta, W [16, 17, 35] and V [36]) have a large range of size effect exponents (m of ~ 0.2 - 0.9) and hcp metal pillars exhibit an exponent depending on slip systems (m of ~ 0.4 for prismatic slip; m of ~ 0.6 for basal slip[8]). When materials dimensions are reduced into the submicrometer-sized regime, even hard and brittle materials exhibit plasticity to a certain extent, such as Si [26], quasicrystals [32], and metallic glasses [37]. They are all found to show minor or almost no size effect. For example, in the sample size range from ~ 100 nm to ~ 1 μ m [38], Si exhibits much smaller size effects than most metals.

One may ask what the Ashby plots look like after taking account of such size effects and whether there is a general law describing the size effects in all these inorganic solids. Here, this work presents material-property plots for micro/nano-pillars, compare the differences among them, and unveils a general trend of the size effects.

2. Results and discussion

This work focuses on the literature of micro/nano-pillars produced by Ga^+ -FIB milling, because a vast majority (over 90%) of reported micro-compression results are based on a Ga^+ -FIB system, which is commonly and commercially available. Although a few well-known issues are found to be associated with the FIB-milling process, such as FIB-induced irradiation damage and taper angle [39]. Nevertheless, the FIB technique has so far been the most important and widely used method to prepare small-sized samples for mechanical measurement. In addition, the Ashby-type plots for small-sized materials are simplified in two aspects: Because m also depends on initial defect density of a sample [40, 41], only well-annealed samples are compared here; For the

reason of legibility, the highest strengths of micro/nano-pillars are compared here, which generally correspond to a pillar diameter of ~100-200 nm.

The highest strength of a micro/nano-pillar sample as a function of its shear modulus, G , is plotted in Figure 1. The critical resolved shear stresses (CRSS) of all the materials fall in the range between $\sim G/30$ and $\sim G/100$. It is interesting to note that the CRSS of some covalent crystals ([26, 27]), quasicrystals [32, 33], and metallic glasses [34] can approach their theoretical values ($\sim G/10$ [42]). As a contrast, most metals, such as Mo, W, Cu, Al and Mg, are near to the lower strength boundary ($\sim G/100$). The difference of strengths might be attributed to relatively low grown-in defect density or FIB-induced damage levels in the former group.

Taking into account of size dependence of material strength, traditional strength–modulus plots that are developed for bulk materials may not be valid anymore, and, therefore, the new plots that include size effect have to be created. Two examples are illustrated here in Figure 2 and Figure 3, showing the relations of CRSS vs. Young’s modulus and CRSS vs. density, respectively. For instance, if Young’s modulus and yield strength are the only determinant parameters, MgO, NbTaMoW HEAs, TiAl, quasicrystals, and Si should be good candidate materials for structural applications. For another example, when specific strength (i.e., strength-to-density ratio) is the most critical factor to be considered, MgO, Si, TiAl, and quasicrystals are good candidates, as shown in Figure 3. Here, Si micro/nano-pillars offer the highest specific strength among all the micro/nano-pillars reported to date, indicating micro- or nanoscale Si is able to store elastic energy as high as ~ 1 MJ/kg, which is comparable to that of lithium battery. However, in real engineering applications, many other important, sometimes even more

dominating, factors should be considered, such as creep resistance, fracture toughness, electrical conductivity, thermal conductivity, etc. Unfortunately, only few of these properties are completely known for materials at such small dimensions.

The other question concerns how one can predict the size effect for a material only based on its known characteristics. It is found, in general, that brittle materials exhibit a minor or no size effect, such as Si [26], metallic glasses [34], and quasicrystals [32, 33], while ductile materials show relatively large size effect, such as fcc metals, basal-slip hcp metals, and ionic crystals on soft slips. It is known that the brittleness of a material can be qualitatively correlated to its energy barrier or force that resists dislocation motion (or shear band propagation for metallic glasses). This force can be described by the Peierls stress, τ_p (or shear stress at 0 K for metallic glasses). Figure 4 illustrates m as a function of τ_p for different types of materials in a linear- logarithmic format. With the value of m ranging from 0 to about 0.8, and τ_p covers over nearly three orders of magnitude from ~ 0.001 GPa to ~ 1 GPa. A general trend of the relation between the Peierls stress and size effect is found: when $\tau_p < \sim 0.1$ GPa, $m \approx 0.6-0.8$, showing a relatively consistent value; when ~ 0.1 GPa $< \tau_p < \sim 1$ GPa, $0 < m < \sim 0.6-0.8$, showing a decreased m with increasing τ_p ; when $\tau_p > \sim 1$ GPa, $m \approx 0$, showing almost no size effect. This observed trend can be associated with the ratio between the required stress for dislocation nucleation and the stress for dislocation motion (or the stress for shear band formation to that for shear band propagation for metallic glasses). For example, in a 100-nm Ni pillar, more than 95% of the flow stress is contributed by dislocation source; while in a 100-nm W pillar, less than 50% of the flow stress is due to source strengthening, figuratively speaking. It should be noted that Figure 4 represents the size effects of materials that are only measured at room temperature and nearly identical strain rate ($\sim 10^{-3} \text{ s}^{-1}$)

and the size dependence of a material strength may depend on the testing temperature and strain rate. Some previous studies demonstrate three-dimensional (3D) size-temperature-strength deformation maps, such as in Si [38] and quasicrystals [43], but the systematic studies on various materials over a large temperature and strain rate range are still scarce. Nevertheless, although the detailed underlying strengthening mechanism may vary among different materials, this general trend in Figure 4 can be technologically important, providing a common guide to predict material strengths at multi-scales.

3. Summary and outlook

In summary, the material-selection plots for micrometer- and submicrometer-sized materials have been created. The strength–modulus plot shows that the highest strengths in various FIB-milled pillars fall in the range of $\sim G/30$ – $G/100$. The strength-to-density plot compares specific strength of various materials at small dimensions, indicating that Si possesses the highest strength-to-density ratio reported to date. The size effect–Peierls stress log-log plot demonstrates three size-effect regimes ($m \approx 0.6$ – 0.8 , $0 < m < \sim 0.6$ – 0.8 and $m \approx 0$) with increasing resistance for the propagation of plasticity mediums – dislocations or shear bands.

The superior and useful mechanical properties of the small-scale materials presented here may permit their implementation in critical applications as well as offer a strong motivation for their further development. For future studies, it is important to collect data and create Ashby-type plots for small-sized materials without FIB effects as well as including other material properties, such as thermal and electrical properties. It is also instrumental to create 3D Ashby-type mechanism maps that takes account of sample size, temperature, and strain rate, in which several

deformation mechanisms may appear, such as dislocation glide, diffusional flow, and dislocation creep.

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Figure captions

Figure 1. The highest critical resolved shear stresses (CRSS) as a function of shear modulus, G , for representative micro-pillars in Table 1. It indicates the highest CRSS of various pillars is in the range of $\sim G/30$ to $\sim G/100$. Shear moduli are obtained from Refs. [44-47]. (For the reason of legibility, some references are not shown in the graph, but can be found in Table 1. the same reason for the other figures).

Figure 2. The highest CRSS as a function of Young's modulus, E , for representative micro-pillars, showing both high strength and Young's modulus for quasicrystals, high-entropy alloys, and MgO (Young's moduli are from Refs. [44-47]).

Figure 3. The CRSS as a function of density for representative micro-pillars, showing Si pillars are among the most high-strength and low-density pillars, while Au pillars have the lowest strength-to-density ratio (densities are calculated according to their compositions).

Figure 4. Size-effect exponent, m , as a function of Peierls stress, τ_p , for representative micro-pillars, indicates that when $\tau_p < \sim 0.1$ GPa, $m \approx 0.6-0.8$, showing a relatively consistent value; when ~ 0.1 GPa $< \tau_p < \sim 1$ GPa, $0 < m < \sim 0.6-0.8$, showing m decreases with increasing τ_p ; when $\tau_p > \sim 1$ GPa, $m \approx 0$, showing almost no size effect; The values of τ_p (or shear stress at 0 K for metallic glasses) are obtained from Refs. [44-48]. (It should be noted that Si, GaAs, quasicrystals (QCs) and metallic glasses (MGs) are all with the $m \approx 0$, the difference of their m values is only for the legibility of the graph.)

Table 1. Summary of representative materials on the compression of FIB-milled micro-/nano-pillars

Materials	Au	Al	Ni	Cu	Nb	Ta	Mo	W	V	Ti	Mg	NaCl	KCl	LiF	MgO
Type	fcc	fcc	fcc	fcc	bcc	bcc	bcc	bcc	bcc	hcp	hcp	ionic crystal	ionic crystal	ionic crystal	ionic crystal
Ref.	[9, 10]	[11, 12]	[13]	[14, 15]	[16, 17]	[16, 17]	[16, 17]	[16, 17]	[36]	[18, 19]	[20]	[21]	[22]	[23, 24]	[25]

Materials	Si	GaAs	TiAl	HEAs	Al₁₃Co₄	Al-Ni-Co	Al-Pd-Mn	Cu-based metallic glass	Zn-based metallic glass
Type	covalent crystal	covalent crystal	ordered intermetallic	disordered intermetallic	complex metallic alloy	decagonal quasicrystal	icosahedral quasicrystal	metallic glass	metallic glass
Ref.	[26]	[27]	[28]	[29, 30]	[31]	[33]	[32]	[34]	[34]