Universal Maximum Strength of Solid Metals and Alloys

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Universal maximum strength of solid metals and alloys

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Interstitial electron density ρ_o is offered as a direct metric for maximum strength in metals, arising from universal properties derived from an electron-gas – ρ_o sets the exchange-correlation parameter r_s in density-functional theory (DFT). It holds also for maximum shear strength τ_{max} in polycrystals [Phys. Rev. Lett. **124**, 125501]. Elastic moduli and τ_{max} for polycrystalline (amorphous) metals are linear with ρ_o and melting T_m (glass-transition T_g) temperature. ρ_o or r_s, even with rule-of-mixture estimate, predicts relative strength for rapid, reliable selection of high-strength alloys with ductility, as confirmed for elements to steels to complex solid-solutions, and validated experimentally.

With rising interest in design of increasingly complex metallic systems, it is critical to deliver fast and reliable physics-based metrics for materials optimization. An approach that links bond strength and strength of metals, and provides fast prediction (without adjustable parameters), remains elusive. A simple metric would facilitate accelerated design of reliable and damage-tolerant, high-strength metallic alloys for high-temperature applications (*e.g.*, higher efficiency energy generation), including multi-principal-element alloys (MPEAs) [1–5], an exciting class of materials with a vast design space and emerging unique properties [6–10]. Metals are limited by their operational temperature and strength.

With perspective from J.J. Gilman [11, 12] on response of materials to applied stress, we offer a simple, unifying, physics-based metric that provides quantitatively correct results to accelerate design that is computationally less burdensome and requires little *a priori* knowledge. For example, bulk modulus (B) reflects volumetric response to hydrostatic stress and data on ionic materials shows $B \sim r_o^{-4}$ [11] (r_o is interatomic spacing), justified by potentials dominated by a Coulomb interaction. Nevertheless, it is surprising that alkali metals and tetrahedrally covalently-bonded crystals and cubic-diamond compounds also exhibit this behavior, while mixed primary-bonded transition-metal carbides do not. For crystalline metals and ionic compounds, Gilman also provided a fairly accurate model for surface energy from Young's moduli (E) and atomic radii, effectively a measure of average bond strength in uniaxial tension [13].

Since Frenkel's work [14], estimates of shear strength based on shear moduli G [15] give maximum shear strength as $\tau_{max} \approx G/30$, an order-of-magnitude estimate – a factor of 1000 too large for dislocation-mediated cases. Using DFT, ideal (dislocation-free) maximum tensile strength estimated from changes of energy-per-atom along an ideal Bain-path [16, 17] gives 10–100 GPa, a factor of 100 too large. With defects, DFT can be quantitative, *e.g.*, twinning stresses [18, 19] and stacking-fault energies [20], but require large supercells that are computational costly. Some bcc metals have variable strength or ductility due to electronic effects [21].

An estimate of E, associated with bond strength (stiffness), is found using scaling (in SI units [15]), *i.e.*,

$$E \approxeq 100\frac{k_B T_m}{V_{atom}}\left[1-0.5\frac{T}{T_m}\right] GPa \xrightarrow{T=0} 100\frac{k_B T_m}{V_{atom}}. \qquad (1)$$

(T_m) T is (melting) temperature in Kelvin and V_{atom} is volume per atom (in Å). At 0 K, (1) is fairly accurate (see Supplemental Material [22] Fig. S1). In isotropic polycrystals with Poisson's ratio ν, $B = E\,[3(1-2\nu)]^{-1}$ and $G = E\,[2(1+\nu)]^{-1}$ will also scale with T_m, giving similar relative elastic strength. Chandross and Argibay [23] recently argued a maximum achievable τ_{max} in a polycrystalline metal (including grain- or sample-size effects) is given by [similar to (1) as $L \propto k_B T_m$ (see Fig. S2)]

$$\tau_{max} \approxeq \left(L\frac{\rho_L}{M}\right)\left[1-\frac{T}{T_m}\right] f_g\; GPa \xrightarrow{T=0} k_B T_m \left(\frac{\rho_L}{M}\right) f_g, \qquad (2)$$

where ($L\ \rho_L/M$) estimates the product of average bond strength and bond density from intrinsic properties L (molar heat of fusion), ρ_L (density of liquid at T_m), M (atomic mass). With d (δ) is grain diameter (grain-boundary width), $f_g = (d-\delta)/d)^3$ is volume fraction of crystalline grains that incur amorphization energy penalty. With f_g=1 (single crystal), Eq. (2) is a good upper bound to maximum strength [23].

We reveal strength measures (*e.g.*, moduli and τ_{max}) in metals (Fig. 1) and alloys (Fig. 2), which are expensive to compute or measure, correlate with an easily computed scalar – average interstitial electron density ρ_o. From properties of a homogeneous-electron gas, ρ_o follows a DFT universal curve (scatter due to alloy stability changes). We show that ρ_o is linear with T_m (glass-transition temperature T_g) for crystalline (amorphous) metals. Thus, ρ_o is a fast relative strength measure for metals, including complex solid solutions and metallic glasses, as validated by measured data. We also find that a rule-of-mixtures (RoM) estimate from the elements provides a reliable ρ_o for an alloy, as confirmed by DFT and measured data. Supplemented with a RoM estimate of Pugh Ratio (PR) assesses whether strength is potentially accompanied by ductility – critical for engineering applications. Our validated RoM ρ_o and PR permits accelerated alloy selection from only trivial computations.

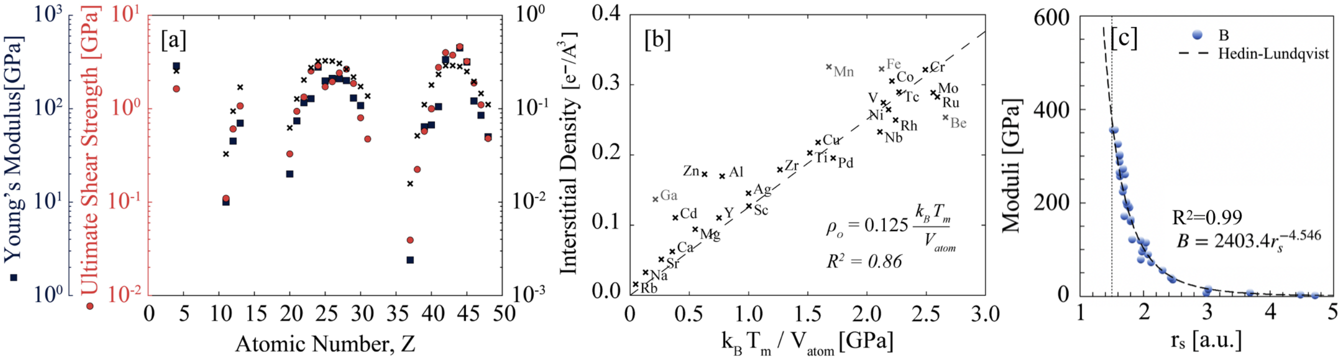

FIG. 1. (Color online). (a) E (■) and τ_{max} (●) [GPa] (from [23]) vs. Z; B is same [24]. On right-vertical axis, DFT ρ_o (×) vs. Z correlates with E, G, and B. (b) ρ_o vs. k_BT_m/V_{atom} shows linear correlation – R^2 is without outliers (Ga, Mn, Fe, Be) having allotropic transitions unaccounted in ρ_o. (c) Measured E, G, B vs. r_s follow Hedin-Lundqvist electron-gas (dashed) curve. Fig. S4 in Supplemental Materials compares all moduli and fits; deviations of E, G arise from Poisson's ratio (deformation anisotropy), where, for $\nu = 1/3$, $E = B$ but $G = (3/8)B$ follows the same curve that is lower (true for all ν).

Measures of strength are reflecting universal behavior and the physics is simple: With applied stress, atoms move closer together within a region containing only interstitial electrons, compressing the electron gas (homogeneous ρ_o in DFT). The larger ρ_o the larger the repulsion – the higher B (E) for hydrostatic (uniaxial) case. This correlation for B in elemental metals was shown by Moruzzi, Janak and Williams [24] (not shown for clarity). See Supplemental Material [22] for comparison to FLAPW [25] and for antiferromagnetic elements [26, 27]. So, we focus on "universality" of ρ_o vs. Z, and, except for scales, B (Eq. in Fig. 1(c)), E (Eq. 1) and τ (Eq. 2) follow directly ρ_o vs. Z (Fig. 1(a)); for ρ_o of 10^{-1} $e/\text{Å}^3$, scales are 10^2 [10^0] for E [τ].

Typically, the interstitial around an atom is considered outside a non-overlapping, inscribed sphere (IS) for a structure. The volumes of unit-cell Ω_{cell} and IS Ω_{IS} are given by geometry (*e.g.*, bcc) and lattice parameters $\{a_i\}$. For elements with Z [28] or solid solutions [29–33] with average $\bar{Z}$, the interstitial ρ_o (or charge Q_o) in interstitial volume $\Omega_o = \Omega_{cell} - \Omega_{IS}$ is

$$\rho_o\Omega_o = Q_o = \bar{Z} - \int_0^{IS} d\mathbf{r}\ \bar{\rho}(\mathbf{r}). \qquad (3)$$

For muffin-tin potentials, the local exchange-correlation (xc) energy functional $\epsilon_{xc}[r_s]$ and potential $\mu_{xc}(r_s)$ is defined [24, 34] by r_s, through ρ_o (with $\frac{4}{3}\pi r_s^3 \equiv 1/\rho_o$). Relative to interstitial reference energy $\mu_{xc}[\rho_o]$, potentials have an electrostatic Ewald term (Ewald energy) dependent linearly on ρ_o (ρ_o^2) [28–31]. For an alloy, the IS radius is determined by saddle-points in the density that depends on environment.[32, 33].

For a binary, E_{form} thus has a large contribution proportional to the square of the difference in ρ_o for the constituent metals [35], similarly for complex solid-solutions [29–32]. Clearly, ρ_o vs. Z and large differences in ρ_o between, say, transition- and alkali-metals, directly affect E_{form} or T_m. We confirm in Fig. 1(b) ρ_o vs. k_BT_m/V_{atom} behaves linearly. (While estimates of T_m are possible by more quantitative methods, *e.g.*, [36], they are demanding.) Takeaway: moduli vs. r_s in Fig. 1(c) (and Fig. S4) follows universal curve and relative maximum strength is indicated by r_s (reflecting $r_s \to \rho_o \propto T_m$, B, E, or τ_{max}).

For metals, compounds, and complex solid-solutions, we use DFT-based Green's function Korringa-Kohn-Rostoker (KKR) combined with the coherent-potential approximation (CPA) to get configurationally-averaged properties for arbitrary random alloys [29–33, 37], including for design [8, 20] and chemically- or vacancy-mediated ordering [38–40]. Due to averaging, KKR-CPA has only 1 (2) atom per cell for fcc/bcc (hcp) phases to get $\bar{\rho}(\mathbf{r})$ and find ρ_o via (3). For the Green's functions, we used a $L_{max} = 3$ spherical harmonic basis (s, p, d, f symmetries) and semi-circular contour integration with 24 complex energies, and Brillouin-zone (BZ) mesh [41] of 18×18×18 for bcc/fcc (16×16×10 for hcp). For pure metals or ordered compounds, KKR and full-potential results agree well [32, 33]. Our KKR-CPA package uses exchange-correlation functionals via LibXC [42], here done with PBEsol [43, 44] or Hedin-Lundqvist [34]. For Pugh ratio in MPEAs, we used Super-Cell Random Approximates (SCRAPs) [45] with 60- (5×3×2) and 90- (5×3×3) atoms to mimic bcc random alloys (no short-range order to 3 neighbor shells). SCRAPs results were from VASP [46] with projector-augmented waves, [47, 48] PBE functional [44], and 520 eV cutoff for plane-wave basis. BZ meshes [41] were 2×5×7 (60-atom) and 2×5×5 (90-atom). Convergence thresholds were 10^{-5} eV (0.01 eV/Å) for energy (forces). KKR-CPA and SCRAPs average a, E$_{form}$, and B agree [45]. For bcc MPEAs, a fully relaxed SCRAP with local lattice distortions has ρ_o closer to CPA value (see Supplemental Materials for result/discussion).

Notably, as for elemental metals (Fig. 2a) with strength in correct measured order (here B) with Ir and

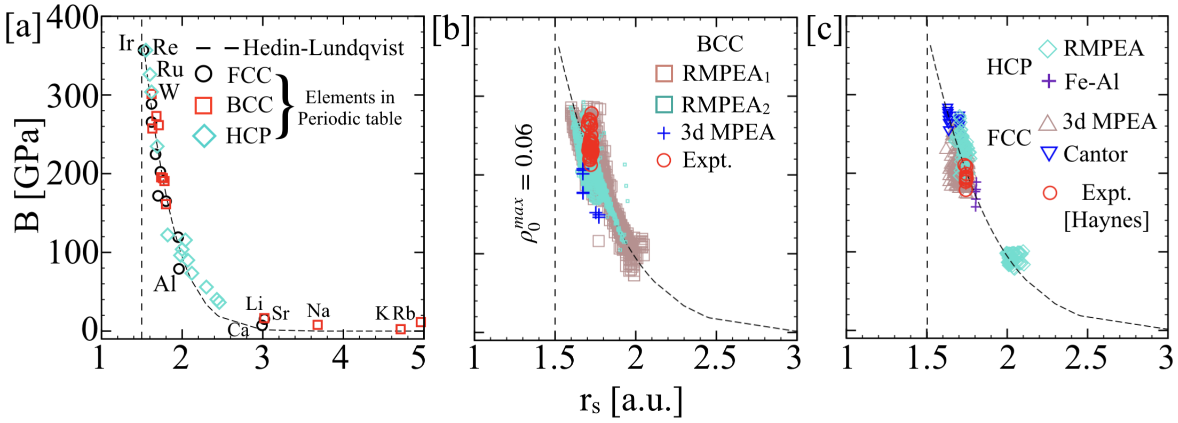

FIG. 2. (Color online) From KKR(CPA), (a) bulk moduli B [GPa] vs. r_s [a.u.] for a homogeneous electron gas ($\left[\frac{4}{3}\pi r_s^3\right]^{-1} = \rho_o$). (b) As in (a) but for bcc refractory (R)MPEAs and $3d$ MPEA, with example measured values. (c) As in (a) or (b) but for fcc/hcp MPEAs, compared to measured Haynes 282 steel values. For Hedin-Lundquist DFT functional (dashed lines), ρ_o values yield B values from the universal behavior. At $r_s \approx 1.5$, a maximum $\rho_o \approx 0.06\ e^-/\AA^3$ yields maximum elemental B.

Re at peak, solid-solution alloy results calculated (over 2800) follow the *universal electron-gas curve*, see Fig. 2b for bcc and Fig. 2c for fcc/hcp phases, including Cantor-type [1, 5] alloys. Some scatter in the data is found along the curve as the alloys have crystal structure (an electron-gas does not), and alloys near the curve are more stable (lowest E_{form}, and higher B), while less stable ones fall below the curve (lower B, see Fig. S5 and discussion). As such, a "vertical" behavior is found within alloy families vs. composition as stability change (Fig. S5). Hence, r_s (ρ_o) provides a correct relative measure of B, E, G, τ, or T_m – but, in contrast to r_s, they are expensive to calculate or time-consuming to measure. $\rho_0^{max}(r_s \approx 1.5)$ governs maximum strength (Fig. 2).

To validate correlations further, we compare measured B data [49] and the universal metric reflected in B vs. r_s, see Fig. 2b for bcc MPEAs (Mo-W-Ta-Ti-Ze-Cr/Al) and Fig. 2c for steels (Haynes-282). Measured data follows the universal r_s curve [again with caveat: most-stable alloys straddle the curve (Fig. S5) and less-stable are below it] and, hence, r_s serves as a relative measure of strength (stability): a smaller r_s has higher strength. Of course, in addition to strength, decreasing grain size (Hall-Petch behavior) can increase yield and ultimate-tensile strength [50]; tuning chemistry can strengthen via twinning- or transformation-induced plasticity [7, 20]; or multi-phase MPEA superalloys can show high specific-strength [51].

For practicality in most technological applications, metals should have high strength and ductility, as needed to avoid brittle behavior and premature failure. Ideally, then, strength combined with a metric to assess ductility quickly for any complex alloy is desired. For MPEAs, we find surprising results involving Pugh's ratio (PR $= B/G$) [52] – which captures for crystalline cases the extent of the plastic range without fracture, reflecting competition between resistance to plastic deformation (G) and fracture strength (B). PR $\gtrsim 1.8$ indicates ductility, brittle below this. For isotropic polycrystalline metals, PR depends only on ν, i.e., $B/G \to \frac{2(1+\nu)}{3(1-2\nu)}$. For simplicity, we tested for MPEAs compositionally-weighted (c_i) elemental rule-of-mixtures (RoM) with

$$\mathrm{PR} = \frac{2(1+\bar{\nu})}{3(1-2\bar{\nu})}\ ,\ \text{and}\ \bar{\nu} = \sum_{i=1}^{N} c_i \nu_i . \tag{4}$$

In Fig. 3, DFT PR vs. (4) for 300 MPEAs agree, as verified experimentally [49]. A higher ρ_o indicates higher B and metallic properties. For Cr-rich MPEAs, Pugh ratio fails to predict the observed ductile-to-brittle crossover; nevertheless the linear behavior remains.

We now turn to bulk-metallic glasses (BMGs) or amorphous metals. To assess ρ_o and evaluate, among other quantities, the shear moduli G, we require su-

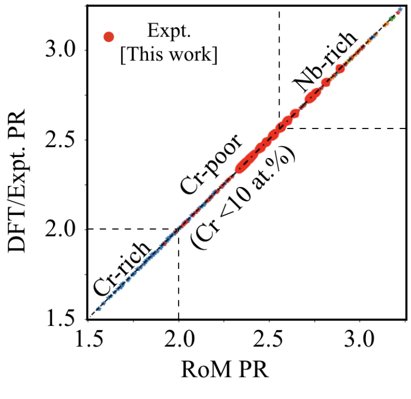

FIG. 3. (Color online). Using SCRAPs, DFT Pugh Ratio (PR) vs. Eq. (4), along with measured data (red circles [49]) for 32 alloys with compositions $(\text{Mo-W})_{1-x-y}(\text{Ti-Zr})_x\text{Ta}_y$. DFT data is for 300 W-Mo-Nb-Ta-Ti-Cr-Al alloys, varying mainly Cr and Nb content.

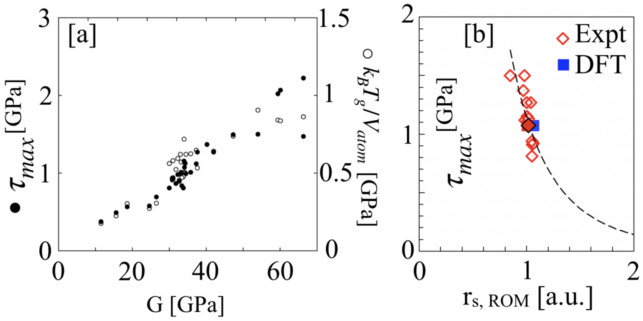

FIG. 4. For BMGs, we compare measured (a) τ_{max} or $k_B T_g / V_{atom}$ vs. G for 32 BMGs (tables in [53, 56]), and (b) τ_{max} vs. RoM-r_s for 12 BMGs (table in [55]). In (a), τ_{max} and T_g show identical linearity with G, differing by a scaling constant. PR above 1.8 [53]. For Vitreloy, KKR-CPA DFT-r_s [blue square] agrees to ∼2% of RoM-r_s [solid diamond].

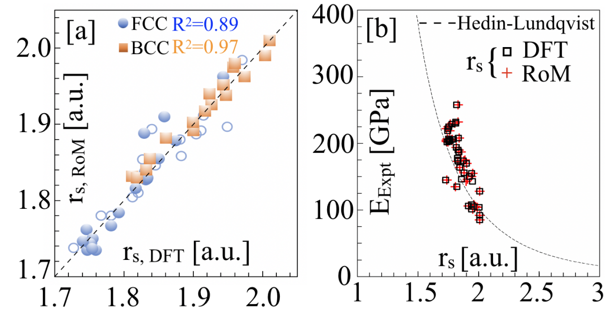

FIG. 5. (Color online). (a) RoM r_s vs. DFT r_s (R^2 from 1:1). RoM r_s uses values in Fig. S6 ("Periodic Table" for elements). Outlier data (off 1:1 line) is for magnetic fcc-MPEAs. (b) For clarity, bcc-MPEA measured [59] E vs. r_s from DFT (squares) and RoM (pluses), relative to universal electron-gas curve.

percells with densities (volumes) mimicking the high-temperature, non-crystalline metal (left for future work). However, as with crystalline metals, we anticipate that ρ_o for amorphous metals will show similar linear behavior with G and $k_B T_g / V_{atom}$. Note that T_g, as often reported, is a surrogate for Kauzmann temperature in limit of infinite heating rate.

Hence, we plot τ_{max} and $k_B T_g / V_{atom}$ vs. G (Fig. 4a) using measured data for BMG [53–55] and amorphous MPEAs [56]. Indeed, both results mirror one another with linear correlation. So, we anticipate that ρ_o for amorphous metals follows the same r_s correlation. Indeed, we plot in Fig. 4b the measured τ_{max} vs. RoM-r_s (G differs by a scale from Fig. 4a), and they follow the r_s curve. For Vitreloy BMG [$Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$], from KKR-CPA in bcc phase with same volume and similar (14-atom) coordination number to BMG (15-atom) found experimentally [57], we find DFT-r_s ∼2% larger than RoM-r_s value in Fig. 4b (likely due to using elemental ground-state crystalline values to estimate BMG phase). In Fig. 4a, measured data below linear is likely due to heating rates or sample defects (*e.g.*, inclusions, voids, and oxide), all of which are common, affecting τ or G due to limited ductility and dependence on quench rate [58].

Before concluding, we offer a "Periodic Table" for elements in hcp/fcc/bcc phases and associated B and ρ_o (Supplemental Material Fig. S6). Within an elemental group, ρ_o (or r_s) should be similar, yielding a similar B; in fact, for atoms in elemental period 2-6, the correlation coefficient is $C(\rho_0, B) \geq 0.95$. The stable phase and its lattice parameters dictate interstitial electron count, and influence the outcome of lowest phase. In Fig. S6, r_s gives the trend in B and takes a minimum at Group VIII, where bcc→hcp→fcc occurs. Notably, for MPEAs at zero pressure, we find good ρ_o or r_s values via RoM from values in Fig. S6 compared to direct DFT results (Fig. 5a). From experiments on bcc MPEAs [59], we confirm E vs. RoM-r_s follows the universal curve (Fig. 5b) – again scatter is from variation with composition (Fig. S5). As values overlay in Fig. 5b, RoM-r_s is a reliable *a priori* estimate of DFT-r_s; i.e., strength by RoM from, *e.g.*, $B[r_s] = 2403.4\ r_s^{-4.546}$ GPa should mirror DFT results. Indeed, RoM-derived compositions for high strength fairly coincide with DFT down-selections that were validated by measurements on refractory MPEAs for high-T applications [49]; the same DFT-guided methods aided and accelerated development of high specific-strength MPEA superalloys [51]. So, in alloys studied thus far, *a priori* RoM-ρ_o estimates could have more quickly narrowed regions with high strength.

Summary. For single- and poly-crystalline metals, we have shown direct correlation between elastic moduli, tensile and shear strengths, and heat of fusion, all of which correlate with properties of an electron gas versus exchange-correlation $r_s[\rho_o]$ parameter – a *universal curve*. This behavior reflects the correlation of ρ_o vs. Z (atomic number) or linear correlation with T_m (Fig. 1-2). Mechanical measures of strength also scale linearly with T_m and ρ_o. But, r_s can quickly assess relative strength in DFT, as confirmed experimentally (Fig. 2). A similar correlation with ρ_o is expected in amorphous metals, as suggested by measured data, where τ scales with G and T_g (Fig. 4). Finally, a rule-of-mixture r_s gives a fast *a priori* estimate strength of MPEA (Fig. 5) or BMGs (Fig. 4) to accelerate design, *e.g.*, for high-temperature strength and ductility (Fig. 3) or to train machine-learning models using a physics-based feature.

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