

Towards a periodic table for the nanomechanical properties of the elements

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Abstract

Starting from a material description involving only two parameters, the cohesion energy and the atomic size, all the fundamental nanomechanical properties for a given chemical element are estimated. In particular, Young's modulus, Poisson's ratio, critical normal and shear stresses and strains, fracture and fragmentation energies, fracture toughness and coefficient of thermal expansion are deduced. Even if the approach partially recalls the classical solid state physics treatment and gives estimations rather than exact predictions, new interesting aspects clearly emerge from the analysis. According to the proposed simple but general model, a preliminary periodic table for the nanomechanical properties of the elements is presented for the first time. The periodicity of the mechanical properties, similarly to the well-known periodicity of the electronic properties, is clearly emphasized. A comparison between our approach and some data present in the literature concludes this paper.

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1. Introduction

Recently, the interest on the mechanical properties of materials at the nanoscale level has been remarkably growing. Just in the last few decades, material scientists have been able to make direct measurements at such a critical size scale, three orders of magnitude smaller than the more known and accessible microscale. An example is given by the exceptional mechanical properties observed in nanotubes (Treacy et al., 1996; Ross, 1991; Yakobson and Smalley, 1997; Yakobson et al., 1996, 1997), since their discovery by Iijima (1991) and other scientists (Weng-Sieh et al., 1995; Chopra et al., 1995; Loiseau et al., 1996). To give an idea of the impact on the scientific community caused by the discovery of nanotubes, it is sufficient to mention that a comparatively recent review paper (Qian et al., 2002), dealing specifically with the mechanics of carbon nanotubes, quotes 349 references. The tremendous mechanical properties coupled with the exceptional electronic ones lead to

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consider nanoscale materials as optimal candidates for innovative materials (e.g., bio-inspired), for biomechanical applications (e.g., nanorobots) or electronics (e.g., nanoelectromechanical systems).

Following the increasing interest in nanomechanics, this paper intends to present new results in the study of the mechanical properties of materials at the nanoscale. We show that only two parameters are needed to describe the nanomechanics of materials: the cohesion energy and the atomic size. The proposed simple but general model gives, as a result, a preliminary periodic table for the nanomechanical properties of elements, in which the periodicity of the mechanical properties is clearly emphasized. A comparison between our estimations and the data present in the literature concludes this paper.

2. Non-linear stress–strain relationship

Let us consider—for the sake of simplicity—a material arranged in the simple cubic lattice. The lattice is spaced of a given size a —coincident with the average interatomic distance—obeying, around the mechanical equilibrium position, to a linear elastic isotropic constitutive law. For larger displacements let a non-linear response be considered. As we will show, the non-linearity in the constitutive equation has to be considered for developing a general model including in particular also the effect of the coefficient of thermal expansion. Anisotropy is not taken into account in our model, the aim of which is to give simple estimations of the nanomechanical properties of materials. However, different types of lattices could be treated by considering as a first approximation an equivalent simple cubic lattice (e.g., by equating the atomic volumes).

The interatomic potential U between atoms depends substantially on their chemical bonding. The atoms do not come into contact owing to Pauli's and nuclei repulsions and reach their equilibrium positions. Even if different chemical bonds imply different interatomic potentials (e.g., Lennard-Jones), we can consider a general form (representing the interaction between one atom and all the others) according to the following series expansion:

$$U(x) = \sum_{n=0}^N c_n x^n, \quad (1)$$

where x is the displacement around the equilibrium position, c_n are unknown coefficients and N is the order of the polynomial approximation. The force F between atoms will be:

$$F(x) = \frac{dU(x)}{dx}. \quad (2)$$

We can assume $c_0 = 0$, the energy being defined through its differential, and we must have $c_1 = 0$, the net force being vanishing at the equilibrium point $x = 0$. The classical harmonic approximation sets $N = 2$ and gives a linear relationship between force and displacement, the so-called Hooke's law. In addition, this symmetric form for the potential energy, related to small displacements, predicts vanishing thermal expansion, in contrast to the experimental evidence. Thus, at least an additional term has to be assumed, so that a value of $N = 3$ is here considered. According to the simplified hypothesis of isotropic regular lattice, a volume $a \times a \times a$ per each atom is considered (simple cubic lattice). The two unknown constants c_2 and c_3 can be obtained by imposing the definitions of Young's modulus and coefficient of thermal expansion, i.e.:

$$\lim_{x \rightarrow 0} \frac{F(x)}{xa} = E, \quad (3a)$$

$$\frac{\langle x \rangle}{aT} = \alpha, \quad (3b)$$

$\langle x \rangle$ being the mean value of the displacement due to the thermal vibration at temperature T . The first condition implies $c_2 = Ea/2$. On the other hand, the second one, evaluating $\langle x \rangle$ by means of the Boltzmann's distribution, i.e.:

$$\langle x \rangle = \frac{\int_{-\infty}^{+\infty} x e^{-\beta U(x)} dx}{\int_{-\infty}^{+\infty} e^{-\beta U(x)} dx} \approx \frac{\int_{-\infty}^{+\infty} x e^{-\beta c_2 x^2} (1 - \beta c_3 x^3) dx}{\int_{-\infty}^{+\infty} e^{-\beta c_2 x^2} dx}, \quad (4)$$

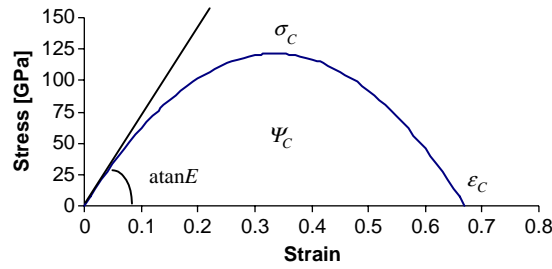


Fig. 1. Nanostress vs. nanostrain relationship (for carbon). Young's modulus E , critical stress σ_C and strain ε_C and energy density (or fragmentation energy) ψ_C .

where $\beta = (k_B T)^{-1}$ and k_B is Boltzmann's constant, gives $c_3 = -E^2 a^3 \alpha / (3k_B)$. In terms of local stress $\sigma = F/a^2$ and strain $\varepsilon = x/a$, the result is:

$$\sigma(\varepsilon) \approx E\varepsilon - \frac{E^2 a^3 \alpha}{k_B} \varepsilon^2 \quad \text{for } \varepsilon \leq \varepsilon_C. \quad (5)$$

Even if the considered approach, based on the interatomic potential, is very simple, classical and well known (Kittel, 1966), the result of Eq. (5) is original and describes a general form for the stress–strain relationship at nanoscale: for small displacements it recovers the well-known Hooke's law, whereas for large displacements a non-Hookean softening regime dominates. Note that the multi-body nature of the atomic interaction is automatically taken into account in Eq. (5) via the Young's modulus. However, more sophisticated multi-body potential could be easily considered (Zhang et al., 2002). The cutoff at ε_C is analogous to the cutoffs classically introduced in the interatomic potentials. This is imposed by the fact that, after the critical (i.e., maximum) strain ε_C for which the stress vanishes, the approximation of Eq. (5) loses its validity. Eq. (5) is general in the sense that the atomic (or electronic or chemical bonding) structure of the solid is traduced in terms of global parameters.

According to Eq. (5), the critical (i.e., maximum) stress and strain are predicted to be:

$$\sigma_C \approx \frac{k_B}{4\alpha a^3}, \quad (6a)$$

$$\varepsilon_C \approx \frac{k_B}{E\alpha a^3}. \quad (6b)$$

Note that ε_C represents the maximum strain assuming a displacement-controlled process. Vice versa, for a force-controlled process, the critical strain is one half of the previous one and will be reached at the maximum stress (e.g., see Fig. 1).

Finally, we note that, at atomic scale, the failure mechanisms could tend towards a unification: the separation between two atoms can be considered a plastic deformation, a brittle fracture or also a melting process. The ratio between the maximum amplitude x_{\max} and its mean value $\langle x \rangle$ gives an estimation of the statistic concentration C_x of the displacements. It is equal to $C_x = x_{\max} / \langle x \rangle \approx \varepsilon / (\alpha T)$. Inverting the previous equation, evaluated in critical conditions, would lead an estimation of the melting temperature as: $T_C \approx \varepsilon_C / (\alpha C_x)$, where C_x is expected to be larger than one.

3. Fracture, fragmentation and cohesion energies

The energy dissipated per unit volume a^3 , that we could call fragmentation energy (Carpinteri and Pugno, 2002), can be calculated starting from the non-linear relationship of Eq. (5) as:

$$\Psi_C \approx \int_0^{\varepsilon_C} \sigma(\varepsilon) d\varepsilon \approx \frac{k_B^2}{6Ea^6\alpha^2}. \quad (7)$$

Thus, the energy dissipated per unit area a^2 , the so-called fracture energy is:

$$G_C \approx \Psi_C a \approx \frac{k_B^2}{6Ea^5\alpha^2}. \quad (8)$$

The fracture energy plays a fundamental role in the prediction of the resistance against brittle crack propagation for a structural element (Pugno and Carpinteri, 2003).

On the other hand, the energy to pull-out an atom from the lattice, the so-called cohesion energy (Kittel, 1966), must be equal to:

$$W_C \approx G_C 6a^2 \approx \frac{k_B^2}{Ea^3\alpha^2}. \quad (9)$$

$6a^2$ being the new surface area created after the pull-out of one atom from the lattice, according to our simplified model.

4. Correlation between Young's modulus and coefficient of thermal expansion

The Young's modulus is an index of the stiffness of a material reacting to mechanical loadings, whereas the coefficient of thermal expansion is an index of the compliance of a material in relation to thermal loadings. The aim of this section is to give, by virtue of a simplified argument, an expression for a correlation between them.

Let us consider the differential of the free energy u , given by (Kittel, 1966) $du = -p dV - S dT$, where the pressure p and the entropy S are defined as $p = -(\frac{\partial u}{\partial V})_T$, $S = -(\frac{\partial u}{\partial T})_V$, and V is the volume. At the thermodynamical equilibrium it is $du = 0$, so that $p = -S \frac{dT}{dV} = (\frac{\partial u}{\partial T})_V \frac{dT}{dV}$. For one atom, the contribution to the free energy due to the thermal vibrations can be classically considered equal to $\sim 3/2 k_B T$. Assuming constant pressure, the coefficient of thermal expansion being defined as $\alpha = (3V)^{-1} dV/dT$, the previous relationship would give $p = \frac{k_B}{2V\alpha}$. On the other hand, assuming constant temperature, differentiating and introducing the stress σ and strain ε under hydrostatic pressure p , for one atom of volume $V \approx a^3$, we have:

$$dp = -d\sigma = -\frac{k_B}{2\alpha} \frac{dV}{V^2} = -\frac{k_B}{2\alpha a^3} 3d\varepsilon. \quad (10)$$

Isotropic linear elastic constitutive laws (see Carpinteri, 1997) are expected for small strains, implying under hydrostatic regime the following relationship:

$$\frac{d\sigma}{d\varepsilon} = \frac{E}{1 - 2\nu}, \quad (11)$$

ν being the Poisson's ratio of the material. The combination of the two previous equations provides the following correlation between Young's modulus and coefficient of thermal expansion as:

$$E \approx \frac{3k_B(1 - 2\nu)}{2\alpha a^3}. \quad (12)$$

As expected, they are inversely related. This result coincides with Grüneisen's relation evaluated for one atom, in which the thermal capacity is assumed to be equal to $3k_B$ (the classical value for T around room temperature) and Grüneisen's experimental constant is assumed to be equal to $3/2$, close to its experimental value for many chemical elements (Slater, 1940). Using Grüneisen's relation instead of Eq. (12) would give more precise results although introducing a new experimental parameter. For this reason, we prefer to consider the simple correlation reported in Eq. (12). However, note that the thermal expansion coefficient and the Young's modulus are functions of the temperature (Jiang et al., 2004).

5. Non-linear shear stress–strain relationship and Poisson's ratio

In Eq. (12) a new elastic constant appears, i.e., the Poisson's ratio ν that, with Young's modulus E , allows one to describe the elastic properties for isotropic materials. What is the expected value for ν at the nanoscale?

To evaluate this coefficient, that thermodynamically must be comprised between -1 and $1/2$, we can alternatively evaluate the shear elastic modulus G .

For small displacements, the shear stress τ is connected with the displacement y (perpendicular to the previously introduced x co-ordinate) by Hooke's law, i.e.:

$$\tau = G \frac{y}{a}. \quad (13)$$

Due to the periodicity of the lattice with respect to shear, the relation shear stress vs. displacement can be assumed as (Frenkel, 1926):

$$\tau \approx \frac{G}{2\pi} \sin \left(2\pi \frac{y}{a} \right), \quad (14)$$

showing a non-Hookean region for large displacements. Obviously, for small displacements it becomes the Hooke's law of Eq. (13). As a consequence, the maximum value of the shear stress is:

$$\tau_C \approx \frac{G}{2\pi}. \quad (15)$$

The ideal shear strength is predicted to be approximately only one order of magnitude smaller than the shear elastic modulus (Frenkel, 1926). Even if the correct coefficient of proportionality remains unknown, depending on the adopted model, this result is experimentally verified and represents an interesting tool to discriminate if the measurements on material strength are close or not to the ideal material strength. The simple approach reported in Section 2 can be considered the extension of this approach for the normal stress–strain relationship.

The shear strain γ is defined by $\tan \gamma = y/a$, so that the non-linear shear stress vs. strain relationship at the nanoscale is predicted as:

$$\tau \approx \frac{G}{2\pi} \sin (2\pi \tan \gamma). \quad (16)$$

The critical value of the shear strain γ will be reached, in a displacement-controlled process, when the shear stress vanishes, for:

$$\gamma_C = \text{atan} 1/2 \approx 27^\circ. \quad (17)$$

On the other hand, if the process is force-controlled then the critical value of the shear strain will be reached when the stress equals its critical value. The corresponding shear strain level is $\text{atan} 1/4 \approx 14^\circ$. This parameter is very large if compared with the measured values at human size scale (of the order of the meter). In addition, it is material independent. This means that, at nanoscale, the ductility—that is not a material property but a size dependent parameter—seems to “universally” prevail over brittleness, independently of the considered material.

Considering the derived strength of Eq. (6a), and replacing α by Eq. (12), gives $\sigma_C \approx \frac{E}{6(1-2\nu)}$. Thus, the model confirms that the ideal strength is expected as a significant fraction of the Young's modulus: such result can be considered a proof of consistency for the simple model that we are proposing. Assuming the well-known tensional Tresca's or energetic von Mises' criteria (see Carpinteri, 1997) (usually considered in plasticity but still applicable if a brittle collapse is assumed):

$$\sigma_C \approx \lambda_{T,VM} \tau_C, \quad (18)$$

where $\lambda_T = 2$ or $\lambda_{VM} = \sqrt{3}$. By comparison between the normal and shear strengths, noting that $G = \frac{E}{2(1+\nu)}$, we deduce an estimation of the Poisson's ratio at the nanoscale as:

$$\nu \approx \frac{3\lambda_{T,VM} - 2\pi}{6\lambda_{T,VM} + 2\pi} \approx 0. \quad (19)$$

According to Tresca's criterion, the prediction is of $\nu_T = -0.015$, as well as for von Mises' criterion of $\nu_{VM} = -0.065$. Practically both criteria suggest Poisson's ratio close to zero. A prediction of ν outside its thermodynamical domain $[-1, 1/2]$ would show an inconsistency of our model. On the contrary and in spite of its

simplicity, it appears *self-consistent*. Obviously, the prediction of Poisson's ratio close to zero has to be taken with caution, representing only an estimation of our simplified model. However, a surprisingly close to zero Poisson's ratio of $\nu \approx 0.07$, has been recently measured for nanotubes by means of Brillouin light scattering (Casari et al., 2001).

6. Nanomechanical property estimations

Eliminating the coefficient of thermal expansion by Eq. (12) in the derived nanomechanical properties, and assuming a Poisson's ratio equal to zero, gives the following estimation for the nanomechanical properties, as a function of the cohesion energy W_C and of the atomic size a :

$$G_C \approx \frac{W_C}{6a^2}, \quad \Psi_C \approx \frac{G_C}{a}, \quad (20a)$$

$$\nu \approx 0, \quad E \approx \frac{27}{2} \Psi_C, \quad (20b)$$

$$\sigma_C \approx \frac{E}{6}, \quad \tau_C \approx \frac{E}{4\pi}, \quad (20c)$$

$$\varepsilon_C \approx \frac{2}{3}, \quad \gamma_C \approx \text{atan} \frac{1}{2}. \quad (20d)$$

Better estimations could be deduced relaxing the simplified hypothesis of $\nu \approx 0$. Note the large general value (around 67%) of the critical strain that, as suggested also by the critical shear strain, implies a very large ductility at the nanoscale, independently of the considered material. Such a result seems to be confirmed by the large ductility shown by classically brittle materials (if considered at the human size scale) like glass or carbon, e.g., glass whiskers or carbon nanotubes (Yakobson et al., 1997).

7. Can our estimations be considered in reasonable agreement with the data reported in the literature?

The most well-known prediction for the ideal strength of crystals was derived by Orowan (1948) in the following form:

$$\sigma_C^{(\text{Orowan})} \approx \sqrt{\frac{EG_C}{2a}}. \quad (21)$$

A detailed comparison between the Orowan's prediction and a large number of experimental observations was reported by Macmillan (1983), demonstrating that, in spite of its simplicity, Eq. (21) can reasonably predict the ideal strength of materials. Thus, if our approach agrees with such a prediction, we conclude that it has to be considered in agreement with the experimental observations on ideal strength of solids. Obviously, our approach as well as the Orowan's estimation have to be considered as reasonable estimations rather than as exact predictions. Rearranging Eqs. (20) we find:

$$\sigma_C \approx \sqrt{\frac{27}{36}} \sqrt{\frac{EG_C}{2a}} \approx 0.9 \sigma_C^{(\text{Orowan})}. \quad (22)$$

Thus, the two estimations are in reciprocal agreement.

Finally, we note that, applying quantized fracture mechanics (Pugno and Ruoff, 2004) considering the fracture quantum as coincident with the atomic size, the prediction of the ideal strength is:

$$\sigma_C^{(\text{QFM})} \approx \sqrt{\frac{4}{\pi}} \sqrt{\frac{EG_C}{2a}} \approx 1.1 \sigma_C^{(\text{Orowan})} \quad (23)$$

again in agreement with the previous model.

Now, let us focus the attention on carbon (graphitic form), for which $a \approx 1.54 \text{ \AA}$ and $W_C \approx 7.36 \text{ eV/atom}$ (Kittel, 1966). Correspondingly, from Eqs. (20) we estimate:

- (1) $\nu \approx 0$; experiments on carbon nanotubes seem to confirm this prediction: a surprisingly close to zero value of $\nu \approx 0.07$ has been recently measured (Casari et al., 2001).
- (2) $E \approx 725 \text{ GPa}$; it is well known that the Young's modulus for ideal carbon nanotubes, or graphite, is expected to be of the order of $E \approx 1 \text{ TPa}$ (Qian et al., 2002). Values close to 800 GPa were measured by Yu et al. (2000).
- (3) $G_C \approx 8.3 \text{ N/m}$ (and $\Psi_C \approx 54 \text{ GPa}$); a reference value for carbon nanotubes is $G_C \approx 8.4 \text{ N/m}$ (Lambin et al., 1998).
- (4) $\varepsilon_C \approx 67\%$ (and $\gamma_C \approx 27^\circ$); based on molecular dynamics atomistic simulations (Yakobson et al., 1997), a value of $\varepsilon_C \approx 40\%$ is locally predicted in monoatomic chains due to high strain fracture of carbon nanotubes.
- (5) $\sigma_C \approx 121 \text{ GPa}$ (and $\tau_C \approx 58 \text{ GPa}$); strength of ideal carbon nanotubes, or graphite, is expected to be of the order of $\sigma_C \approx 100 \text{ GPa}$ (Qian et al., 2002). Values up to 64 GPa were measured by Yu et al. (2000).

Eventually, the toughness at the nanoscale is predicted by definition as $K_{IC} = \sqrt{G_C E} \approx 2.45 \text{ MPa } \sqrt{\text{m}}$, and, from Eq. (12), the coefficient of thermal expansion is $\alpha \approx 8 \times 10^{-6} \text{ K}^{-1}$, whereas, considering $T_C \approx 4000 \text{ K}$ would give a displacement localization (ratio between maximum and mean values of the displacement during thermal vibrations) $C_x \approx 20$.

The nanoscale stress–strain relationship of carbon (Eq. (5)) is reported in Fig. 1.

It is important to note that the predicted values substantially agree with the experimental results at the nanoscale and that they are completely different from the corresponding values at the macroscale. In fact, strong size-effects on material properties are expected (Carpinteri and Pugno, 2004).

8. Nanomechanics as the borderline between classical and quantum mechanics: Young's modulus and crack propagation

The last considerations are on brittle crack propagation at the nanoscale. The velocity of the crack propagation, as well as of the elastic waves, is of the order of $\sqrt{E/\rho}$, ρ being the density of the considered material. According to special relativity, it must be smaller than light velocity c , so that the corresponding maximum value of the Young's modulus results to be $E_{\text{SR}}^{\text{max}} \approx \rho c^2$, e.g., and therefore around 10^{20} Pa for $\rho \approx 10^3 \text{ kg/m}^3$ (thus, much larger than the observed values).

A more interesting upper-bound for Young's modulus is imposed by quantum mechanics, considering fracture propagation at the nanoscale coupled with the Heisenberg's principle. In one of its forms, the principle states that $\Delta W \Delta t \geq \hbar$, ΔW and Δt being respectively the energy and the time spent in the process, and $\hbar = h/2\pi$, where h is the Planck's constant. With reference to fracture propagation, evaluating the time as $\Delta t \approx a/\sqrt{E/\rho}$, and the energy as $\Delta W \approx G_C a^2$, we obtain:

$$E_{\text{QM}}^{\text{max}} \approx \frac{\rho G_C^2 a^6}{\hbar^2}, \quad (24)$$

that, for $\rho \approx 10^3 \text{ kg/m}^3$, $G_C \approx 10 \text{ N/m}$ and $a \approx 1 \text{ \AA}$, results to be around 10 TPa and of the same order of magnitude (TPa) observed for example in carbon nanotubes. This very simple argument is intended to show that nanomechanics can be considered at the borderline between classical and quantum mechanics (and, obviously, outside the domain of special relativity). This is the reason why both classical and quantum mechanics have been successfully applied in nanomechanical treatments.

9. A preliminary periodic table for the nanomechanical properties of elements

According to Eq. (22), and based on the values of the interatomic distances in the stable lattice reported (table of periodic properties of the elements by Sargent-Scientific Laboratory Equipment Catalog Number S18806) and of the cohesion energies (Kittel, 1966; referred to 0 K), the nanomechanical properties of the

elements (for which both the interatomic distance and cohesion energy are known) as functions of their atomic number are depicted in Figs. 2–8. A preliminary periodic table for the nanomechanical properties of elements

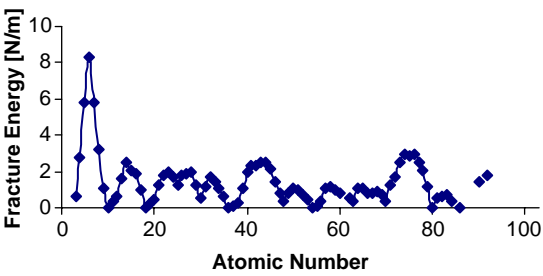


Fig. 2. Nanofracture energy G_C of elements vs. atomic number.

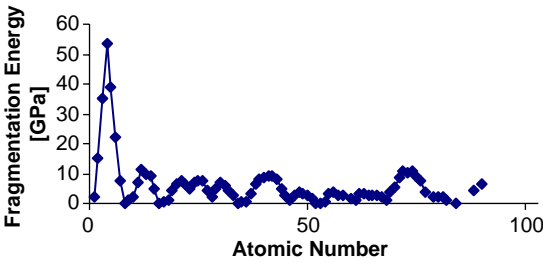


Fig. 3. Nanofragmentation energy ψ_C of elements vs. atomic number.

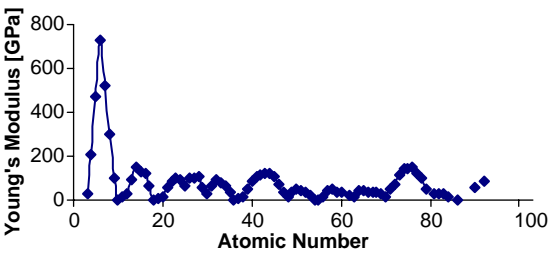


Fig. 4. Nano-Young's modulus E of elements vs. atomic number.

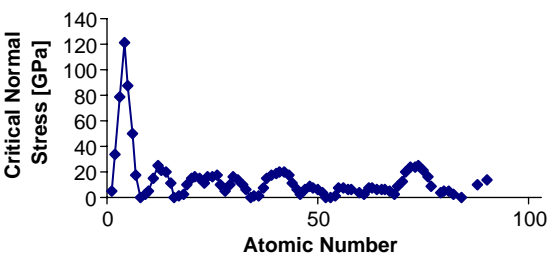


Fig. 5. Nanonormal strength σ_C of elements vs. atomic number.

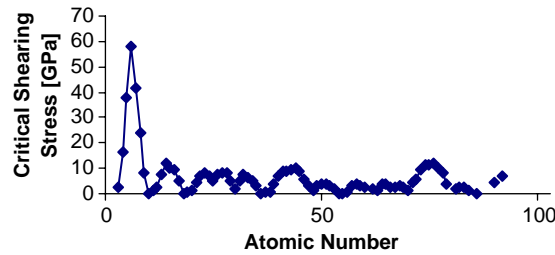
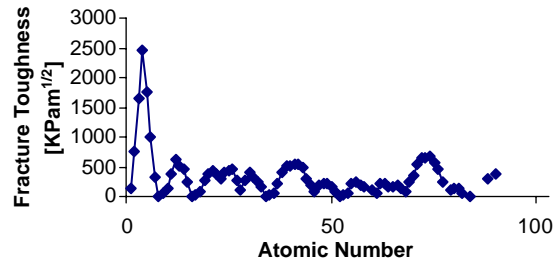
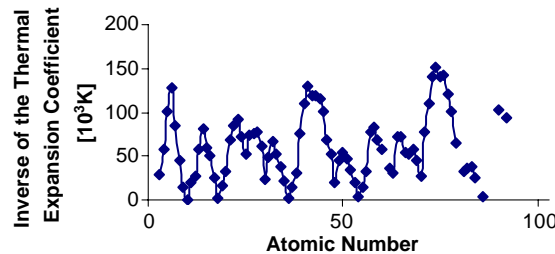
Fig. 6. Nanoshear strength τ_C of elements vs. atomic number.Fig. 7. Nanofracture toughness K_{IC} of elements vs. atomic number.Fig. 8. Inverse of the coefficient of thermal expansion α of elements vs. atomic number.

Table 1

A preliminary periodic table for the nanomechanical properties of the elements

¹ H																																				² He																	
³ Li ⁵ ₃₇		⁴ Be ³⁴ ₇₅₁		<div><div>Z=6</div><div>$E[\text{GPa}]=725$</div><div>$C_{121}=\sigma_C[\text{GPa}]$</div><div>$2450=K_{IC}[\text{KPa}\sqrt{\text{m}}]$</div></div>																								⁴⁷ B ⁷⁹ ₁₆₅₃		⁶ C ¹²¹ ₇₂₅		⁷ N ⁸⁷ ₅₂₅		⁸ O ⁵⁰ ₃₀₁		⁹ F ¹⁷ ₁₀₁		¹⁰ Ne ^{0.07} _{0.4}															
¹¹ Na ⁶⁷ ₁₄		¹² Mg ⁵ ₃₈																										¹³ Al ¹⁵ ₉₁		¹⁴ Si ²⁵ ₁₅₃		¹⁵ P ²² ₁₃₀		¹⁶ S ²⁰ ₁₂₁		¹⁷ Cl ¹¹ ₆₅		¹⁸ Ar ^{0.1} _{0.7}															
¹⁹ K ¹ ₆		²⁰ Ca ³ ₁₆		²¹ Sc ¹⁰ ₅₉		²² Ti ¹⁴ ₈₇		²³ V ¹⁷ ₉₉		²⁴ Cr ¹⁵ ₉₀		²⁵ Mn ¹¹ ₆₇		²⁶ Fe ¹⁶ ₁₁₇		²⁷ Co ¹⁷ ₁₀₃		²⁸ Ni ¹⁷ ₁₀₅		²⁹ Cu ¹⁰ ₆₀		³⁰ Zn ⁵ ₂₇		³¹ Ga ¹⁰ ₆₃		³² Ge ¹⁶ ₉₆		³³ As ¹³ ₈₀		³⁴ Se ¹⁰ ₆₁		³⁵ Br ⁶ ₃₇		³⁶ Kr ^{0.1} _{0.8}																			
³⁷ Rb ²³ ₁₁		³⁸ Sr ² ₁₁		³⁹ Y ⁸ ₄₆		⁴⁰ Zr ¹⁵ ₈₈		⁴¹ Nb ¹⁸ ₁₀₈		⁴² Mo ¹⁹ ₁₁₄		⁴³ Tc ²⁰ ₁₂₃		⁴⁴ Ru ²¹ ₁₀₈		⁴⁵ Rh ¹⁸ ₁₀₈		⁴⁶ Pd ¹¹ ₆₉		⁴⁷ Ag ⁶ ₃₇		⁴⁸ Cd ³ ₁₆		⁴⁹ In ⁷ ₃₉		⁵⁰ Sn ⁸ ₅₀		⁵¹ Sb ⁸ ₄₆		⁵² Te ⁶ ₃₇		⁵³ I ⁴ ₂₁		⁵⁴ Xe ^{0.1} _{0.8}																			
⁵⁵ Cs ¹ ₃		⁵⁶ Ba ² ₁₁		⁵⁷ La ⁷ ₄₂		⁷² Hf ¹² ₇₂		⁷³ Ta ¹⁹ ₁₁₇		⁷⁴ W ²⁴ ₁₄₅		⁷⁵ Re ²⁴ ₁₄₂		⁷⁶ Os ²⁵ ₁₄₉		⁷⁷ Ir ²¹ ₁₂₄		⁷⁸ Pt ¹⁷ ₁₀₀		⁷⁹ Au ⁸ ₅₈		⁸⁰ Hg		⁸¹ Tl ¹ ₂₆		⁸² Pb ⁵ ₂₉		⁸³ Bi ⁵ ₃₁		⁸⁴ Po ² ₁₂₄		⁸⁵ At		⁸⁶ Rn ^{0.2} _{0.9}																			
⁸⁷ Fr		⁸⁸ Ra		⁸⁹ Ac																																																	
⁵⁸ Ce ⁸ ₄₈		⁵⁹ Pr ⁷ ₃₉		⁶⁰ Nd ⁶ ₃₄		⁶¹ Pm		⁶² Sm ³ ₂₁		⁶³ Eu ² ₁₃		⁶⁴ Gd ⁷ ₄₅		⁶⁵ Tb ⁸ ₄₆		⁶⁶ Dy ⁶ ₃₅		⁶⁷ Ho ⁶ ₃₄		⁶⁸ Er ⁶ ₃₈		⁶⁹ Tm ⁵ ₃₁		⁷⁰ Yb ² ₁₅		⁷¹ Lu ⁹ ₅₅																											
⁹⁰ Th ¹⁰ ₉₀		⁹¹ Pa		⁹² U ¹⁴ ₈₅		⁹³ Np		⁹⁴ Np		⁹⁵ Am		⁹⁶ Cm		⁹⁷ Bk		⁹⁸ Cf		⁹⁹ Es		¹⁰⁰ Fm		¹⁰¹ Md		¹⁰² No		¹⁰³ Lw																											

Based on:

$$G_C \approx \frac{W_C}{6a^2} \quad \Psi_C \approx \frac{G_C}{a} \quad \nu \approx 0 \quad E \approx \frac{27}{2} \Psi_C \quad \sigma_C \approx \frac{E}{6} \quad \tau_C \approx \frac{E}{4\pi} \quad \varepsilon_C \approx \frac{2}{3} \quad \gamma_C \approx \text{atan} \frac{1}{2}$$

ν = Poisson's ratio (material-independent), E = Young's modulus, σ_C = critical normal stress, τ = critical shear stress, ε_C = critical normal strain (material-independent), γ_C = critical shear strain (material-independent), G_C = fracture energy (per unit area), Ψ_C = fragmentation energy (per unit volume), $K_{IC} = \sqrt{G_C E}$ = fracture toughness, W_C = cohesion energy, a = interatomic distance, Z = atomic number (material properties referred to 0 K).

is reported in Table 1. We have focused our attention on the main mechanical properties of materials, i.e., the Young's modulus, the strength and the fracture toughness. The periodicity in the nanomechanical properties appears in a very clear way. Carbon—the chemical foundation of life—appears to be the strongest element.

10. Model limitations and conclusions

The values that we have reported in the “preliminary periodic table for the nanomechanical properties of elements”, Table 1, are affected by different uncertainties. In particular, we have simply assumed the Poisson's ratio equal to zero, as suggested by the considerations reported in Section 5; however, zero represents an intermediate value between its thermodynamic limits of -1 and $1/2$. Furthermore, we have to note that the Poisson's ratio is an anisotropic parameter, depending on the crystallographic direction along which it is measured: thus, different values should be considered for each different crystallographic direction. For the sake of simplicity, to present a preliminary periodic table, we have chosen to ignore anisotropy. Note that the classical periodic table of the elements itself ignores anisotropy, reporting mean values, as for example for the electrical or thermal conductivity, as well as for the atomic radius. The “atomic radius” itself has a degree of uncertainty, that affects our predictions. In fact, different types of atomic radii can be defined through different models, e.g., Hartree–Fock approach, rigid spheres, and so on. A few of them are reported in the periodic table of elements in terms of atomic (or also covalent or ionic) radius or volume. We note that the atomic radius and volume are independent parameters, thus representing a first reason of uncertainty. In addition, as previously emphasized, we have neglected anisotropy. However, in our approach different values for each crystallographic direction of the parameter a could allow us to roughly take into account anisotropy, as well as a “mean value” (e.g., the cubic root of the volume per atom) would allow us to consider not only simple cubic lattice. Finally, our model ignores plastic deformations.

To clarify the previous points, we can treat as a simple example the case of sodium, considering its lattice parameter (BCC, 0.42906 nm) and applying the rigid sphere model (2 atoms per cell in BCC). The Young's modulus of the sodium usually reported in the literature is close to 10 GPa, against our preliminary prediction of 14 GPa. According to the periodic table of the elements, the atomic radius of the sodium (that we have used) is 0.190 nm, whereas the atomic radius that we calculate, remembering that the closed packed direction is $[111]$ (diagonal), is 0.186 nm. The same value is deduced starting from the volume of the unit cell (cube of the lattice parameter for BCC) and taking into account the packing factor for BCC (0.68). Thus, considering 0.186 nm instead of 0.190 nm would yield $E \approx 14 \times 0.190^3 / 0.186^3 \approx 15$ GPa. On the other hand, removing the approximation of a vanishing Poisson's ratio, $\frac{E}{(1-2\nu)} \approx 15$ GPa, so that to capture the correct value of $E \approx 10$ GPa, a value of $\nu \approx 0.17$ is deduced.

We conclude that our preliminary predictions must be considered only simple estimations; however in spite of its limits, the approach reported in this paper could be of interest due to its simplicity and generality.

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