A Note on the Transition from Nano- to Mega-Mechanics: The Role of the Stress Quantization

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ABSTRACT

This short note addresses the following question: Can the same physical theory be successfully applied to model phenomena and processes varying from the nano to the mega size-scale? And if so, what are the necessary modifications that need to be introduced? A partial answer is given here within the framework of continuum mechanics provided that a stress quantization procedure is considered. It has recently been shown that such an approach may successfully be utilized to justify the discrepancies emerging from actual on-silicon experiments in comparison with related model predictions based on standard continuum approaches. Two examples, on the smallest and largest spherical object existing on our planet, i.e. a fullerene molecule (having a radius of a few nanometers) and the Earth itself (having a radius of a few megameters), are discussed spanning a length size spectrum of ~15 orders of magnitude.

1. INTRODUCTION

Continuum theories, such as classical elasticity, are not capable of treating objects spanning several orders of magnitude in size, such as the long-known planet Earth and the recently discovered fullerene molecule which span length scales differing by 15 orders of magnitude. The simplest indication in support of this claim is to imagine a linear elastic plate containing a hole and subjected to a far field stress. Obviously, the strength of the plate will depend on the size of the hole, thus a hole-size-effect on the plate strength is expected. In passing, we note that "holes" are common both in geotechnical and mining engineering on the Earth scale, as well as in MEMS/NEMS nanoengineering applications on the Fullerene scale. Since elasticity does not possess an internal characteristic material length one can easily conclude, without making any calculation, that this prediction for the plate strength will erroneously be hole-size independent, a fact only recently attended by the experimental literature. In other words, the absence of an internal characteristic length disables such a continuum theory from discriminating between "small" and "large" holes. In fact, by conventionally assuming that failure of the plate occurs when the maximum stress σ_{max} reaches the theoretical material strength σ_{th}, the corresponding failure stress is predicted to be $\sigma_f = \sigma_{th}/S_c$, where S_c is the stress-concentration factor at the hole perimeter (e.g., $S_c = 3$ for uniaxial load, $S_c = 2$ for uniform biaxial load, $S_c = 4$ for pure shear, see /1/).

Modifications of linear elasticity to allow for additional "stretching" and "rotational" degrees of freedom for the material point "mimicking" the translation and rotation of the atomic bonds have been proposed in the literature starting with the works of Cauchy and Voigt in the 18^{th} century, continuing with the celebrated work of brothers Cosserat in 1906, and concluding with the works of Truesdell, Toupin, Rivlin and Mindlin (for a historical account one can consult, for example, the review by Altan and Aifantis /2/), among others, half a century later. Despite their mathematical rigor and elegance these theories did not make it possible to dispense with elastic singularities at crack tips, even though a large number of phenomenological constants were used. Moreover, the complexity of the associated boundary conditions has prevented the derivation of easy-to-use results to describe, for example, size effects. A simplified gradient elasticity theory was proposed by the second author in 1992 /3/ involving only one extra coefficient (commonly known as gradient coefficient, the square root of which was identified with the dominant internal length of the underlying elastic microstructure). Moreover, solutions of boundary value problems of this gradient elasticity model (departing from the classical Hooke's elastic model by only one term involving the Laplacian of the Hookean stress) could be reduced to solutions of an inhomogeneous Helmholtz equation with the source term being the solution of the corresponding classical elasticity boundary value problem. Elastic singularities from dislocation lines and crack tips were readily eliminated by this model and size effects were conveniently interpreted (see, for example /4,5/). In particular, size effects for hollowed specimens are discussed in two accompanying papers contained in this Journal's issue /6,7/. For this reason, we are not elaborating further on gradient elasticity in this short note, but we describe briefly an alternative approach, namely, the so-called "quantized elasticity" approach for discussing scale effects.

Quantized elasticity could simply be formulated from its classical continuum counterpart by substituting the stress σ with its mean value on a quantum of volume a^3 (or surface a^2, or length a), i.e., $\sigma \to \sigma^* = \langle \sigma \rangle_{a^3}$, recovering Classical Elasticity in the limit of a vanishing quantization (i.e. $a \to 0$, correspondence principle). The term "quantized" is here simply used as a synonym of "discrete", for consistency with the literature /8, 9/. It is clear that such a simple extension automatically includes a characteristic length, i.e. a. Returning to the example of the perforated plate, this extension allows us to discriminate between a small (radius smaller than a) or large (radius larger than a) hole. In addition, this new parameter a is directly related to the discrete internal structure of the material at small size-scales (e.g. atoms /9/) or, in general, to a characteristic length defining the departure from homogeneity, at larger size-scales (e.g. grains, inclusions and so on). In the fracture mechanics community this idea has already been successfully applied. In particular, Linear Elastic Fracture Mechanics (LEFM /10/) has recently been extended by the first author by removing the hypothesis of the continuous crack propagation, by using Quantized Fracture Mechanics (QFM /9/), as a generalization of previous nonlocal approaches /8, 11/. According to this view, instead of the local stress the corresponding force acting on a fracture quantum of length a, or equivalently the mean value of the stress σ along it, has to be considered in fracture phenomena, namely $\sigma \to \sigma^* = \langle \sigma \rangle_a$.

This stress quantization is the key for removing the discrepancies between classical elasticity-based theory and actual on-silicon experiments, as we are going to demonstrate below for completely different size-scales.

2. NANOSCALE

Consider a fullerene /12/, of radius R and thickness δ (~0.34 nm for carbon) subjected to an internal pressure p; such a pressure will cause a stretching on its wall equal to $\sigma \approx pR/(2\delta)$, as concluded from the equilibrium requirements imposed on half of this spherical shell structure. Assume the presence on the wall of a nano-hole of radius r << R (e.g. an atomic vacancy cluster). According to classical elasticity theory, the circumferential stress field around the hole is $\sigma_y = \sigma\left(1 + r^2/x^2\right)$ /1/, where $x \geq r$ is the radial coordinate starting from the hole center. Setting $\sigma_{y\max} \equiv \sigma_y(x = r) = 2\sigma = \sigma_{th}$ the failure stress is predicted to be $\sigma_f = \sigma_{th}/S_c$ with $S_c = 2$, that is the related stress-concentration in the vicinity of the hole. On the other hand, by applying a quantized fracture criterion /8/, i.e., by setting $\sigma_y^* = (1/a)\int_r^{r+a} \sigma_y(x)\,dx = \sigma_{th}$, we deduce the following failure stress σ_f (or failure pressure $p_f \approx 2\sigma_f \delta/R$):

$$\sigma_f(r/a) = \frac{\sigma_{th}}{S_c^*} \quad ; \qquad S_c^* = \frac{S_c\, r/a + 1}{r/a + 1} \;, \tag{1}$$

with $S_c = 2$. Eq. (1) implies $\sigma_f/\sigma_{th} \to 1/S_c$ only for $r/a \to \infty$, i.e. vanishing quantization or large holes. [Note that Eq. (1) does not consider defect self-interactions, i.e. r << R)]. On the other hand, for $r/a \to 0$, $\sigma_f/\sigma_{th} \to 1$, i.e. holes with vanishing size do not affect the structural strength, as expected. Computational researchers /13, 14/ performed quantum mechanical calculations using density functional theory, semiempirical methods and molecular mechanics to explore the role of vacancy defects on the fracture of carbon fullerene nanotubes /12/ under tension. Their simulations can be compared with Eq. (1) by considering $S_c = 3$ (uniaxial tension, for which the exact solution is reported in /9/), since we have assumed R >> r, thus neglecting the elastic energy associated to the curvature for both cases. Eq. (1) closely describes their strength predictions, computed for (50,0) (100,0) and (29,29) carbon nanotubes containing nano-holes of six different sizes. In fact, Eq. (1) with a = 0.25 nm or a = 1 nm corresponds to two curves basically capable of enveloping all their results based on the above mentioned atomistic simulations (see Figure 1). Note that such fracture quanta are comparable with the distance between two adjacent chemical bonds (broken during carbon fracture), confirming a relation between a and the internal structure of the material. Thus, the agreement between the quantized approach and the on-silicon experiments is remarkable, justifying, at the same time, the deviation from the standard prediction (1/3) of continuum classical elasticity.

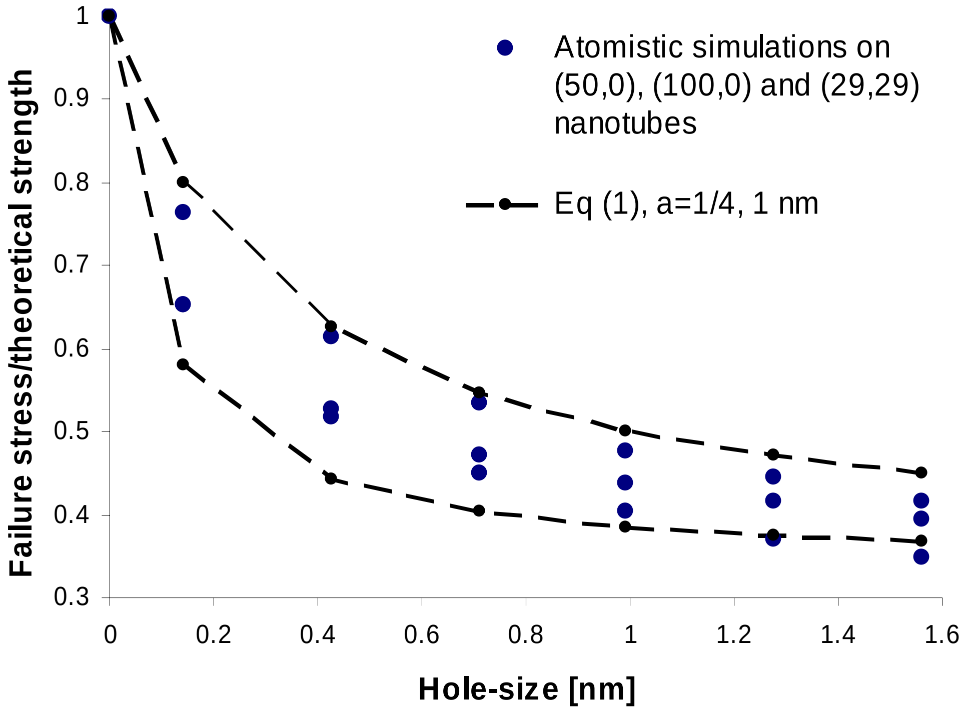

Fig. 1: Atomistic simulations [13, 14] interpreted here by assuming a stress quantization (Eq. (1) with a = 0.25 nm and a = 1 nm, respectively). Note that classical elasticity (i.e. the continuum counterpart of the “quantized” approach) would trivially yield a straight horizontal line at 1/3, independently of the hole-size. Thus, the role of the stress quantization is crucial.

3. MEGASCALE

Next, let us abandon fracture mechanics to consider the coefficient of geostatic stress k_0, i.e. the ratio between the horizontal and vertical geostatic stresses; a geophysical parameter fundamental in the tunnelling design /15/. This problem has recently been considered by Efremidis and Aifantis /16/ through the use of gradient elasticity to explain the departure of this ratio from classical elasticity predictions, but in accordance with existing, even though scattered, experimental measurements. The vertical pressure at a depth z is given by γz , where γ is the specific weight of the Earth's crust. Thus, the horizontal stress is given, according to linear elastic isotropic laws of continuum elasticity (see, for example, /1/) by $\sigma_H = \nu / \left((1-\nu)\gamma z\right)$, where ν is the Poisson's ratio. Consequently the geostatic ratio $k_0 = \sigma_H / (\gamma z) = \nu / (1-\nu)$ is in the range 0.3-0.5 for rocks. In contrast to this straightforward prediction, and as a consequence of extensive experimental work /15/, the coefficient of geostatic stress was observed to obey an empirical law of the form $k \approx k_0 + c/z$, in which c represented an empirical correction term. In fact, by considering the two sets of parameters ($k_0 = 0.3$, c = 0.1 km) and ($k_0 = 0.5$, c = 1.5 km) all the collated worldwide *in situ* stress data can be enveloped, as shown in Figure 2 /15/. By considering instead of σ_H its quantized version $\sigma_H^* = (1/a)\int_z^{z+a} \sigma_H dz$, as a method to include the effect of the layered crust structure of the Earth, we immediately deduce

$$k = \frac{\sigma_H^*}{\gamma z} = k_0 + \frac{k_0 a}{2z} \quad , \tag{2}$$

which is identical to the observed experimental relationship, with $c = k_0 a/2$. Thus, for the above mentioned two envelope curves, we set a = 0.7 km and a = 6 km. Accordingly, the agreement between the quantized approach and the large scale experiments is remarkable, justifying, at the same time, the deviation from the standard prediction (~0.4) of continuum classical elasticity. As already mentioned, a result similar to that reported in Eq. (2) can be derived by using gradient elasticity /16/, even though the calculation is not as simple in that case.

4. CONCLUSIONS

We have shown that for the two extreme cases discussed here, the same physical theory /9,17,17/ can be applied to objects spanning sizes within ~15 orders of magnitude, by simply modifying the extension of the stress quantization domain. At the nanoscale a is found to be of the order of the Angström, whereas at the megascale a is of the order of the kilometer. It would be of interest to further substantiate such conclusions by considering other examples at the nanoscale (fracture of protein chains and NEMS) and the megascale (earthquakes and tectonic fractures). It is difficult to envision methods of analysis enabling conclusions on phenomena with so huge differences in their size-scale range, suggesting that this method may be an interesting candidate to explore for further multiscale applications, all the way from the nano- to the mega-regime.

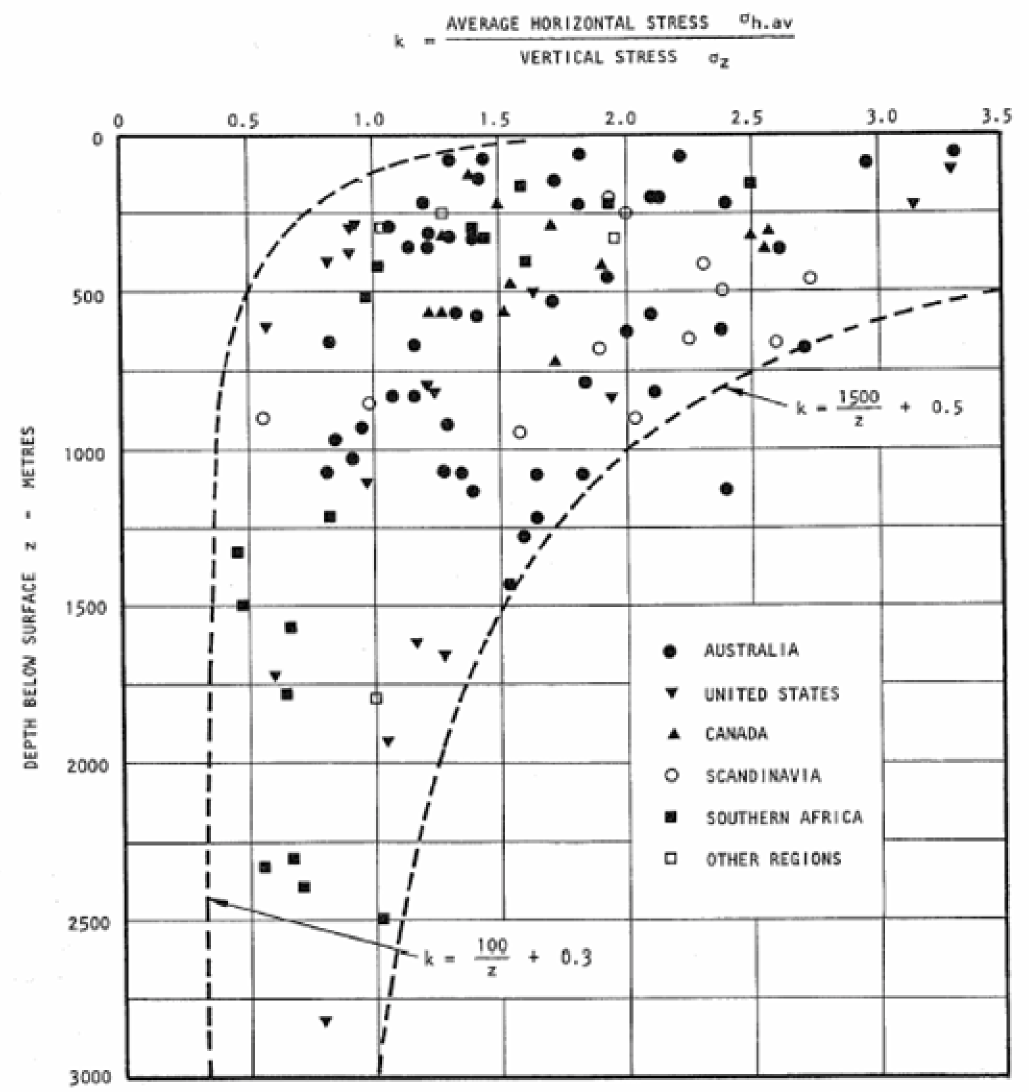

Fig. 2: Large-scale experiments /15/ interpreted by assuming a stress quantization (Eq. (2) with a = 0.7 km and a = 6 km). Note that classical elasticity (i.e. the continuum counterpart of the "quantized" approach) would trivially yield a vertical straight line at ~0.4, independently of the depth below the Earth's surface. Thus, the role of the stress quantization is crucial.

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