Emergent properties in interface mechanical problems

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SUMMARY.

1 INTRODUCTION

Modern measurement techniques have shown that both the geometry of typical micro-defects and the topography of rough surfaces exhibit fractal qualities over several length scales. Evidence is mounting that this multi-scale character is an important factor in the determination of macro-scale properties [1]. In general, it is not possible to predict the global system behavior just from the knowledge of the constitutive models at the micro-scale. The global properties, in fact, emerge from the nonlinear interactions between the system components, a feature typical of organized complex systems. Hence, the understanding of these phenomena is very challenging and demands modeling and extensive computational simulations.

Examples in physics and engineering investigated by the present author regard the size-scale effects on the frictional response of rough surfaces [2], the thermal and electromagnetic properties of heterogeneous materials [3,4], the anomalous fatigue behavior of short-cracks [5,6], as well as the ability of hierarchical polycrystals to tolerate defects through the presence of interfaces at different length scales [7].

In this work, two interface problems related to contact and fracture mechanics of solids are presented as a paradigm of emergent properties in complex mechanical systems. The former concerns the determination of the relation between contact conductance and applied pressure of a rough surface. The latter shows the condition of flaw-tolerance in hierarchical polycrystals as a result of the interplay of cohesive interfaces across multiple scales. The solution of these problems requires the use of dimensional analysis, fractal geometry, computational mechanics, as well as optimization methods.

2 EMERGENT PROPERTIES IN CONTACT MECHANICS: THE CASE OF THE INTERFACE CONTACT CONDUCTANCE

Heat conduction across a rough surface is an important problem, both from the theoretical and the applied point of views. As schematically shown in Fig.1, heat flows in the direction from the warmer body towards to cooler one. At the interface, heat conduction takes place through the asperities in contact. Convection through gas and radiation are also admissible. However, in vacuum and in applications with moderate temperature jumps, conduction is prevailing and convection and radiation can be generally neglected without committing a significant error.

Due to the fact that the contact surface is not completely flat due to roughness, an imperfect contact condition takes place and a temperature jump is observed at the interface. The relation between heat flux q and temperature jump at the interface has the following expression:

$$q = -C\,\Delta T, \tag{1}$$

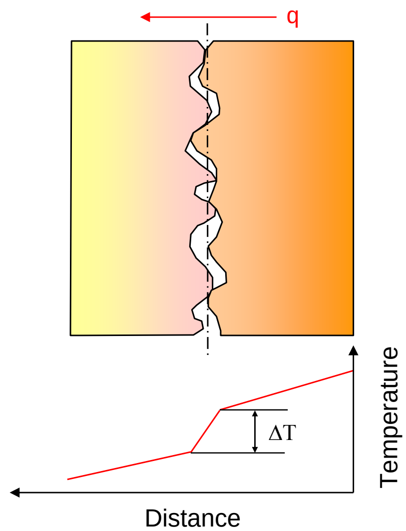

Figure 1: Heat flux and temperature profile for two bodies in contact along a rough interface.

where C is the specific (per unit area) interface contact conductance.

The specific thermal contact conductance of rough surfaces can be correlated to the the derivative of the force-indentation curve, i.e., to the incremental stiffness, as mathematically proven in [8]:

$$C = -\frac{2}{\rho E}\frac{\mathrm{d}p}{\mathrm{d}d}, \tag{2}$$

where p is the nominal applied pressure and d is the mean plane separation between the rough surfaces. The material properties E and ρ are the composite elastic modulus and resistivity of bodies 1 and 2 in contact.

An alternative description of the contact conductance can be obtained by noting that the imperfect contact at the interface is equivalent to the interposition of a fictitious layer of the same material whose thickness h is given by $h = 1/(\rho C)$.

Let us consider a plane rough surface subjected to uniform nominal contact pressure. If the surface is fractal in Weierstrass-Mandelbrot sense — i.e. if it has no largest or smallest length scale in wavelength — than there will be a cut-off in wavenumber at small values (long wavelengths) corresponding to the finite dimensions of the contact area, Δ. Such a surface can be completely characterized by the parameters Δ, σ, D, where σ is the RMS roughness or variance of the height distribution and D is the fractal dimension.

According to the results in [3], the most synthetic dependence of C on the model parameters can be achieved by using the following dimensionless form:

$$\widetilde{C} = \frac{\Delta}{h} = f\left(\widetilde{p}, D\right), \tag{3}$$

where $\widetilde{C} = C\rho\Delta$ is the dimensionless contact conductance and $\widetilde{p} = \dfrac{p\Delta}{E\sigma}$ is the dimensionless contact pressure.

Considerations of incomplete self-similarity in [3] suggested a further simplification of Eq.(3) by admitting a power-law dependence between dimensionless contact conductance and dimensionless pressure, confirmed by experimental and numerical investigations (see [3, 9–12] for a review of the literature on this matter):

$$\widetilde{C} = \widetilde{p}^{\beta}\Phi\left(D\right), \tag{4}$$

where β is the incomplete self-similarity exponent and Φ is a dimensionless function possibly dependent on D.

Numerical (virtual) experiments can be performed to assess the validity of Eq.(4) and to identify the model parameters β and Φ. Considering a numerical method based on the identification of 3D maxima of the surface heights (asperities) and their geometric mean radius of curvature, Paggi and Barber [3] investigated the problem of thermal contact conductance in case of fractal roughness. Linear elastic materials were considered and the contact problem at the asperity level was governed by the Hertzian equations with 1st order elastic interactions.

The surfaces were generated using the random midpoint displacement (RMD) method [13], which is an algorithm originally introduced in the field of computer graphics and used to model rough landscapes and surfaces.

In order to decouple the contact resistance due to surface roughness from that due to the macroscopic geometry, the longest wavelength Δ has to be significantly smaller than the length dimension of the nominal contact area, i.e., $\Delta \ll L$. This condition, however, is not fulfilled when a single square RMD surface is considered. To solve this problem, a series of statistically similar RMD surfaces (patches) is generated. These patches are subsequently collected together to form the rough surface to be numerically tested. Increasing the number of patches, the condition of scale separation is better reproduced. A final adjustment of the height fields of the RMD patches in order to obtain a coincidence of the average planes permits also to remove induced undesirable waviness effects.

It is remarkable to note that the contact response of the rough surface generated in this way is not equivalent to averaging over different realizations of RMD patches. *The collective property of interface conductance emerges from the nonlinear interactions between the asperities and it cannot be predicted a priori from the knowledge of the constitutive response of the single asperity (ruled by Hertzian contact laws).*

To quantify this effect, a square rough surface with $D = 2.3$, $L/\Delta = 2$ (2 RMD patches per side) and $\delta/\Delta = 1/64$ is tested up to a final mean plane separation of $d = 0$. The dimensionless contact conductance $\widetilde{C}$ is plotted vs. the dimensionless pressure $\widetilde{p}$ in Fig. 2, considering different approximations of contact interactions. The empty blue dots correspond to neglecting elastic interactions between asperities. The result is therefore the sum of the Hertzian contributions of the various asperities for each mean plane separation. The obtained trend is well approximated by a linear function in the bilogarithmic plane, suggesting a power-law relation between $\widetilde{C}$ and $\widetilde{p}$ with $\beta = 0.82$.

Considering elastic interactions within the asperities of each RMD patch –but with the patches behaving independently of each other– the result is shown in Fig.2 with a solid red line. Elastic interactions reduce the contact conductance at a given pressure level with respect to the previous case. A single power-law relation between $\widetilde{C}$ and $\widetilde{p}$ cannot be proposed. In particular, a necking point is observed for $\widetilde{p} \sim 1 \times 10^{-1}$. Finally, full interaction effects can be considered (filled blue dots in Fig.2), with asperities interacting within the whole surface. The difference with respect to the previous predictions gives an estimate of the effect of clustering and contact spot distributions across patches that cannot be assessed when they are tested independently. In this case, two regimes can be distinguished. For low contact pressures, $\widetilde{p} \lesssim 1 \times 10^{-1}$, the contact conductance can be

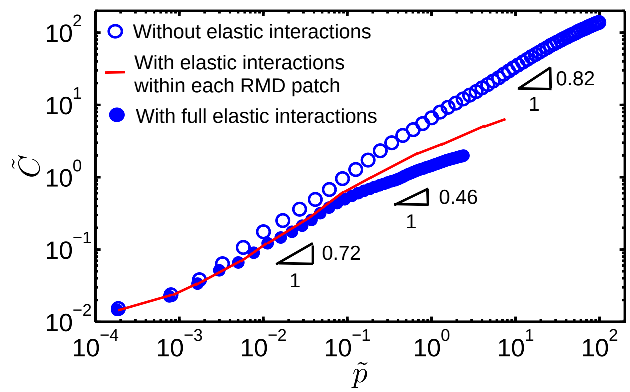

Figure 2: Emergent relation between $\widetilde{C}$ and $\widetilde{p}$, considering different approximations for the elastic interaction between asperities.

approximated by a power-law function of the pressure with an exponent $\beta \sim 0.72$. At higher pressures, the slope reduces to $\beta \sim 0.46$.

3 EMERGENT PROPERTIES IN FRACTURE MECHANICS: THE CASE OF STRENGTH OF HIERARCHICAL MATERIALS

Another interesting problem in the mechanics of interfaces regards the nonlinear interaction of cohesive interfaces across multiple scales in hierarchical materials. This problem is of conceptual and practical interest for the design of bio-inspired heterogeneous materials mimicking the microstructure of bones. It is in fact well-known that, although bones are composed of biological materials with relatively poor mechanical properties, they are very tough and are able to withstand a large number of fatigue cycles. This phenomenon was firstly explained in [14] according to a consideration of *flaw tolerance* related to the interplay between the toughness of cracks and the size of the microstructure.

This condition of flaw tolerance was found to be valid also for the two-level hierarchical polycrystalline material shown in Fig.3.

In [7], a new cohesive zone model for finite thickness interfaces [15] has been used to model the nonlinear fracture behaviour of the thick material interfaces of WC-Co surrounding the polycrystalline diamond rods in the framework of the finite element method. This model, based on a nonlocal damage mechanics formulation to account for the stiffness reduction induced by defects and microcracks coalescing and propagating inside the interface region, suggests that the thicker the interface, the lower the peak stress of the cohesive traction-separation curve representative of the interface response. This trend is consistent with statistical considerations, i.e., the larger the interface region, the higher the probability to find a defect of a given size. This seems also to be confirmed by molecular dynamics simulations in [16], where the peak stress of Mode I simulations is found to be approximately a linear decreasing function of the layer thickness h, see Fig.4.

When this nonlinear fracture mechanics model is applied to the hierarchical microstructure in Fig.3, it is found that, when interface cracks inside the rods (having a size $a \leq d^{\text{level 1}}$) are such that $l_{\text{CZM}}^{\text{level 2}} > d^{\text{level 1}}$, their maximum opening displacement lies within the range of cohesive interactions. Here, $l_{\text{CZM}}^{\text{level 2}}$ is the process zone size of the grain boundary interface cracks of polycrystalline

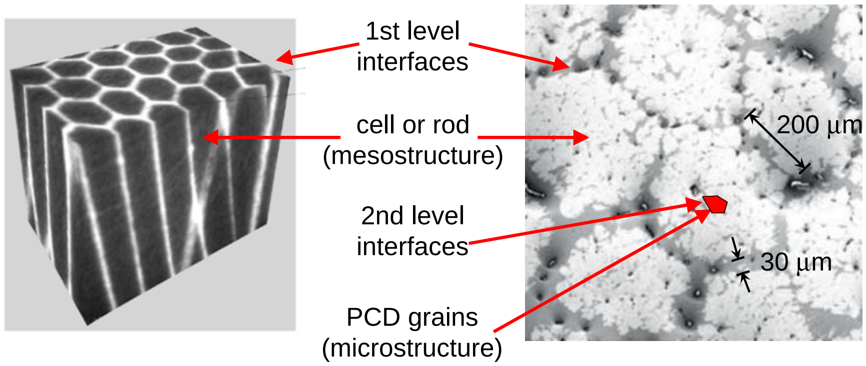

Figure 3: A two-level hierarchical polycrystalline material whose fracture response has been numerically investigated in [7].

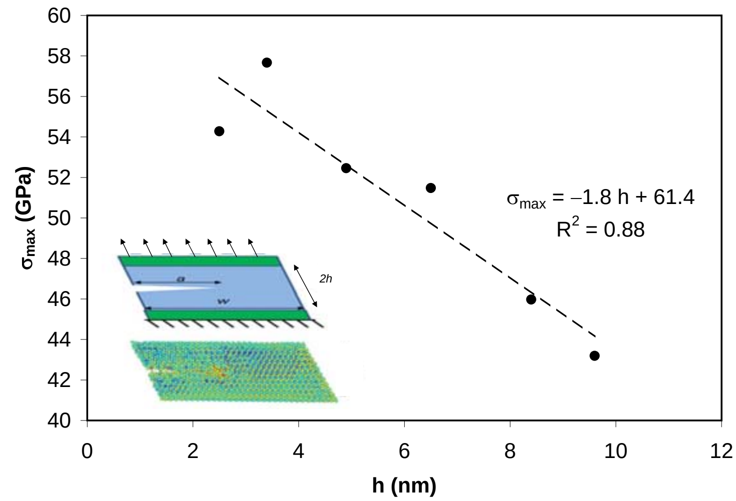

Figure 4: Molecular dynamics results [16] showing the linear decreasing peak cohesive traction by increasing the interface thickness, in agreement with the prediction of the nonlocal cohesive zone model for finite thickness interfaces [15].

diamond. Therefore, no stress-free cracks develop in the cellular rods, which are able to tolerate intrinsic defects of any size. Hence, fracture has to involve the finite thickness upper scale interfaces at the level 1 and the strength is maximized.

These results are important for the application of homogenization techniques and domain decomposition methods. A separation of scales, leading to vanishing interactions between the interfaces at the different hierarchical levels, is fulfilled only for $l_{\mathrm{CZM}}^{\mathrm{level}\,2}/d^{\mathrm{level}\,1} \gtrsim 1$, see Fig.5. When this condition is not achieved, *the mechanical strength is again a collective emergent property resulting from the nonlinear interactions of the interfaces at the various scales* and it cannot be predicted a priori or by simplified models artificially separating the length scales.

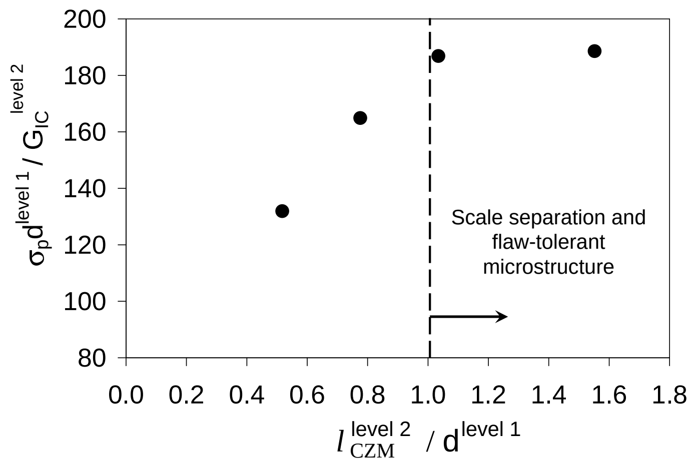

Figure 5: Numerical prediction of the tensile strength of the hierarchical polycrystalline material in Fig.3 by varying the ratio between the process zone size of the interfaces inside the rods, $l_{\mathrm{CZM}}^{\mathrm{level2}}$, and the diameter of the rods, d^{level1}.

4 CONCLUSIONS

In the present study, two examples of emergent properties related to interface contact and fracture mechanics have been reviewed. Focus is given to the fact that, when multiple scales are present in the mechanical system, it is not possible to predict a priori its global response from the knowledge of the nonlinear constitutive laws of the various constituents. As is typical of complex systems, in fact, the collective properties emerge from the nonlinear and nonlocal interactions between the system constituents and can solely be predicted by using numerical methods. Further research in this field will regard optimization, which is very important for the design and control of these systems.

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