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BIOINSPIRED NANOMECHANICS:
A CONTRIBUTION FOR THE CENTENARY OF THE GRIFFITH'S THEORY

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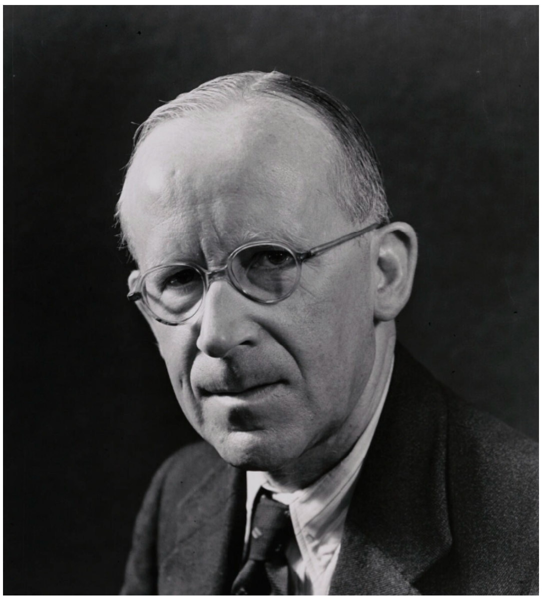
(nicola.pugno@unitn.it, extended abstract of the opening plenary lecture of the XXV ICTAM)

Summary The Italian artist, inventor and scientist Leonardo da Vinci (1452-1519) can probably be considered the father of bio-inspired design, as illustrated for example by his artificial wings and flying machines, based on bird observation and dissection. Five centuries from his death, bioinspiration is attracting widespread attention worldwide, both in academia and industry. This paper, related to the planned opening plenary lecture at XXV ICTAM, provides 3 new ideas in line with Griffith's theory of Linear Elastic Fracture Mechanics (LEFM): (i) a simple proposal to further generalize Dynamic/Quantized Fracture Mechanics theory and thus LEFM; (ii) the introduction of multiscale 3D Ashby's plots, to account for the role of size-effects on material properties for an improved material/structural selection and comparison; (iii) a new fundamental toughening mechanism that we -with Massimiliano Fraldi and colleagues- believe could be the key to better understand the fracture of bones, including related diseases (e.g. osteoporosis) and treatments; it is based on the evidence of stress alternating in sign in lamellae, thanks to symmetry breaking and hierarchy, simultaneously helping the crack opening needed for bone remodeling and the crack arrest needed for preserving its integrity and thus life, also suggesting new bio-inspired designs for tough composites. The inspiration for this work derives not only from Nature (and from da Vinci), but also from fundamental papers published by estimated colleagues of our community, all of whom I cannot mention here for brevity, starting from A. A. Griffith, who 100 years ago published his seminal paper. The following considerations thus represent my contribution for the centenary of Griffith's theory.

GRIFFITH/GENERALIZED DYNAMIC QUANTIZED FRACTURE MECHANICS

In 1921 Griffith published his seminal paper, submitted in 1920, basically describing the theory of Linear Elastic Fracture Mechanics (LEFM) [1], Fig. 1.



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VI. *The Phenomena of Rupture and Flow in Solids.*

By A. A. Griffith, *M. Eng.* (*of the Royal Aircraft Establishment*).

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1. *Introduction.*

In the course of an investigation of the effect of surface scratches on the mechanical strength of solids, some general conclusions were reached which appear to have a direct bearing on the problem of rupture, from an engineering standpoint, and also on the larger question of the nature of intermolecular cohesion.

The original object of the work, which was carried out at the Royal Aircraft Establishment, was the discovery of the effect of surface treatment—such as, for instance, filing, grinding or polishing—on the strength of metallic machine parts subjected to alternating or repeated loads. In the case of steel, and some other metals in common use, the results of fatigue tests indicated that the range of alternating stress which could be permanently sustained by the material was smaller than the range within which it was sensibly elastic, after being subjected to a great number of reversals. Hence it was inferred that the safe range of loading of a part, having a scratched or

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Figure 1. (left) Sir A. A. Griffith published his pioneering paper 100 years ago: The phenomena of rupture and flow in solids. Philosophical Transactions of the Royal Society of London. Series A, Containing Papers of a Mathematical or Physical Character. 1921 IV. 221: 163-198. (right) The first page of his pioneering paper.

According to LEFM, not the (maximal) stress but the energy release rate, or equivalently the stress intensity factor, must reach a critical value for the onset of crack propagation. In order to solve some limitations of LEFM, including the remaining paradox of infinite strength for vanishing crack length, I extended LEFM by introducing Quantized Fracture Mechanics (QFM, [2]): mathematically, differentials are simply substituted by finite differences in Griffith's energy balance. This corresponds to considering the onset of crack propagation not when the energy release rate reaches a critical value (the fracture energy per unit area of the material) but when its mean value along a fracture quantum of crack surface area ΔA -the previously introduced finite difference- reaches the material fracture energy. Equivalently, it is not the stress intensity factor (for the different crack propagation modes) $K \equiv K_{LEFM}$ that must reach a critical value (the fracture toughness of the material, K_C) for crack propagation, but instead the square root of the mean value of the square of the stress intensity factor along a fracture quantum, which is by definition the quantized stress intensity factor K_{QFM}. This theory is thus based on the removal of the hypothesis of continuous crack growth, i.e. on the existence of a quantum of energy dissipation/crack advancement, as postulated in the stress-analogue approach by Novozhilov [3]. In dynamic fracture, and considering the existence of a quantum of action, the mean value must be considered also along a quantum of time Δt -thus defining the dynamic quantized stress intensity factor K_{DQFM} [4]- as introduced again by the Russian's School in the stress-analogue incubation time fracture mechanics approach [5].

The exponent of 2 can in principle be generalized to a positive real number α, thus proposing a Griffith/Generalized (Dynamic) Quantized Fracture Mechanics (GQFM), predicting crack propagation according to:

$$K_{GQFM}^{(\alpha,\Delta A,\Delta t)} \equiv \sqrt[\alpha]{\frac{1}{\Delta A \Delta t}\int_{t-\Delta t}^{t}\int_{A}^{A+\Delta A} K(A,t)^{\alpha}\,\mathrm{d}A\mathrm{d}t} = K_C \quad (1)$$

Note that $K_{GQFM}^{(\alpha,\Delta A=0,\Delta t=0)} = K_{LEFM}$, $K_{GQFM}^{(\alpha=2,\Delta A,\Delta t=0)} = K_{QFM}$, $K_{GQFM}^{(\alpha=2,\Delta A,\Delta t)} = K_{DQFM}$ and $K_{GQFM}^{(\alpha=1,\Delta A=0,\Delta t)} = K_{ITFM}$, where K_{ITFM} is the equivalent stress-intensity factor according to the incubation time fracture mechanics [5]. Accordingly, all these limiting-case theories, which have been proved to capture experimental observations that LEFM cannot describe, are recovered and thus the correspondence principle is satisfied, as expected in the limit of vanishing fracture energy and action quanta.

The generalized stress intensity factor in (1) could also extend stress-intensity factor based laws such as those of fatigue, as proven for $\alpha = 2$ to capture both long and short crack behaviours even in fatigue (thus from the Wöhler to the Paris regimes) [6]. With the criterion (1), apparent R-curve behaviours and strain-rate effects emerge naturally as a consequence of the existence of fracture and time quanta, rendering fracture toughness no longer, or less crack-length and strain-rate dependent, and thus a more realistic material property, as it must be by definition. This could also help in the formulation of more realistic Ashby's plots.

MULTISCALE 3D ASHBY'S PLOTS

Asbhy's plots are fundamental for material selection [7]. As is well known, simply assuming in Griffith's theory a crack length $a \propto l^k$, where l is the structural size, would result in a scaling law for the strength of the type $\sigma \propto l^{-k/2}$, as similarly predicted by Weibull's statistics [8] or by other interpretations, e.g. fractal geometry [9]. I do not wish to comment here about the details of size-effect laws, but rather to emphasize that with the advent of nanotechnology, it is not infrequent to see papers reporting the fabrication of a new material using an Ashby's plot, even if it has been tested at a smaller size-scale. The need to adopt different Ashby's plots at the micro- and nano-scales has already been highlighted [10]. Here, I propose to use 3D Asbhy's plots for an improved multiscale representation, material/structural selection and comparison.

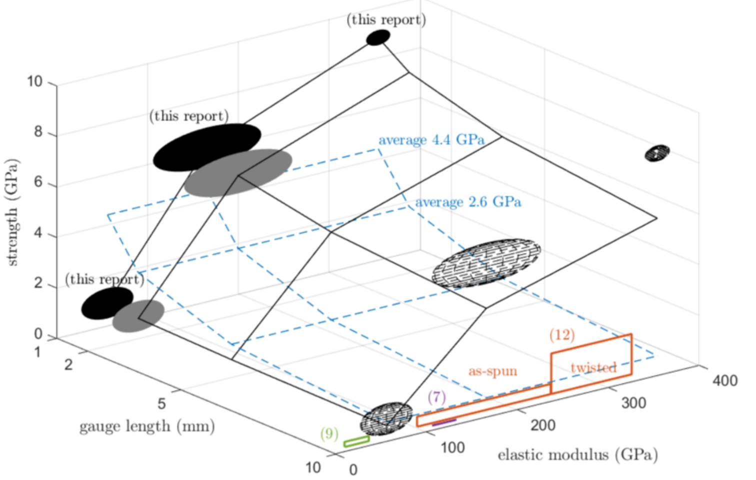

Figure 2. The black ellipses represent the strength vs elastic modulus data collected by the authors in [11] corresponding to samples with 1-mm gauge length (their fig. 4B). The overall average of this data is 4.4 GPa, while I have computed a total average of 2.6 GPa for the data at 2-mm gauge length (their fig. 3A). The corresponding scaling law, considering in a first approximation the independence of the elastic modulus, is of the type $\sigma \propto l^{-k/2}$ with a large value of $k/2 \cong 0.75$ (blue dashed lines). This scaling law predicts strength values comparable to those taken from the literature (green, purple or red areas, 1-cm gauge length). When considering the low- and high-strength regions (peaks in their fig. 3A), the average for the ellipse centred at a strength of 6.2 GPa for 1-mm gauge length falls to 5.6 GPa for a 2-mm gauge length, thus giving a scaling law with $k/2 \cong 0.15$ (black solid lines). The dashed ellipses are the projections at 10-mm gauge length of those at 1-mm gauge length, as reported in [11], whereas mean or maximal predictions at 10-mm are those reported with the blue dashed or black continuous lines, respectively. This case study must be considered just a preliminary example, such as the deduced size-effects.

As an example, I treat the case reported in Figure 2, where nanotube bundles are considered according to the paper in [11]. Asbhy's plot presented by the authors was inevitably classical, i.e. 2D, without considering the role of the bundle/gauge length, even if these authors perfectly recognized the role of size-effects and thus tested samples at different gauge lengths. A 3D Asbhy's plot, with a new axis corresponding to the size-scale (here gauge length) could thus be a better choice for comparison with other experiments, as described in Fig. 2. The experiments from the literature reported for comparison in [11] where performed at a gauge length of 1 cm, which I have considered in the 3D plot. I have also reported their experiments [11], not in the same plane but in their correct positions (1-mm or 2-mm gauge length planes). According to the same authors' experiments at different gauge lengths and assuming the simple mentioned scaling law of $\sigma \propto l^{-k/2}$, I could predict mean or maximal strength values expected at larger gauge lengths, including 10 mm, as reported respectively with the blue dashed or black solid lines.

The need for multiscale 3D Asbhy's plots is thus evident if we wish to move towards a standardization in material property comparisons. Regarding fracture toughness, the use of criterion (1) could further help the standardization, as previously mentioned. In general, the understanding of the toughness mechanisms is fundamental in Nature and Engineering. We believe that we have discovered a new fundamental one in bones.

A RECENTLY DISCOVERED TOUGHENING MECHANISM IN BONES

Bone tissue is a hybrid material made of an inorganic calcium phosphate phase nucleated into a collagenous matrix and organized hierarchically, from nanofibrillary components, to osteons (hundreds of micrometers in size), up to the cortical/trabecular macrostructure. It behaves as a complex composite able to adapt its internal organization to optimize the mechanical response under externally applied loads, contemporarily minimizing weight and resisting severe impacts and fatigue stress cycles by exhibiting surprising and not yet completely understood crack arresting mechanisms to avoid catastrophic fracture. In particular, it seems to be suitably designed to resist fracture at multiple size scales, thus achieving remarkable strength and toughness. However, the exceptional mechanical properties of bone can deteriorate with ageing and/or diseases: therefore, it is necessary to fully understand the mechanisms that confer these properties, also to develop therapies able to preserve or even rescue tissue functionality. Osteons, the fundamental bone units (Fig. 3a), are nearly hollow cylinders made of several concentric layers (lamellae) comprising helically arranged fibres wrapped nearly alternately clockwise and counterclockwise. With the Basic Multicellular Unit (BMU) osteocytes sense mechanical signals and activate and coordinate osteoblasts and osteoclasts for bone remodelling, i.e. resorption of preexisting bone by osteoclasts followed by *de novo* bone formation by osteoblasts (this process being impaired during ageing and diseases). It is ascertained that micro-damaging occurring across the scales plays a crucial role in bone mechanobiology, the micro-cracks opening at the osteon-matrix interfaces and within osteons working to trigger the BMU activities and the level of damage being an indicator of the need to locally increase mineral content through bone remodelling processes. However, how the crack propagation is triggered and arrested nearly simultaneously, both in compression and in tension (and thus also in bending) in such a stiff material, is still a partially unsolved enigma.

The most recognised hypothesis to explain the crack stopping/slowing phenomenon is based on the material inhomogeneity and anisotropy and the layered architecture of osteons: after nucleating, cracks would be halted when radially travelling across the osteon lamellae since they encounter the nearly alternating and in any case different arrangement of the wrapped fibres that make them decelerate at the lamellar interfaces and deviate along the circumferential direction. This leads to the dissipation of energy by increasing the length of the crack path, as well as by breaking micro-bridge elements and encountering a number of micro-voids and discontinuities generating micro-cracking. This mechanism surely plays an important role in arresting cracks in bone, but both theoretical calculations to estimate stress intensity factors at the crack tips and numerical analyses simulating crack propagation within osteons under static/cyclic loads as well as experimental findings [12], highlight that this is not sufficient to hinder fracture, suggesting that some yet undiscovered mechanisms should cooperate with (or exploit) bone hierarchy to halt crack progression [13]. Theoretical results also suggest that tensile hoop stresses in the lamellae, responsible for micro-crack opening in the radial direction, would occur only in case of compressive loads, while experimental observations show diffuse radial micro-cracks generated by tensile loads too [14].

Motivated by these incomplete and somehow contradictory results, we (the authors of ref. [15]) deeply explored an additional crack opening and stopping thus smart toughening mechanism with respect to those widely accepted in the literature, for which we have now clear theoretical evidences as well as experimental confirmation on 3D printed artificial hierarchical bones. For the occasion of this XXV ICTAM conference, we have rendered the paper public in the *Arxiv* [15]. Our results, obtained from an accurate mechanical model (Fig. 3a) of elastic anisotropy (Fig. 3b), show a counterintuitive radially distribution alternating in sign of both hoop and shear stresses in the lamellae and sub-lamellae (Fig. 3c,d), which could simultaneously act to open and halt cracks (Fig. 3e) thanks to hierarchy and symmetry breaking (Fig. 3f). This could also better stimulate the osteocyte activity by amplifying the mechanical signal, thus finally producing a "perfect" system capable to work both under compression or tension and thus bending.

Accordingly, this indeed unveils a powerful crack opening and simultaneously arresting mechanism, mediated by both the helical microstructure of the collagen fibrils in lamellae and sub-lamellae and the currently neglected small discrepancy in the nearly symmetric staggered angles of their wrapping in adjacent lamellae/sub-lamellae. The latter symmetry breaking generates this mechanism of Alternating Stresses in Lamellae (ASL, Fig. 3f), also occuring in sub-lamellae (ASL2) and hierarchy is shown to further enhance its power (Fig. 3c,d). Thus if ASL plays a fundamental role in bone toughening, its disappearance could be strictly related with bone ageing and common bone degenerative diseases, such as osteoporosis. Therefore, investigating the mechanosignaling pathways linking ASL to cellular response(s) and tissue remodelling could have important and wide-ranging implications for both the comprehension of bone disorders and the conception of new therapies, essentially based on the idea of restoring ASL when lost. Additionally, with this ASL*n*-based toughening mechanism, a new design of bio-inspired *n*-level hierarchical composites is envisioned, e.g. in the next generation of self-healing materials where both crack opening and arrest could be required.

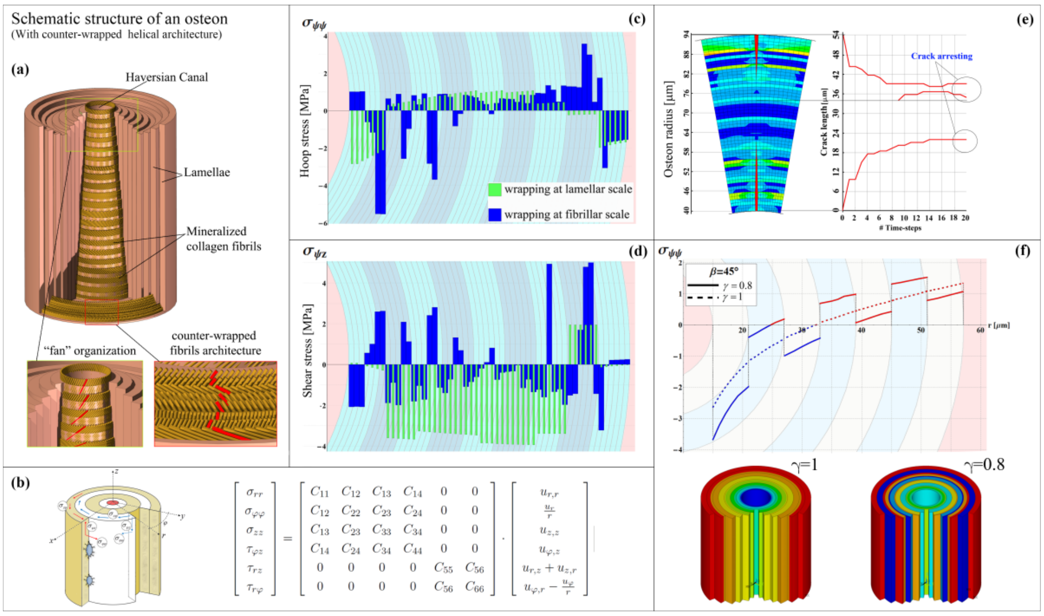

Figure 3. a) Osteon schematic structure. b) Anisotropic (monoclinic) elastic global equations resulting from the local helicoidal transversal isotropy (5 elastic constants). c)-d) Alternating in sign hoop and shear stresses without or with the presence of sub-lamellae, with stress jump amplification in the latter hierarchical case. e) Numerically (finite element) simulated crack progression and halting across osteon lamellae. f) Alternating in sign hoop and shear stresses in adjacent lamellae with fibril wrapping angles of β and $-\gamma\beta$ respectively and related stress jump amplification for symmetry breaking ($\gamma\neq 1$). For details see [15].

CONCLUSIONS

To celebrate the centenary of Griffith's theory (1921), in this paper -related to the opening plenary lecture at XXV ICTAM- I have presented 3 new concepts in the field of fracture: (i) a new extension of Griffith's theory, following the previous proposals by the author on Dynamic/Quantized Fracture Mechanics; (ii) the proposal of multiscale 3D Asbhy's plots, to include in these plots the fundamental role of the size-scale on the strength and in general on the mechanical properties of materials, for an improved material/structural selection and comparison; (iii) a new fundamental bone toughening mechanism, deriving from evidence of stress alternating in sign in osteon lamellae, emerging from the rupture of the symmetry of fibrils and empowered by hierarchy of sub-lamellae, suggesting also inspired solutions in Leonardo da Vinci's spirit [16].

As our lamellae, alone we are fragile but altogether we are resilient: this is why the pandemic is not stopping us, thanks to the new frontiers of Science and Technology and especially solidarity among peoples.

References

[1] Griffith, A. A. The phenomena of rupture and flow in solids. *Philosophical Transactions of the Royal Society of London*. Series A, Containing Papers of a Mathematical or Physical Character. IV. **221**: 163-198, 1921.
[2] Pugno N. M., Ruoff R. Quantized Fracture Mechanics. *Philosophical Magazine* **84**: 2829-2845, 2004.
[3] Novozhilov V. On a necessary and sufficient criterion for brittle strength, *Prik. Mat. Mek.* **33**: 212-222, 1969.
[4] Pugno N. M. Dynamic Quantized Fracture Mechanics. *International Journal of Fracture* **140**: 159-168, 2006.
[5] Petrov Y. and Morozov N. On the Modeling of Fracture of Brittle Solids, *Journal of Applied Mechanics* **61**: 710-712, 1994.
[6] Pugno N. M., Cornetti N., Carpinteri A. New unified laws in fatigue: from the Wöhler's to the Paris' regime. *Engineering Fracture Mechanics* **601**: 595-601, 2007.
[7] Ashby M. F. A first report on deformation-mechanism maps. *Acta Metallurgica* **20**: 887-897, 1972.
[8] Weibull W. A statistical distribution function of wide applicability. *Journal of Applied Mechanics* **18**: 293-297, 1951.
[9] Carpinteri A., Pugno N. M. Are the scaling laws on strength of solids related to mechanics or to geometry? *Nature Materials* **4**: 421-423, 2005.
[10] Zou, Y. Materials selection in micro- or nano-mechanical design: Towards new Ashby plots for small-sized materials, *Materials Science and Engineering: A* **680**: 421-425, 2017.
[11] Koziol K., Vilatela J., Moisala A., Motta M., Cunniff P., Sennett M., Windle A. High-Performance Carbon Nanotube Fiber. *Science* **318**, 1892-1895, 2007.
[12] Sabet F., Najafi A., Hamed E., Jasiuk I. Modelling of bone fracture and strength at different length scales: a review. *Interface Focus* **6**: 20150055, 2016.
[13] Ritchie R. O. The conflicts between strength and toughness. *Nature Materials* **10**: 817-822, 2011.
[14] Yeni Y. N., Hou F., Ciarelli T., Vashishth D., Fyhrie D. P. Trabecular shear stresses predict in vivo linear microcrack density but not diffuse damage in human vertebral cancellous bone. *Annals of Biomedical Engineering* **31**: 726-732, 2003.
[15] Fraldi M., Cutolo A., Carotenuto A., Palumbo S., Bosia F., Pugno N. M. Alternating in sign lamellar stresses, thanks to symmetry breaking and hierarchy, provide a new fundamental bone toughening mechanism, *Arxiv,* August 2021.
[16] Pugno N. M. The commemoration of Leonardo da Vinci. *Meccanica* **54**: 2317-2324, 2019.