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Structural integrity of hierarchical composites

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ABSTRACT. Interface mechanical problems are of paramount importance in engineering and materials science. Traditionally, due to the complexity of modelling their mechanical behaviour, interfaces are often treated as defects and their features are not explored. In this study, a different approach is illustrated, where the interfaces play an active role in the design of innovative hierarchical composites and are fundamental for their structural integrity. Numerical examples regarding cutting tools made of hierarchical cellular polycrystalline materials are proposed, showing that tailoring of interface properties at the different scales is the way to achieve superior mechanical responses that cannot be obtained using standard materials

KEYWORDS. Hierarchical composites; Fracture mechanics; Finite element method; Cohesive zone model.

INTRODUCTION

A significant advancement in the field of strength of materials has been achieved with the advent of composites. Combining different materials together allows us to realize structures with enhanced mechanical properties. Fiber reinforced materials are just one of these successful examples. The matrix contributes to the toughness and the density of the material, whereas fibers significantly increase the strength. Notable applications regard metal matrix composites used for aerospace applications, as well as fiber reinforced concrete for civil engineering purposes [1]. Similar strategies are accomplished with laminates and sandwich structures, where superior mechanical properties are achieved through the suitable combination of the individual material constituents [2].

In this context, the mechanical behaviour and the overall performance of composites are usually not limited by bulk properties, but by the interface characteristics. Debonding between matrix and reinforcement develops from early stage of deformation under monotonic and cyclic loading [3]. This damage affects the tensile strength, the fatigue strength, the fracture toughness, as well as the main mechanical properties.

Therefore, to understand the effect of the interface properties upon the mechanical response, several theoretical, numerical and experimental studies have been put forward in the last decades. Although research progresses are evident, especially from the computational point of view, a lot of work has still to be done to understand the mechanics of interfaces and their effect on the global structural response. In general, interfaces are commonly considered as defects, i.e., weak points of the material microstructure that limit the achievement of the maximum theoretical strength. This way of thinking, in conjunction with the difficulty of defining appropriate physical and mathematical models for interfaces, leads to a passive design approach. The attention is therefore focused on preserving the structural integrity by remaining in the elastic regime, covering all the modelling uncertainties with severe safety coefficients.

A different approach, leading to an active design, could however be pursued. Once suitable models are developed for characterizing the mechanics of interfaces, then structural analysis should pay attention to the failure modes, optimizing the material microstructure and the structural component performance through a suitable tailoring of the interface properties.

This way of thinking is clearly inspired by biological structures, where interfaces play an active role in the realization of an optimized structured by using individual constituents of relatively poor mechanical properties [4]. For instance, bone tissue undergoes microcracking as a result of repeated daily loading cycles. Fracture toughness capabilities are related to the osteonal structure. A ductile osteon-matrix interface promotes crack initiation, but, at the same time, it reduces the velocity of crack propagation in compact bone by blunting the crack tip and trapping it within the lamellar structure [4]. Therefore, design of biological structures suggests not to avoid microcracks and defects, but rather include them as an important parameter for the optimization of the material microstructure. Recent research on this field has focused on the characterization of biological interfaces, which is considered nowadays as a topic of extreme importance. The investigation of the constituent materials organization and distribution is also a compelling need. Preliminary results show that the realization of hierarchical microstructures is the way how biological materials achieve superior material properties. Robust and reliable adhesion systems of geckos are obtained through a hierarchical assembly of fibrils [5]. Similarly, toughness and defect tolerance of biological hard tissues are the result of hierarchical microstructures ranging over several length scales, from nano to macro [6].

The outcome of this research may contribute to a future development of new nanocomposite materials, mimicking the structures of biological materials. A pioneering effort in this direction is given by cellular polycrystalline materials recently designed by Fang et al. [7]. Extruded single fibers were packed together and put through a further extrusion process. The result is a honeycomb microstructure as sketched in Fig. 1, in which the cores are of polycrystalline diamond (PCD) and the cell walls are of WC/Co. Toughness and hardness of these new materials are considerably higher than those of standard homogeneous PCD, as also analytically predicted in [8]. This seems to be primarily attributed to the cell boundary material, which deters crack propagation and absorbs fracture energies, while the high hardness of the cell material provides wear resistance.

In this context, to understand the role of the process variables on the mechanical response, it is urgent to move from real experiments to virtual (numerical) simulations. In this paper, an example of active design is proposed, where it is shown that the interfaces in hierarchical cellular materials are determinant for the realization of desired material responses.

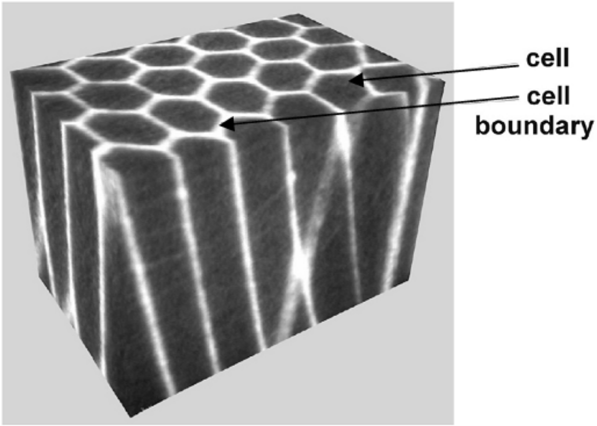

Figure 1: Scheme of a functionally designed cellular microstructure (adapted from [9]).

FRACTURE MECHANICS OF HIERARCHICAL CELLULAR MATERIALS

The effect of the upper scale interfaces on crack growth

Let us consider a bimaterial component where an external layer composed of polycrystalline cells is bonded to a substrate (see Fig. 1). This is for instance the case of the bit of a cutting tool, where the external layer is usually made of polycrystalline diamond (PCD) and the substrate is hardmetal. This composite structure is then joined to a steel support (for more details about geometry and material properties, please refer to [10,11]). When subjected to repeated loadings, as during cutting operations, different failure modes (micro-, meso- and macro-chipping) may occur, depending on the initiation point of a crack on the vertical side in tension. Different failure mechanisms (brittle crack propagation, fatigue crack growth) may also occur. In general, chipping leads to a premature failure of the bit ad therefore to a reduced lifetime of the tool.

In case of a standard PCD layer, where the size of the polycrystals is much smaller than the size of the layer, the material can be considered as homogeneous from the modelling point of view. As a consequence, crack propagation takes place under prevailing Mode I conditions and the crack path is curvilinear, as shown in Fig. 2.

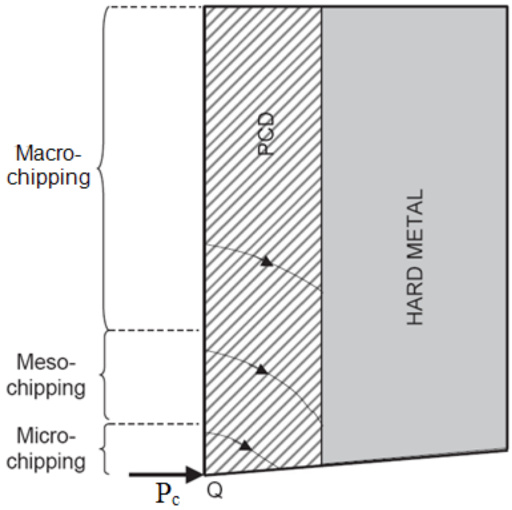

Figure 2: Sketch of a PCD bit used in cutting tools [10]. The critical impact load is denoted by Pc and different possible failure modes ranging from micro- to macro-chipping are sketched.

If heterogeneous cellular materials are used instead of a homogeneous layer, then a different crack path can be obtained. More specifically, considering the mechanical stress field due to a horizontal force acting at the tool tip, a magnification of the crack path for macro-chipping is shown in Fig. 3.

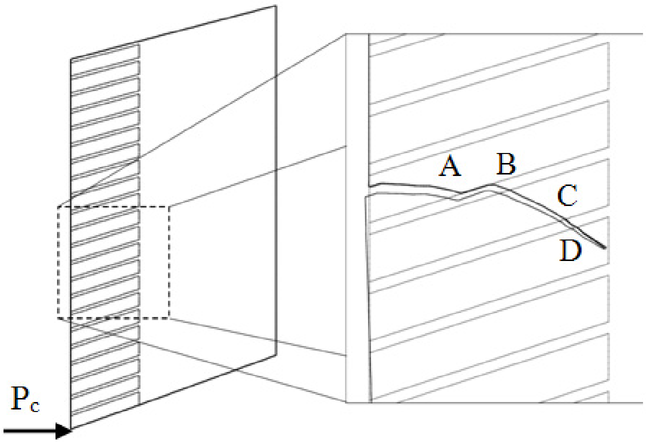

Figure 3: Fracture of a cutter with a cellular microstructure: scheme of the compact bit (left) and magnification of the crack path in the region inside the rectangular dashed box (right).

This result is obtained by performing a finite element analysis of the bimaterial structure using linear elastic fracture mechanics as in [10]. The simulations are carried out exploiting the interface fracture mechanics features of FRANC2D [13]. More specifically, the fracture parameters of the bimaterial interfaces are assumed equal to the average value of those of the neighboring materials. The rod diameter is equal to 200 μm and the thickness of the binder between the cells is 50 μm (see [9] for more details about the geometry of the material microstructure).

The critical load for crack propagation, P_c, which corresponds to the condition of $K_I = K_{IC}$ at the crack tip, is shown in Fig. 4 vs. the crack length a. The load P^* represents the average load typically experienced during experimental tests and a_{max} is the final crack length, when the crack meets the hardmetal substrate. At the beginning of the simulation, the crack propagates into a PCD road, and therefore there is no difference with respect to a standard homogeneous material, at least in 2D simulations. Interestingly, when the crack tip meets the bi-material interface, delamination of the rod cell takes place (path A-B). Since the interface fracture energy is higher than that of the PCD, the external applied load required for crack propagation has to be significantly increased with respect to the homogeneous case. Subsequently, crack deviates again into the rod (path B-C). A second peak is finally observed when the crack propagates through the binder between the cells (path C-D).

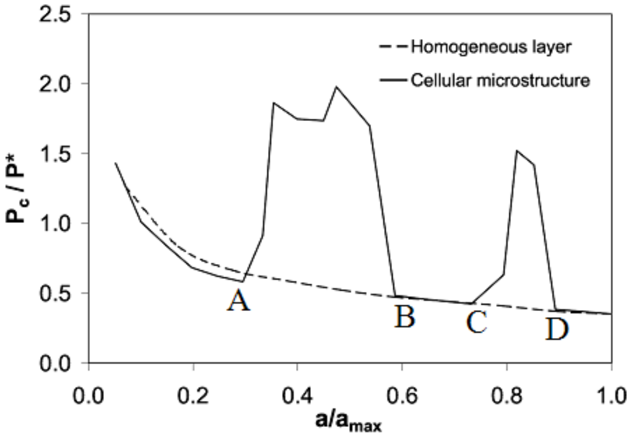

Figure 4: Dimensionless critical load for brittle crack propagation vs. dimensionless crack length. The response of a cellular microstructure is compared with that of a homogeneous layer.

These results are important for two reasons. First, a crack would arrest its propagation at the first interface if the dimensionless applied load is lower than 2.0. This situation is substantially different from the case of a homogeneous layer, where the critical dimensionless load is a monotonic decreasing function of the crack length. Therefore, when the dimensionless applied load exceeds 1.5, then the crack cannot be arrested. Therefore, the use of a cellular microstructure acts as a *crack-arrester*, controlling the evolution of chipping failure modes.

On the other hand, interfaces tougher than the rods is not always a desirable situation. In case of micro-chipping, weak interfaces may promote crack propagation along the rod boundaries. This would be suitable to activate a *self-resharpening* process of the tool tip, which progressively loses its cutting efficiency due to wear. Therefore, the optimal material microstructure would correspond to cellular rods embedded into a tougher matrix, with interface properties depending on the vertical coordinate on the cutting edge.

The effect of a hierarchical assembly of interfaces

It is also possible to quantify the effect of structural hierarchy by simulating the mechanical behaviour of a cellular microstructure using the finite element method and nonlinear fracture mechanics. To this purpose, let us consider the material microstructure depicted in Fig. 5.

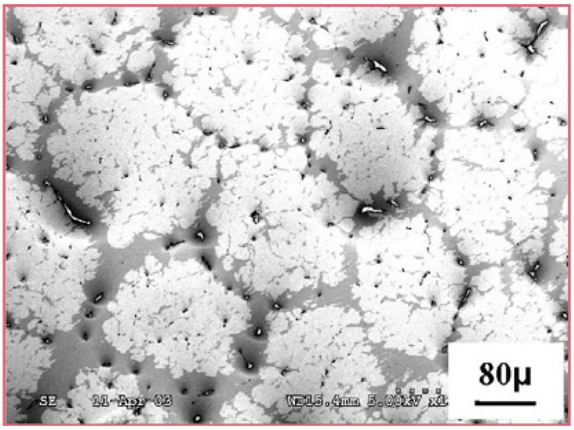

Figure 5: Cross-section of cellular rods with bright cells and dark grey cell boundaries (adapted from [9]).

Each exagonal rod (mesostructure) is composed of a standard polycrystalline material (microstructure). At the microscopic scale (called level 1 in this work), polycrystalline grains are separated by interfaces. Such polycrystals compose the material mesostructure (level 2), which is represented by the exagonal rods. Such rods are also separated from each others by interfaces, much thicker and with different composition with respect to the interfaces of level 1. As proposed in [13,14] interface fracture can be modelled by simplifying the real material microstructure and considering zero-thickness interface elements between the grains. Then, a suitable cohesive zone model (CZM) which takes into account the properties of finite thickness interfaces has to be used. In the present study, we consider the nonlocal CZM recently proposed by Paggi and Wriggers [13,14].

A sketch of the interfaces of a standard polycrystalline material is shown in Fig. 6. Ideal exagonal shapes are considered for the polycrystals. The constitutive model of each interface is described by a Mixed Mode stress-separation relation, given by the nonlocal CZM [13,14].

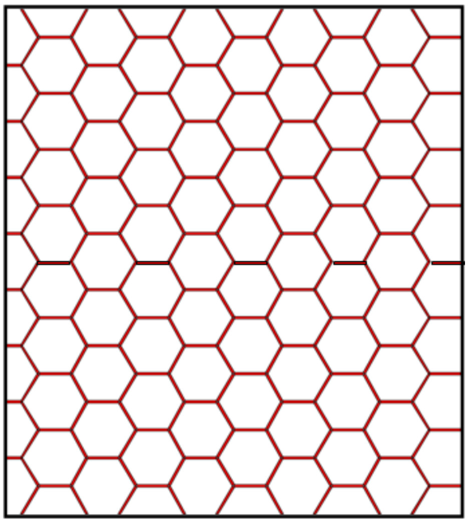

Figure 6: 2D model of a polycrystal (CZM interface elements are shown in red with a suitably amplified thickness, for visual representation).

To model the present materials processing, we remark that each rod is realized first through sintering of polycrystalline materials as those shown in Fig. 6. Then, the individual roads are joined together using high pressure and temperature conditions, such that the interfaces of level 2 develop. This configuration is sketched in Fig. 7, where yellow interfaces define the boundaries of the rod cells. A direct comparison between Figs. 6 and 7 clearly shows that the two microstructures are not physically similar, if different constitutive laws are used for the interfaces at the two levels.

As an example, let us consider interfaces at the second level tougher than those of the first level. In particular, we select $G_{\mathrm{IC}}^{l2} / G_{\mathrm{IC}}^{l1} = 5$. Keeping constant the CZM parameters of the interfaces of level 1, different CZM shapes are considered for the interfaces of level 2, as shown in Fig. 8 in case of pure Mode I deformation. Here, $\sigma_{\max}^{l1}$ denotes the peak cohesive stress of the interfaces of level 1, and g_{Nc}^{l1} is the critical relative opening displacement corresponding to vanishing cohesive stresses for the interfaces of level 1. Considering virtual tensile tests, imposing a monotonic horizontal displacement to the nodes on the vertical right side of the material microstructure, the homogenized response of the representative volume element of the hierarchical material is determined.

The peak stresses for the various simulations are plotted in Fig. 9 vs. $\sigma_{\max}^{l2} / \sigma_{\max}^{l1}$. These peak stresses are made dimensionless using the Mode I fracture energy of level 1 and the grain size diameter of the polycrystals composing the rods, d^{l1}. In this diagram, the response of a standard polycrystalline material without structural hierarchy, as that shown in Fig. 6, is represented by the red dot in correspondence of $\sigma_{\max}^{l2} / \sigma_{\max}^{l1} = 1$. The results clearly show that the tensile strength of the material can be significantly increased by using a hierarchical microstructure. The interfaces of the level 2 act as *crack-arresters* for the microcracks propagating into level 1. The main effect of material hierarchy is therefore to increase the ability of a heterogeneous material to tolerate defects.

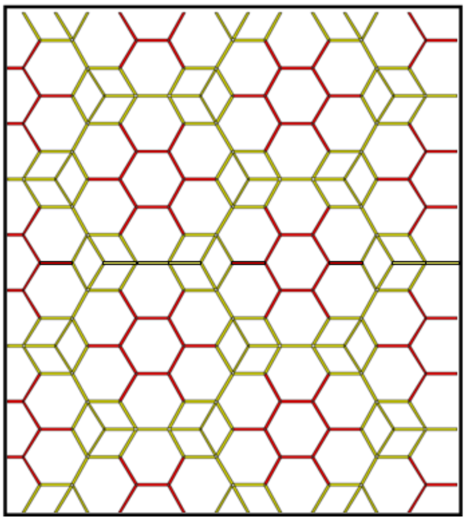

Figure 7: 2D model of a hierarchical polycrystal (CZM interface elements are shown in yellow and red, at the different scales).

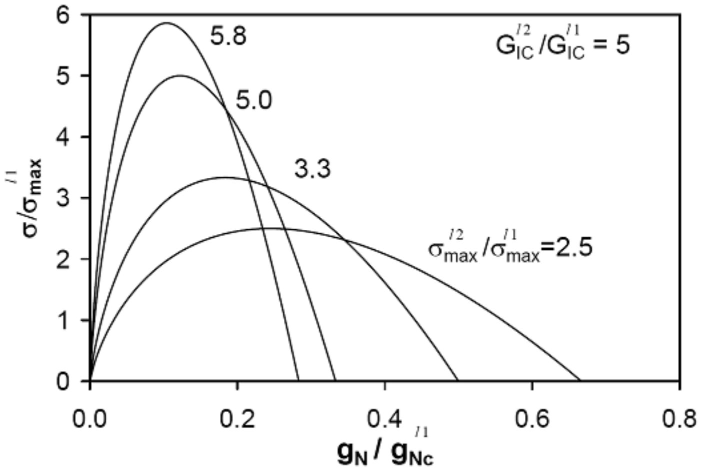

Figure 8: Shapes of the CZMs of the interfaces between the rods (level 2 or mesostructure).

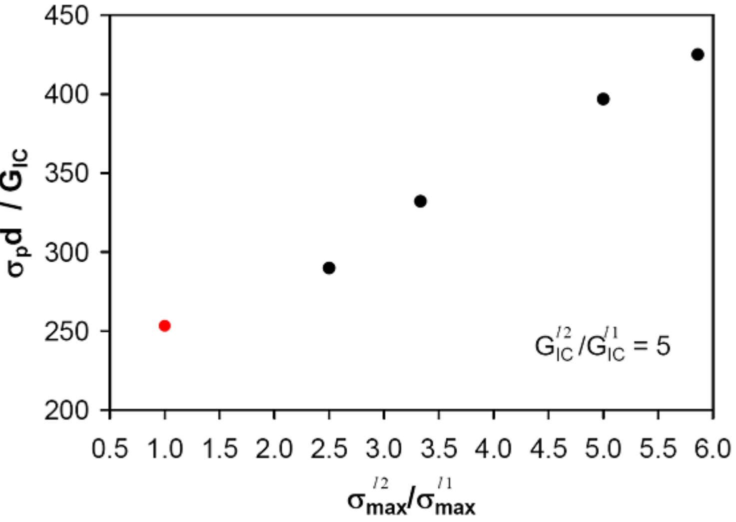

Figure 9: dimensionless tensile strength vs. CZM peak stress ratio between levels 2 and 1.

The peak stresses for the various simulations are plotted in Fig. 9 vs. $\sigma_{\max}^{l2}/\sigma_{\max}^{l1}$. These peak stresses are made dimensionless using the Mode I fracture energy of level 1 and the grain size diameter of the polycrystals composing the rods, d^{l1}. In this diagram, the response of a standard polycrystalline material without structural hierarchy, as that shown in Fig. 6, is represented by the red dot in correspondence of $\sigma_{\max}^{l2}/\sigma_{\max}^{l1}=1$. The results clearly show that the tensile strength of the material can be significantly increased by using a hierarchical microstructure. The interfaces of the level 2 act as *crack-arresters* for the microcracks propagating into level 1. The main effect of material hierarchy is therefore to increase the ability of a heterogeneous material to tolerate defects.

CONCLUSIONS

In this paper it has been shown that functionally designed microstructures can offer enhanced mechanical properties as compared to traditional heterogeneous materials. Tailoring the interfaces properties allows us to enforce crack propagation along desired paths. In this way, self-resharpening effects can be achieved. Structural hierarchy is also particularly important. In this study it has been demonstrated that the interaction of interfaces with different properties at the different hierarchical levels may explain the experimental results in [7].

Further work has to be done in this direction, especially for the 3D simulation of crack propagation in polycrystalline materials. Finite element analyses should also consider coupled thermo-elastic problems, an issue particularly important in cutting technology due to the high temperature conditions. The present study has been limited to a two-level hierarchical composite material. More hierarchical level should be investigated in the future research. However, due to very different length scales involved in the problem, ranging from the size of the sample to the size of the smallest heterogeneity, modelling the mechanical behaviour is a challenging task and multiscale computational methods should be invoked [15]. One possibility is to define representative volume elements (RVE) that provide a homogenized constitutive relationship to be used at the upper level. However, although such an approach is very appealing and has been pursued by several authors [16], some aspects require special attention. For instance, the definition of a RVE is not obvious, especially in case of localized phenomena, like crack nucleation and propagation. Moreover, the condition of scales separation has to be checked with care, otherwise the risk is to exclude coupling effects between length scales that may influence the mechanical response of the material.

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