

# MECHANICS OF INTRA-HIERARCHICAL INTERACTIONS AND ITS POTENTIAL IN DESIGN OF TOUGH MATERIALS

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## 1 Introduction

While nanotechnology has been immensely successful in applications that operate on “small” scales such as medicine and electronics, it is struggling to find its way into the world of “large” scale applications such as transportation, civil and mechanical engineering. The difficulty to realize potential of nanotechnology in design of tough structural materials, to a large extent, reflects a poor understanding of how to overcome three fundamental challenges:

- 1) Challenge to transfer superior mechanical properties of nano-materials to the macro scale;
- 2) Challenge to design materials with a combination of properties that are governed by competing mechanisms (for example, materials that are stiff AND strong AND tough at the same time).
- 3) Challenge to achieve a discontinuous leap in the improvement of a certain property.

In our view, the three challenges are well related and are a simple consequence of a fundamental problem of the “defect driven failure”. Indeed, failure of a material, as we know it today, is driven by stress concentrations generated at internal inhomogeneities and defects. The order, in which failure events occur, is controlled by hierarchical structure of the material and the scale of the inhomogeneities and defects: large defects are more dangerous than small ones. One important drawback of the defect driven failure is that it does not allow for simultaneous improvement of such material properties as strength and ductility/toughness: one is always achieved at the expense of the other. This coupling is a universal problem, irrespective of the material type (metal, polymer, composite, etc).

## 2 Failure of biological composites

With more and more data being accumulated these days on properties of biological materials [1,2], some striking differences in the failure behavior of these and conventional materials begin to emerge. One of the puzzling phenomena is insensitivity of some biological composites to the presence of defects on the nano- and even micro-scale. These materials are able to undergo uniform deformation without localization of damage. Moreover, they exhibit a unique combination of properties that are traditionally considered to be difficult to improve simultaneously (including strength and ductility). The main differences are summarized in Fig. 1. They are a product of the extensive literature survey on failure of structural biological composites (for example, such as bone and spider silk). There are reasons to believe that nature’s secret to control failure mechanisms lies in the intelligent use of a structural hierarchy.

In the present work we hypothesize that if one could create a heterogeneous material that does not generate any stress concentrations when subjected to loading, such a material would possess superior resistance to failure. It would fail due to uniform deformation and simultaneously exhibit high strength and ductility (and, therefore, toughness). Since heterogeneities and defects always introduce stress fluctuations, the very suggestion that a material can be insensitive to its microstructure may seem absurd. The only known way to eliminate stress concentrations is to remove all inhomogeneities and defects.

The objective of this work is to illustrate that material structure can be exploited to eliminate stress concentrations in the material and thus to change its failure behavior in a profound way. With the help of a newly developed model of a virtual material we show that this synergetic effect is possible due to sophisticated communication between-and-within hierarchical levels (referred here as intra-hierarchical interactions). The idea of paying more attention to intra-hierarchical interactions is originated from our previous modeling work inspired by structure of spider silk [3].

### 3. Model

In [3] the current authors proved that a material with two levels of hierarchy can exhibit different mechanisms of failure initiation (from brittle to ductile) depending on the structure of the lower level.

The current work arrives at a stronger conclusion that it is feasible to design hierarchical materials that generate no stress concentrations upon loading despite their heterogeneous microstructure. We use rigid-line inclusions as a tool to model the reinforcing component in the material. The model is combined with the method of interactions developed in [3]. The method was formulated specifically to be able to capture novel effects. It accounts for a number of features that are not present in conventional models of composite materials. For example, the method of interactions is able to treat at least two levels of a hierarchy simultaneously, to consider strong interactions between inhomogeneities, to account for their mutual positions explicitly, etc. The advantage of the developed method is in its transparent analytical basis and simple numerical implementation. For more details the reader is referred to [3].

<b>Failure in conventional materials</b>	<b>Failure in biological composites and materials on the nano-level</b>
<p>Driven by stress concentrations</p> <p>Damage is localized</p> <p>Strength and ductility are coupled</p> <p>Resilience to failure is limited</p>	<p>Not sensitive to stress concentration sites</p> <p>Uniform deformation</p> <p>Strength and ductility are NOT coupled</p> <p>Robust against failure</p>

Fig.1 Differences in the failure behavior of conventional and biological composites.

### 4. Case studies

We investigate two case studies: I) an isolated large inclusion with an array of small inclusions around its tips; II) two interacting collinear inclusions with two arrays of small inclusions near the inner tips of the large inclusions. The length of the small and large inclusions is noted as  $a_{small}$  and  $a_{large}$ , respectively. All inclusions are assumed to be parallel to each other. While position of the large inclusion(s) is fixed, position of the small inclusions is not known. The aim is to find position of the small inclusions with respect to the position of the large inclusions such that stress intensity factors (SIFs) at the tips of the large inclusions reduce to zero (or at least become 0.001 of the value in the absence of the small inclusions). We refer here to the mode II stress intensity factor  $L_{II}$  that is calculated by approaching the tip of the

inclusion from its interface [3]. Reducing the SIF to almost zero by introducing “structure” in the surrounding area with an array of small inclusions is very difficult to meet as SIFs are linearly dependant on the square root of the inclusion length. Indeed, in the case study I it was impossible to find the placement of the small inclusions such that the above condition was satisfied. In the case study II, however, this was possible. There was, however, a certain downside of meeting the condition, namely that the SIFs at the tips of the small inclusions increased in this case significantly. Since SIFs are dependent on the inclusion size it was decided to explore the possibility of reducing the size of small inclusions in order to reduce SIFs at their tips. Fig.2 shows the mode II SIF at the tip of a small inclusion (normalized to the SIF in its isolated state  $L_{II}^{isolated}$ ) as a function of the length of a small inclusion (normalized to the length of a

large inclusion). Interestingly, the synergetic effect of the small inclusions on the SIFs of the large inclusions remained to be present even for inclusions with a very small size.

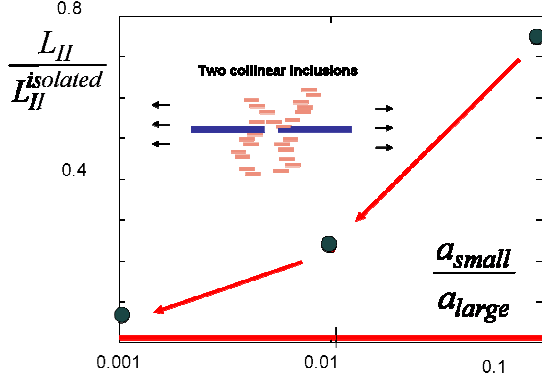


Fig.2 Decrease of the SIF at the tip of a small inclusion as a function of its length.

## 5. Parametric study

We performed a parametric study to examine the effect on the SIFs of the following parameters:

- the length of small inclusions (Fig. 3);
- the number of inclusions in the path (Fig. 4);
- the distance between small inclusions (Fig. 5);
- the number of paths in the array of small inclusions.

We found that SIFs at small inclusions decreased with the size of small inclusions, while SIFs at the large inclusions were almost not affected. A certain number of small inclusions were needed to eliminate the SIFs on the large inclusions. By increasing the number of small inclusions in a band or by decreasing the distance between them, the chance for finding the synergetic effect affecting the SIFs of the large inclusions is improved.

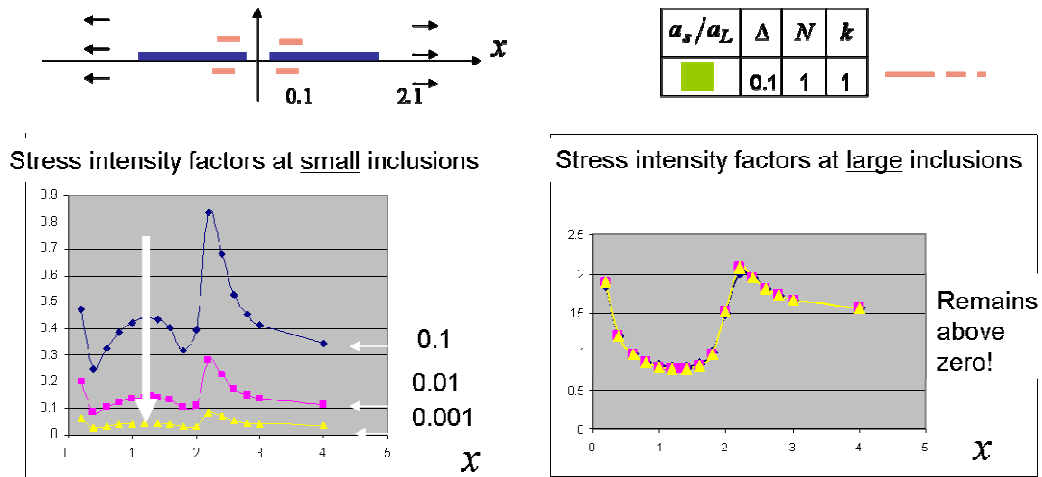


Fig. 3 SIFs at the large and small inclusions for different sizes of small inclusions and at different locations.

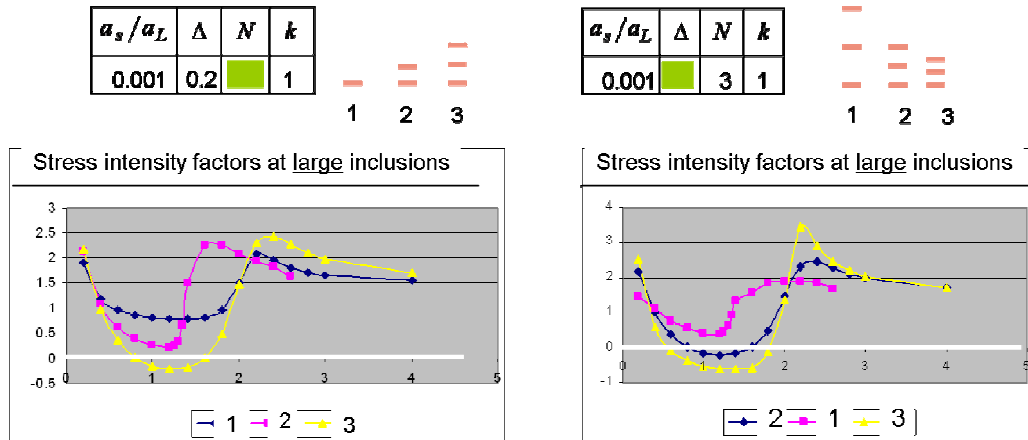


Fig. 4 SIFs at the large inclusions for different number of the small inclusions and distance between them.

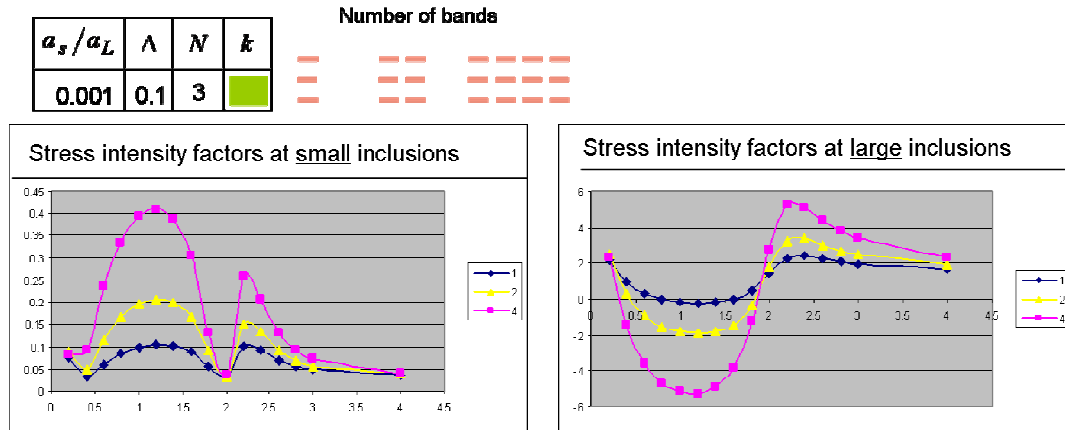


Fig. 5 SIFs at the large and small inclusions for a different number of pathways of small inclusions.

On a simple example of two interacting inclusions we showed that, theoretically speaking, all stress intensity factors can be eliminated. For the large inclusions this can be done by creating structure in the material around them, while for the small inclusions this can be achieved by reducing their size. This means that stress concentrations can be eliminated not only on the nano-scale but also on the micro scale (and theoretically at higher scales).

Interestingly, the position of small inclusion is not unique, i.e. different structures can be created. The phenomenon is observed only in systems with already interacting inclusions (no elimination of the SIF was found for an isolated large inclusion). Positioning of small inclusions is dictated by already existing interactions in the system. It means that structure on the lower level should be created when structure on the upper level is already in place (for example, by means of self-assembly). It is also plausible that the structure should be created under

the loading conditions at which the material will later be operational.

What remains unclear is whether the placement of small inclusions can be found without solving a complex optimization problem. The physics behind this phenomenon is also not explained.

The ambition of this work was to show (conceptually) that it is feasible to design hierarchical materials that are insensitive to their internal structural organization (i.e. that generate no stress concentrations upon loading). With this work, we put forward a new hypothesis that the elimination of stress concentrations on the  $n$ -th level of a material hierarchy (for example, the micro-level) can be achieved by creating a certain structure on the  $(n-1)$ th level (namely, the nano-level). The precise morphology of the lower level is to be dictated by the structure on the higher level and by intelligent interactions between-and-within these levels.

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## References

- [1] M.A. Meyers, P. Chen, A.Y. Lin, Y. Seki. “Biological materials: structure and mechanical properties”. *Progress in Materials Science* 53, 1–206, 2008.
- [2] P. Fratzl, R. Weinkamer. “Nature’s hierarchical materials”. *Progress in Materials Science* 52, 1263–1334, 2007.
- [3] L. Gorbatikh., S.V. Lomov, I. Verpoest. “Original mechanism of failure initiation revealed through modeling of naturally occurring microstructures”. *Journal of the Mechanics and Physics of Solids* 58, 735–750, 2011.