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Crack propagation in staggered structures of biological and biomimetic composites

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ABSTRACT

A phase field model is used to study crack propagation in staggered structures that are commonly found in several biological and biomimetic composites. The composite is modelled by creating an elastic mismatch between the two phases, 'mineral' and 'organic' which form into a staggered brick and mortar type micro-structure. The huge disparity in the stiffness of the two constituent phases gives rise to a non-uniform stress field near crack tips in these materials. Depending on the arrangement of the mineral platelets, different mechanisms of crack propagation may be observed. We find that cracks propagate straight when the aspect ratio of the mineral platelets is higher than a critical value. For lower values of aspect ratio, the cracks tend to exhibit a tortuous crack path in which fracture predominantly occurs in the soft organic phase. This critical aspect ratio is found to be a function of the mineral volume fraction as well as the elastic modulus mismatch. For some configurations, micro cracking in regions close to the crack tips is also observed. A simple theory is presented to analyse the observed crack paths in staggered composites.

1. Introduction

Biocomposites such as bones and nacre are naturally occurring materials that possess remarkable mechanical properties [1–7]. Interestingly the individual constituents of these composites are often found to be weak and/or brittle in nature [8]. Yet, the combination of these constituents in a very complex hierarchical manner comprising several length scales is believed to be the reason for the extraordinary fracture toughness of biocomposites [9,10]. How these microstructural arrangements of the constituents affect the fracture toughness and the effective stiffness of the biocomposites has attracted lot of research interest [1,2,11–19]. Such knowledge would immensely help in creating artificial materials with high fracture toughness and strength combined with low densities which can be exploited in several engineering applications [20–22].

While the actual microstructure of the naturally evolved biocomposites such as bone is very complex comprising of several levels of hierarchies [9,10], a simplified model such as the one shown in Fig. 1 is often found to be useful for analytical and computer simulations for the study of fracture mechanisms in biocomposites [23–28].

Wagner and Weiner [2] have studied the relationship between the microstructure of bone and its mechanical stiffness. Baron and Wagner [4] have investigated the elastic modulus of hard biological tissues by considering their staggered platelet microstructure. Zhang et al. [19] showed the existence of an optimum level of structural hierarchies due to the limited selection of structural proteins. In their study, they predict the optimum level of hierarchies for a human bone as six which is close to what is actually observed.

Although, the above mentioned studies shed important light on the structure-mechanical properties correlation of biocomposites, a detailed analysis of how crack paths are influenced by the underlying mineral-organic microstructure is still lacking. For predicting crack paths in staggered composites, a model which can describe the thermodynamics of the fracture process as well the dynamics of cracks is essential. The phase field models [29–37] for crack propagation are ideally suited for such problems since they can describe crack dynamics, without making any a priori assumptions on the crack path. In this work we use phase field approach for studying crack propagation in composites made up of staggered micro structures in which the elastic modulus mismatch plays an important role in determining the crack trajectories. In particular, we study the effects micro-structural parameters such as aspect ratio α and volume fraction f of the mineral platelets and modulus mismatch characterised by the ratio of Young's modulus of the

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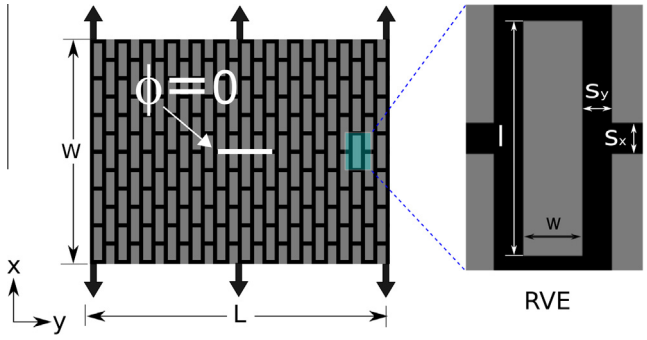

Fig. 1. A schematic of the staggered structure model used in phase field crack simulations. Representative volume element (RVE) used for calculating the effective modulus and the energy densities is shown on the right.

organic to that of the mineral (E_o/E_m), on the crack propagation behaviour in these composites.

This paper is organised in the following way. The next section presents the details of phase field model for crack propagation. Section 3 gives the details of crack simulations, numerical scheme and the boundary conditions of the present study. The results of the crack simulations are presented in Section 4. In Section 5, a simple theory is presented which is used in explaining some of our simulation results and also helpful in generalising the trends predicted by the phase field crack simulations. Section 6 gives a brief summary and concluding remarks of the present work.

2. Phase field model

Phase field modelling (PFM) of crack propagation in solids is emerging as an important tool for studying fracture behaviour especially due to its simplicity and flexibility in handling dynamic crack growth in complex microstructure [31,32,38–40]. The PFM is a variational approach in which a free energy functional $F[\phi(\vec{r}), \nabla\phi(\vec{r})]$ is constructed which depends on a spatially varying order parameter $\phi(\vec{r})$ and its gradient $\vec{\nabla}\phi(\vec{r})$ representing the interface. The time evolution equation for ϕ is obtained so as to drive the free energy to its minimum. In the present model $\phi(\vec{r})$ denotes the degree of brokenness of the solid where $\phi(\vec{r}) = 1$ represents a fully intact solid and $\phi(\vec{r}) = 0$ a fully broken solid or the crack region. $\phi(\vec{r})$ is coupled to the elastic energy density $\mathcal{E}$ and enters the free energy functional in the following way:

$$F = \int \left\{ g(\phi)[\mathcal{E}(\vec{r}) - \mathcal{E}_{th}] + \frac{\kappa}{2} |\vec{\nabla}\phi|^2 \right\} dA, \tag{1}$$

where $g(\phi) = 4\phi^3 - 3\phi^4, \mathcal{E} = \frac{1}{2}\boldsymbol{\epsilon}(\mathbf{u})$. $\mathbb{C}\boldsymbol{\epsilon}(\mathbf{u})$ is the elastic energy density; $\mathbb{C}$ is the elastic stiffness, $\mathbf{u}(\vec{r})$ is the displacement field and $\boldsymbol{\epsilon} = \frac{1}{2}(\nabla\mathbf{u} + \nabla\mathbf{u}^T)$ is the linearised strain tensor. $\mathcal{E}_{th}$ is the threshold elastic energy density for fracture. κ is a gradient coefficient which is related to the surface energy γ by $\kappa = \frac{\gamma^2}{\mathcal{E}_{th}}$. Crack growth is simulated by evolving ϕ in the presence of externally applied loads. The evolution of the ϕ is governed by the variation of the free energy functional in the following way:

$$\frac{d\phi}{dt} = -M\frac{\delta F}{\delta \phi} = -M[-\kappa\nabla^2\phi + (\mathcal{E} - \mathcal{E}_{th})g'(\phi)] \tag{2}$$

M is the rate coefficient which determines the rate of material failure. Elastic equilibrium is achieved by simultaneously solving the following momentum balance equation with a damping parameter η,

$$\rho\frac{\partial^2\mathbf{u}}{\partial t^2} = \vec{\nabla}\cdot\boldsymbol{\sigma} + \eta\nabla^2\frac{d\mathbf{u}}{dt}. \tag{3}$$

Here, ρ is the material density and $\boldsymbol{\sigma}$ is the Cauchy stress tensor which is assumed to be linearly related to the strain ϵ following a generalised Hooke's law (i.e. $\boldsymbol{\sigma} = g(\phi)\mathbb{C}\boldsymbol{\epsilon}$). Note that the stress components are uniformly multiplied by a scaling factor $g(\phi)$ which render zero stresses inside the crack thus providing traction-free boundary condition on the crack surface.

Crack simulations are performed by numerically solving Eqs. (2) and (3) using an explicit finite difference method. The lengths and time are expressed in units of $\xi = \sqrt{\frac{\kappa}{\mathcal{E}_{th}}}$ and $\tau = \frac{1}{M\mathcal{E}_{th}}$ respectively. In terms of these units the finite difference grid spacing and time step are chosen as $\Delta x = \Delta y = \xi$ and $\Delta t = 0.01\tau$. All the variables and parameters are non-dimensionalized by dividing with appropriate scaling factors shown in Table 1. The values chosen for each of the non-dimensionalized parameters are also present in this table.

3. Crack simulations

Crack propagation simulations are conducted on staggered composites with a typical configuration as shown in Fig. 1. In this figure, the dark grey regions correspond to mineral platelets and the black region corresponds to the organic matrix while the thin white portion is the initial crack with $\phi = 0$. The simulation domain is an $L \times W$ rectangular area with a central crack of length a. We have applied periodic boundary conditions in both x and y directions and have chosen $L \approx W \approx 1200\xi$ and $a = 100\xi$. The reference x-axis is always parallel to the longitudinal direction of the platelets and the specimen is loaded in this direction with a constant applied strain rate $\dot{\epsilon}_x = 10^{-4}\tau^{-1}$. The strain rate is small enough to maintain quasi-static conditions and rule out any possibility of dynamic crack branching to kick-in. This has been verified by conducting simulations on pure mineral which resulted in straight crack propagation. The mineral and the organic materials are assumed to have different values of Young's modulus E_m and E_o respectively, but identical Poisson's ratios ($\nu = 0.25$) and $\mathcal{E}_{th}$ values.

The structural details of the composite are shown in the magnified view adjacent to the specimen configuration depicting the unit representative volume element (RVE) of the sample. The length and width of the mineral platelets are denoted by l and w while their spacings in the x and y directions are denoted by s_x and s_y respectively. The volume fraction of the mineral is given by $f = lw/[(l + s_x)(w + s_y)]$ and the aspect ratio by $\alpha = l/w$. In the simulations, the width of the mineral platelet $w = 20\xi$ is fixed while the spacings $s_x = s_y$ and the length of the mineral platelet l are calculated in terms of f and α for this fixed w.

Because of the elastic mismatch between the mineral and organic phases, the crack tip experiences variable driving forces in each direction and manoeuvres according to the local elastic fields. The objective of the present study is to understand the relationship between the structural parameters f, α and the elastic modulus ratio E_o/E_m on the crack path trajectories. To this end we perform crack propagation simulations on specimens of different geometries and correlate the crack trajectory patterns with $\alpha, E_o/E_m$ and f.

Table 1
Values of the non dimensional parameters used in the phase field crack simulations.

Parameter	Scaling factor	Value
κ	$\mathcal{E}_{th}\xi^2$	4
ρ	$\left(\frac{\tau}{\xi}\right)^2\mathcal{E}_{th}$	1
γ	$\mathcal{E}_{th}\xi$	1
$\mathcal{E}_{th}$	$\mathcal{E}_{th}$	1
η	$\mathcal{E}_{th}\tau$	2