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Influence of initial flaws on the mechanical properties of nacre

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ABSTRACT

Nacre is a bio-composite made up of hard mineral and soft protein, and has excellent mechanical properties. This paper examines the effect of naturally occurring defects (initial flaws) in nacre on its mechanical properties such as toughness and strength. A random fuse model is developed incorporating initial flaws. Numerical simulations show that initial flaws affect different mechanical properties at different rates. The variation in the experimentally obtained mechanical properties of nacre reported in the literature is shown to be due to initial flaws. The stress in the mineral and protein increases due to initial flaws, but by different amounts. The results obtained in this study are useful for gaining insight into the failure of nacre and development of nacre-inspired composites.

1. Introduction

Biological materials such as bone and nacre are composites of soft organic protein and hard, brittle mineral. They possess interesting features and properties. The toughness of these bio-composites is excellent, especially when compared to their very weak constituents.

Consider the case of nacre. This is the inner layer of the mollusk shell (Shao et al., 2012). At the micro-scale, nacre consists of aragonite (calcium carbonate) platelets arranged in a staggered fashion. An organic matrix material fills the space between the platelets. This arrangement is referred to as the "Brick and Mortar structure" (Gao et al., 2003; Katti and Katti, 2006). The organic matrix consists of domains, which unfold one after the other without causing the molecular backbone to break (Smith et al., 1999). This leads to a saw tooth type force deflection curve for the organic matrix with a very large deformation. The fracture toughness of nacre is about 3–7 MPa m $^{1/2}$, though the constituent, mineral has a fracture toughness much less than 1 MPa m$^{1/2}$ (Ji and Gao, 2004). Many studies were conducted to examine the reasons for the excellent toughness of nacre (Okumura and de Gennes, 2001; Jackson et al., 1988). Barthelat and Rabiei (2011) conducted experiments and found out that there is a large fracture process zone around the crack tip, enabling high energy dissipation and thereby providing high resistance to fracture. Nukala and Simunovic (2005) found out that domain unfolding plays an important role in the toughness of nacre.

A number of defects are present in the microstructure of nacre (Barthelat and Espinosa, 2007). In this paper, we refer to the defects as initial flaws. The defects that could occur include platelet breakage and matrix flaws. However, nacre is supposed to be defect-tolerant (Huang and Li, 2013). Many researchers have investigated the reasons for the flaw tolerance of nacre (Barthelat et al., 2007; Wang et al., 2001; Huang and Li, 2013). Though this is the case, studies about the influence of existing defects on the mechanical properties are not available in open literature, especially how the various types of initial flaws affect the strength and toughness. There is a need to systematically study the effect of initial flaws in the matrix and platelet on the mechanical properties such as strength and toughness of nacre. The understanding of how existing defects affect failure, would be useful not only for

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getting insight into the failure of nacre, but also for developing nacre-inspired artificial materials.

Discrete lattice models have been proposed for analysis of deformation and fracture of materials. In a discrete lattice model, the continuum is discretised into one-dimensional elements. The random fuse model is a special case of a discrete lattice model where these one dimensional elements are modelled as resistors (de Arcangelis et al., 1985; Kahng et al., 1988). In a random fuse model, displacement and force are replaced by their electrical analogues; voltage and current. In short, a resistor network replaces the continuum. The random fuse model (RFM) is a scalar analogue of an elastic discrete lattice model. The solution of an electrical network (Zienkiewicz, 1971) is very similar to that of an elastic network. The random fuse model provides a simpler way of solving the discretised continuum. This is because of the scalar nature of the equations used in RFM. Moreover, RFM has only one degree of freedom per node per element. However, the corresponding spring and beam elements have higher degrees of freedom (Skjetne et al., 2001). The random fuse model can incorporate disorder much more easily than finite element models (Alava et al., 2006). RFM has been extensively used to simulate the mechanical behaviour of materials, especially when randomness in the properties and structure is to be introduced in the model (Hansen, 2005; Sahimi, 2003; Herrmann and Roux, 1990).

In order to account for evolving failure of materials, a continuous damage random fuse model (CDRFM) has also been proposed (Zapperi et al., 1997). CDRFM has been employed to model domain unfolding in failure simulation of biological composites (Nukala and Šmunović, 2005; Anup et al., 2008). However, in these models, the effect of initial flaws has not been considered.

In this paper, we develop a 2D CDRFM model taking into account initial flaws. Initial flaws of the platelet and the matrix are introduced separately into the model. Numerical solution of the model gives the stress–strain response of the composite. Mechanical properties are derived from this response and the effect of initial flaws on these mechanical properties are examined.

2. Formulation of the problem

In order to develop a model for failure of nacre, CDRFM is employed. Fig. 1 shows a schematic structure of nacre with the mineral platelets and organic matrix. The model used for simulation is based on this structure and is similar to that employed by other researchers (Nukala and Šmunović, 2005; Anup et al., 2008). A square lattice network of L × L size is used. A part of the network used is shown in Fig. 2. In CDRFM, a current–voltage analogue of the elastic model is employed (Zapperi et al., 1997; Nukala and Simunovic, 2005). Ji and Gao (2004) have developed a tension-shear chain model to explain the stress transfer in nacre-like composites. In this model, the mineral platelets are assumed to carry only tensile forces. The matrix is assumed to transfer shear forces between platelets. Based on this model, we assume that platelet elements carry tensile stresses and matrix elements carry shear stresses. These elements are shown in Fig. 2. Tensile matrix elements could be used to connect the horizontal edges of platelets in the gap region. However, stresses carried by the matrix connecting these horizontal edges of platelets are negligible (Ji and Gao, 2004; Jäger and Fratzl, 2000; Nukala and Šmunović, 2005). Therefore, these tensile matrix elements are given zero stiffness values.

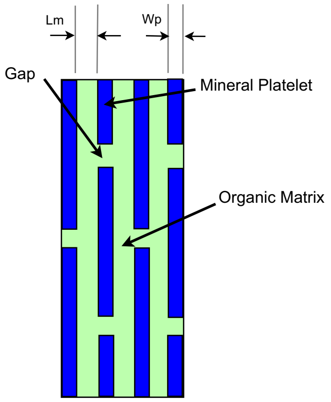

Fig. 1 – Schematic diagram showing the structure of nacre. Note the staggered arrangement of the mineral platelets in the organic matrix.

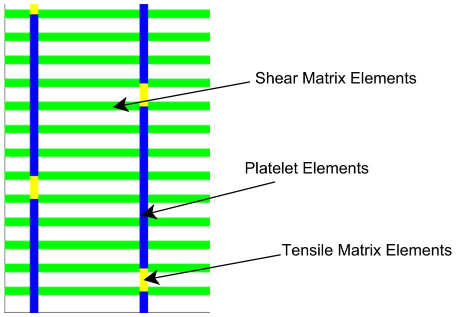

Fig. 2 – A part of the CDRFM model showing the various types of elements. Tension elements are used to represent mineral platelets. Shear elements represent matrix connecting the vertical faces of the platelet; tensile matrix elements connect horizontal faces of the platelets.

In this model, all dimensions are normalised with respect to the width of the platelet, W_p (see Fig. 1). A unit width is assumed in the out of plane direction. Therefore, the area of the platelet, A_p is equal to unity. The platelet is divided into a number of elements equal to the normalised length of the platelet, so that the normalised length of each platelet element is unity. A matrix element has a length equal to L_m as shown in Fig. 1. The width of the matrix element is equal to the length of the matrix element. Therefore, the cross-sectional area of a matrix element is also equal to one.

Stiffness (conductance) of each element is given by $C_e = A_e E_e / L_e$, where E_e is Young's Modulus, A_e is the area, and L_e is the length of the element. The stiffness of a platelet element is equal to Young's modulus, E_p since both area and length are unity. The stiffness of a matrix element is found out to be $C_m = G_m / L_m$, where L_m is the normalised length of a matrix element and G is the shear modulus of the matrix (Nukala and Šmunović, 2005).