STATISTICAL ANALYSIS OF THE MECHANICAL PROPERTIES OF NACRE

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Abstract

A representative model of nacre (mother-of-pearl) was modelled using the finite element software Abaqus to determine the material heterogeneity effect on the overall material behaviour. Nacre constitutes of aragonite tablets (95% Vol) and organic bio polymer layers (5% Vol) arranged in a staggered manner.The tablets were assigned with homogeneous isotropic elastic properties,whereas the constitutive behaviour of bio polymer layers were defined using a cohesive law whose parameters were stochastically generated according to a continuous distribution. Later, the model was imposed with periodic boundary conditions and Monte Carlo simulations were carried out on the random samples subjected to uni-axial tension . It was observed that the heterogeneous material exhibited non uniform failure pattern as compared to the homogeneous material which exhibited an unrealistic uniform failure pattern.Moreover, it was also observed that the RVE size had significant impact on the mean tensile peak strength as well on the standard deviation of the tensile peak strength.

1. Introduction

Mollusks such as pearl oyster, snails etc. Possess a shell made of two protective layers to safeguard themselves from external agents. The outer layer is known as calcite layer, whereas the inner layer is known as nacreous layer or mother-of pearl (Fig. 1.b). The calcite layer is hard, brittle and provides high resistance to penetration,whereas the nacre layer is soft and exhibits large inelastic deformation with high energy dissipation. Nacre constitutes of aragonite tablets (95% Vol) and thin organic bio polymer layers (5% Vol) arranged in a staggered manner (Fig. 1.c). The aragonite ($Caco_3$) tablets are polygonal tablets with thickness of about 0.2 to 1.5m and each tablet is separated from other by the bio polymer layers of thickness varying from 27 to 30nm.Nacre has attracted the attention of many researchers due to its remarkable properties compared to its constituents.

There are several research articles in literature to determine the mechanical properties of nacre assuming homogeneous properties and uniform geometrical features for the nacre's constituents([1],[2],[3]),

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homogeneous properties and stochastic geometrical features ([4],[5]).However,in the present work material properties of the bio polymer layers were varied according to Gaussian distribution and the effect of material heterogeneity on the failure pattern and tensile strength of red abalone (Haliotis Rufescens) nacre over several length scales was determined by carrying out Monte Carlo simulations on a finite element based representative model of nacre(Fig. 1.d) subjected to uni-axial tension.

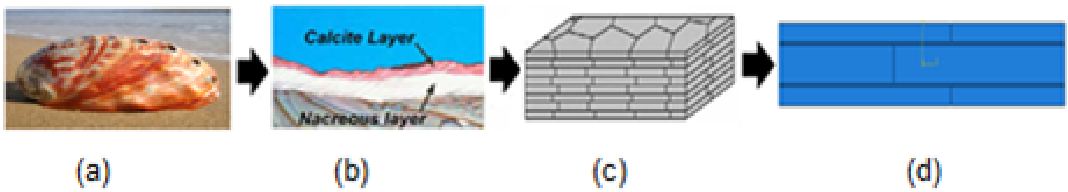

Figure 1. (a) Red abalone shell, (b) Cross sectional view of shell[1], (c) Microstructure of nacre[1], (d) Representative volume element of nacre

2. Methodology

2.1. Finite Element Model

A two dimensional representative volume element (RVE) of nacre under plain strain condition was modelled using the finite element software Abaqus (Version 6.12-3).The major constituent of nacre, aragonite tablets were modelled considering their length(L_x=L_{x1}+L_o+L_{x2}), width (L_y) and thickness (L_z) to be 9027nm, 452nm and 1nm respectively. In addition to that the overlap distance (L_o) between the tablets was considered as 20 % of the tablet's length. Organic bio polymer layers, the other constituent of nacre was considered to have an initial thickness (T_o) of 27nm and the vertical and horizontal bio polymer layers are known as junctions and interfaces respectively. Later, RVE of different sizes were generated by assembling the tablets and organic bio polymer layers in a staggered manner(Fig. 2).In addition to that periodic boundary conditions were imposed on the RVE boundaries to represent the model as infinite periodic medium and also to eliminate the boundary effects.

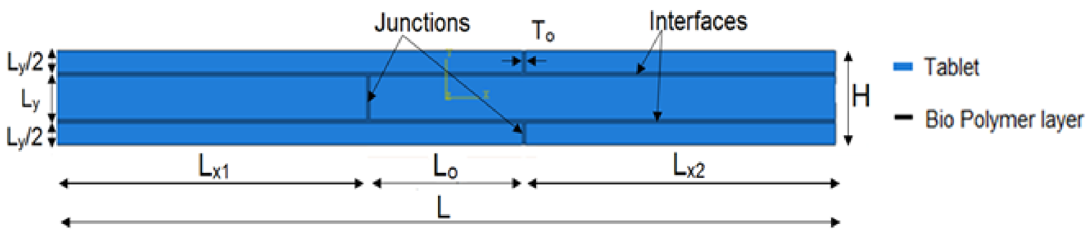

Figure 2. Representative volume element (RVE) of nacre

The aragonite tablets were modelled with 4-noded quadrilateral reduced integration plain strain elements and were assigned with isotropic elastic properties (E_{tablet}=100GPa, ν=0.2), whereas the organic bio polymer layers were modelled with 4-noded cohesive elements and their constitutive behaviour were defined using an isotropic bi-linear traction separation law adapted from [1](Fig. 3).The tensile strength of bio polymer layers (E_n) were generated according to Gaussian distribution with a mean and standard deviation of 1.5GPa and 0.27GPa respectively, whereas the failure displacement ($\delta_{failure}$) and damage initiation displacement ($\delta_{Initiation}$) were considered to be 847nm and 0.9nm respectively. The maximum tensile stress(σ_n) at which the damage initiates was calculated by ($\delta_{Initiation}$/T_o)E_n. Moreover,the shear strength (E_s) and stress (σ_s) were assumed to be half of the tensile strength and stress respectively.

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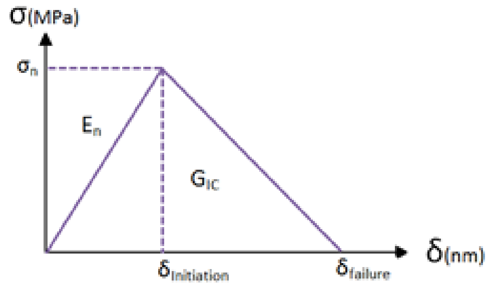

Figure 3. Traction separation law for bio polymer layer

2.2. Numerical Simulation

Numerical uni-axial tension tests were carried out by applying a constant strain of about 1% on the boundary of the RVE and the boundary conditions used are as follows (compare with Fig. 4).

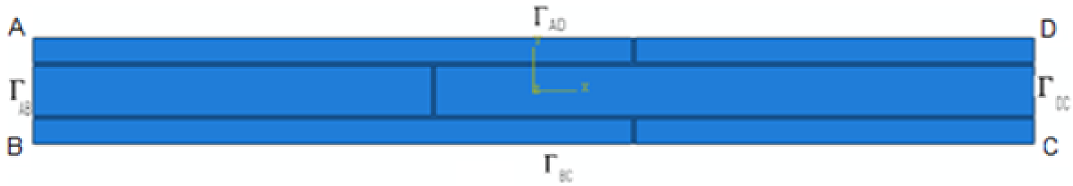

Figure 4. Representative volume element with the boundaries details

$$U_y|_{\Gamma_{AD}} - U_y|_{\Gamma_{BC}} = 0 \tag{1}$$

$$U_x|_{\Gamma_{DC}} - U_x|_{\Gamma_{AB}} = 0.01L \tag{2}$$

$$U_x|_{B} - U_y|_{B} = 0 \tag{3}$$

The rigid body motion of the RVE was constrained using (Eq. 3),whereas the displacements along the longitudinal and transverse directions were applied using (Eq. 2) and (Eq. 1) respectively .Finally, the boundary value problem was solved using Abaqus /Standard solver.

The tensile strength(σ_{xx}) of the RVE was calculated by using the following relation:

$$\sigma_{xx} = \frac{\sum_{\Gamma_{DC}} R_x}{HW} \tag{4}$$

R_x is the reaction forces along the longitudinal direction at the nodes on the edge Γ_{DC} of the RVE, whereas L, H, W are the length, width and thickness (1nm) of the RVE respectively.

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3. Results and Discussion

3.1. Effect of material heterogeneity

Failure pattern of a 2x2 RVE with homogeneous properties is shown in the (Fig. 5) and it can be observed that the cohesive elements in both the left and right junctions had failed at the same rate and is displayed in red (red colour represents complete damage to cohesive elements). It can also be observed from (Fig. 6) that along with the vertical junctions a small region of horizontal interface displayed in red between the vertical cohesive elements also have failed and this is due to shearing of cohesive elements, whereas the remaining regions of horizontal interface remain intact as they doesn't undergo shear. The regions that are intact are displayed in blue(blue colour represents no damage to cohesive elements) .

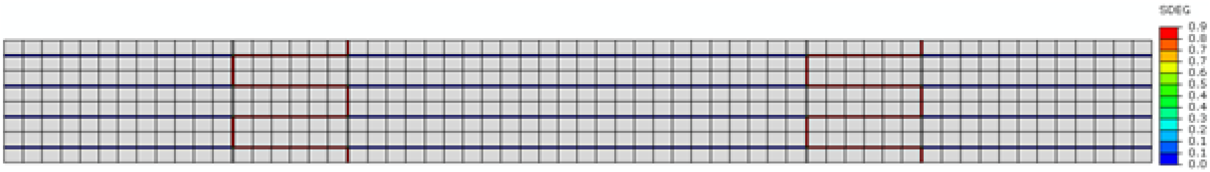

Figure 5. Failure pattern predicted using 2x2 homogeneous RVE model

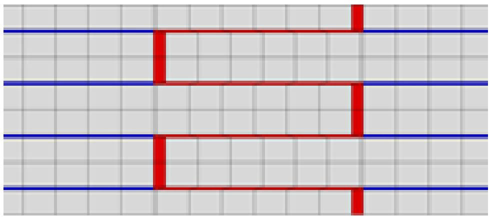

Figure 6. Closer view of the failed left and right junctions of 2x2 homogeneous RVE model

(Fig. 7) represents the failure pattern of a 2x2 RVE with heterogeneous properties and it can be observed that the cohesive elements in the left junctions had failed completely,whereas the elements in the right junctions had failed partially(green colour) . A closer view(Fig. 8) of the RVE suggest that left junctions and the region of horizontal interface close to it have failed completely whereas the regions of horizontal interface close to the right junctions are intact. From the stress-strain curve (Fig. 9)it can be seen that the homogeneous RVE displayed higher tensile peak strength(135MPa)compared to that of heterogeneous RVE(130MPa) .In addition to that it can also be observed that the post damage initiation slope of homogeneous model was less than the heterogeneous model indicating that the homogeneous RVE can withstand large strain compared to that of heterogeneous model.

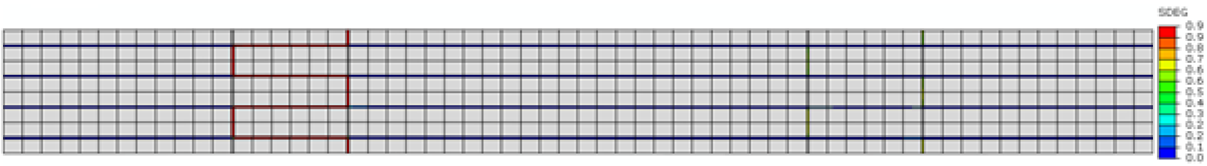

Figure 7. Failure pattern predicted using 2x2 heterogeneous RVE model

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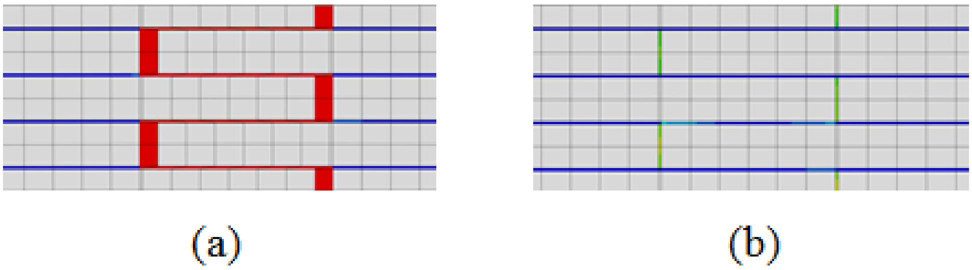

Figure 8. Closer view of the failed a) left and b) right junctions of 2x2 heterogeneous RVE model

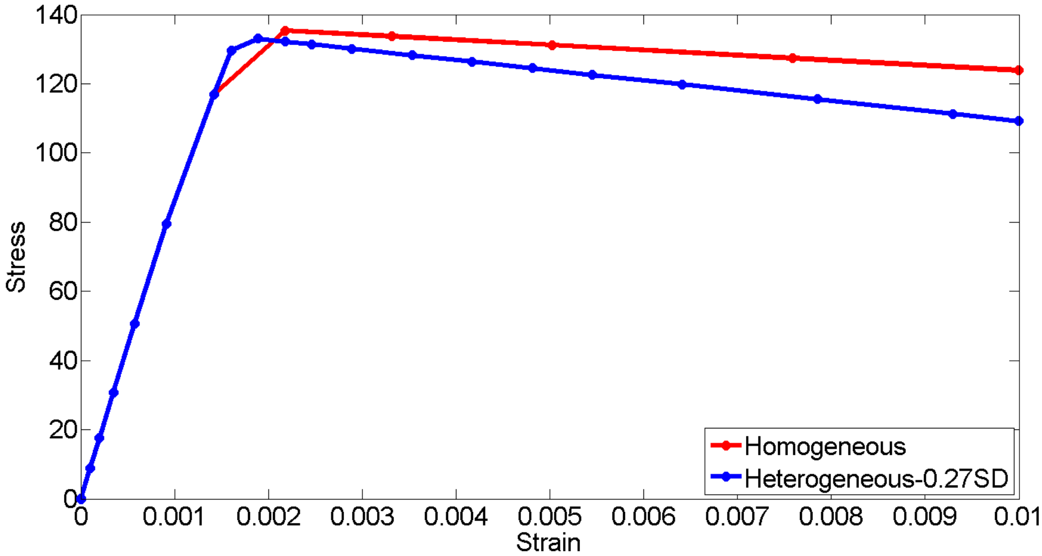

Figure 9. Stress vs strain curve for 2x2 RVE

3.2. Size effect

For each RVE size ,Monte Carlo simulations with 500 random samples were carried out and the overall peak strength of the RVE was determined. It can be observed from (Table 1) that the mean peak strength of the RVE decreases as the size of the RVE increases indicating that the failure occurs in accordance with the weakest link theory.In addition to that it can also be seen that the standard deviation in peak strength decreases as the RVE size increases indicating that peak strength predictions are more reliable as the size of the RVE increases.

Table 1. Statistics of Monte Carlo simulation results

RVE Size	Mean Peak Strength (MPa)	Std Dev in Peak Strength (MPa)
2x2	129.684	6.786
4x4	128.094	4.237
8x8	127.477	2.612

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4. Conclusion

A finite element based representative model of nacre with random heterogeneous properties was modelled to determine the tensile peak strength of the RVE.To emphasize the material heterogeneity effect on the RVE failure pattern, homogeneous and heterogeneous RVE models of different sizes were considered and it was shown that the heterogeneous model exhibited non uniform failure patterns,whereas the homogeneous model exhibited uniform failure pattern.In addition to that the size effect on the mean tensile peak strength and on the standard deviation in the peak strength was also presented.

Acknowledgments

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