MODELLING CLAY GALLERY FAILURE IN CLAY NANOCOMPOSITES

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1 Introduction

Clay gallery failures have recently been observed to precede propagating cracks in an epoxy/clay nanocomposite and they are hypothesized to be a key mechanism to increasing the fracture toughness of the nanocomposites [1]. However, the effects of clay gallery failure are not well understood and modelling this failure mechanism is required. In particular, its effects on deformation and fracture properties of the nanocomposite need understanding.

In this work, a numerical model to study the effects of clay gallery failure at different clay concentration is introduced. The numerical model is used to study the dilatation resulting from clay gallery failure. The dilation behaviour is akin to hydrostatic-pressure-dependent yield. The establishment of a hydrostatic-pressure-dependent "yield" criterion and its associated flow rule will enable the crack growth resistance of epoxy/clay nanocomposite to be modelled.

2 The Model

The model assumes clay gallery failure will cause a clay nanocomposite to be a hydrostatic-pressure-dependent material. The model idealises an epoxy/clay nanocomposite into a representative volume element (RVE) that comprised of an elastic-plastic matrix filled with intercalated clay particles that are randomly orientated and dispersed at the nano-scale. The intercalated clay particle consists of two effective clay layers that are isotropic elastic and a gallery layer that is governed by a cohesive traction-separation law that behaves initially in a linear elastic manner with the stiffness in the planar direction assumed to be half of the normal stiffness of the gallery. Damage initiates upon satisfying a stress criterion. Damage propagation is linear and full damage (or failure) occurs when the scalar cohesive energy of the gallery is exceeded. More details of the numerical model are given in [2].

An in-house program is developed to generate the numerical model with randomly distributed and randomly orientated intercalated clay particles, of a given volume fraction, that do not intersect with the model's boundary and with other clay particles. To overcome issues of a denuded zone forming at the model's boundary, the model dimensions are made large compared to the diameter of the clay particle. The in-house program also develops the PYTHON scripts for ABAQUS/CAE to generate the finite element mesh of the numerical models. Fig. 1 shows a cartoon of idealised model of the intercalated clay nanocomposite.

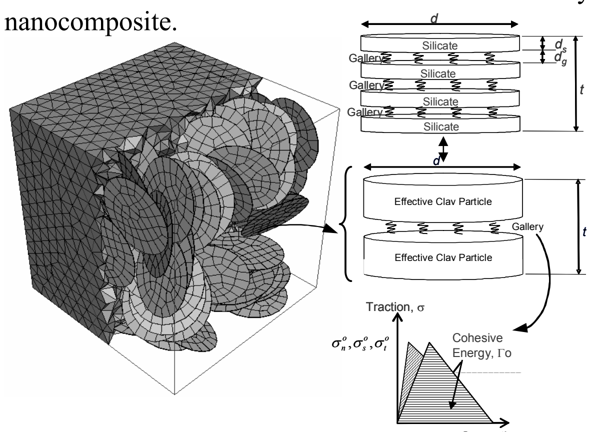

Fig. 1. Schematic of a typical numerical model of an intercalated clay nanocomposite.

3 Results & Discussions

The numerical model of the clay nanocomposite at different clay concentration has been developed and subjected to loading conditions ranging from pure hydrostatic tension to pure shear state. Fig 2 shows the typical hydrostatic stress and volumetric strain behaviour of an intercalated clay nanocomposite with 0.5%, 1% and 2% clay volume fraction (V_f).

The figure shows that clay gallery failure or clay delamination is the mechanism responsible for the onset of non-linearity in the hydrostatic stress-volumetric strain behaviour of the nanocomposite. The clay gallery failure typically propagates at constant stress and the corresponding dilatation (i.e. the increase in volumetric strain) develops up to a critical value. Thereafter, the dilatation in the nanocomposite increased proportionally with the hydrostatic load bearing capacity of the nanocomposite.

For low concentration of clay particles, i.e. V_f = 0.5% & 1%, the dilatation at constant hydrostatic tension stress saturate when 50% percent of the total number of clay particles are delaminated. Subsequently, the dilatation caused by clay delamination increased linearly with the hydrostatic stress.

For higher clay concentration, i.e. $V_f \geq 2\%$, the hydrostatic stress initially drops as the clay particles delaminates followed by an increase in hydrostatic stress as more clay particles delaminate. The hydrostatic stress level at which 50% percent of the total number of clay particles are delaminated is significantly higher than the stress level at which the clay delamination is initiated. Or in other words a lower percentage of clay particles are delaminated after dilatation propagation reached the hydrostatic stress at which clay delamination is initiated.

The mechanism for changing the dilatation trend of a nanocomposite containing low and higher concentration of clay particle is inter-particle interaction, which develops when clay particles clusters or agglomerates. Computational evidences to support this hypothesis will be provided during the conference presentation. Also, the nature of the hydrostatic-pressure-dependent yield criterion of the nanocomposite will be presented.

4 Conclusions

A numerical model that considers the development of clay gallery failure in clay nanocomposites has been developed. Clay gallery failure has been shown to cause the nanocomposite to dilate under a hydrostatic strain state. The dilatation trends of the nanocomposite are shown to be dependent on the clay concentration or the development of inter-particle interaction.

Acknowledgements

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References

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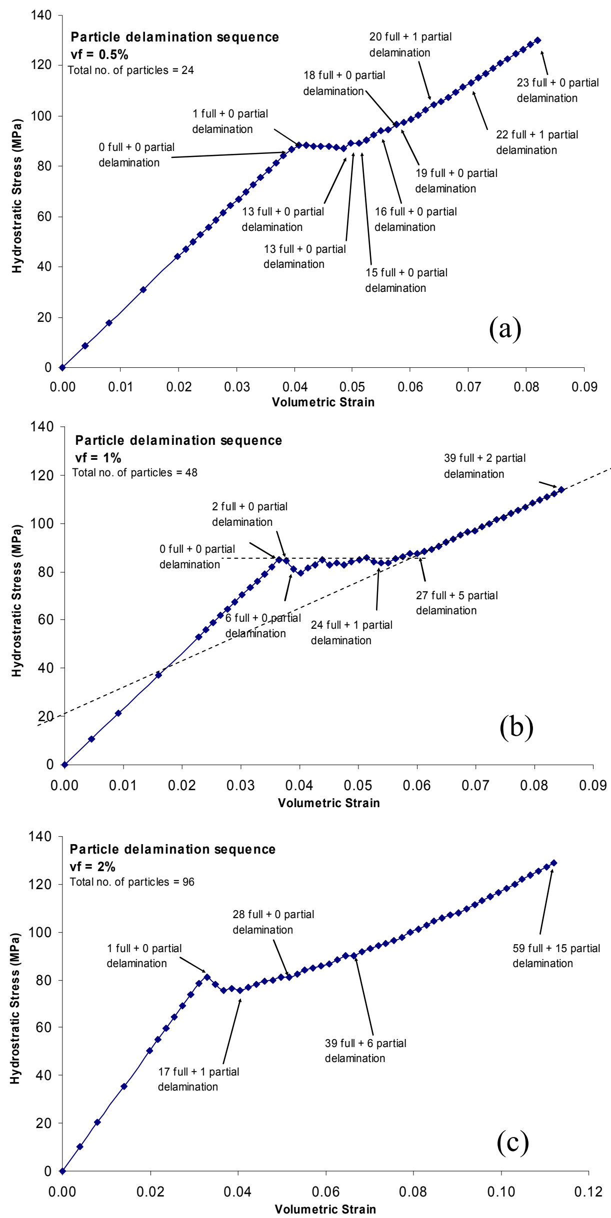

Fig. 2. The hydrostatic stress-volumetric strain curve of an intercalated clay nanocomposite at (a) V_f =0.5%, (b) V_f=1% and (c) V_f=2%.