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APPLICATION OF ANALYSIS ON GRAPHS TO SITE-BOND MODELS FOR DAMAGE EVOLUTION IN HETEROGENEOUS MATERIALS

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Damage in heterogeneous materials is a mechanism for dissipation of strain energy, often associated with the generation and growth of micro-cracks. Initially these are of the size of specific microstructure features, but consequently coalesce to form larger micro-cracks. The application of continuum-based computational strategies to analyse the microstructure-controlled evolution of micro-crack populations is unrealistic. A realistic methodology needs to account for the heterogeneity and the mechanisms of micro-crack generation. Discrete lattice models provide frameworks for incorporating relevant materials and physics information. Lattices have generating cell complexes, so that lattice sites located in cells are linked by lattice bonds resisting relative deformations between cells.

The site-bond method [1], based on a tessellation of space into truncated octahedral cells, was shown to reproduce any isotropic material in contrast to previously used lattices [2]. With bonds represented by beam elements, the methodology was applied to predict the damage evolution in cement [3] and concrete under complex loadings [4]. To address theoretical problems with the beam representation, the method was developed recently to represent bonds by spring bundles resisting axial and transversal relative displacements between sites [5]. A new formulation, allowing for the incorporation of a richer set of microstructure characteristics than in [3, 4], was proposed and applied to the analysis of microstructure-properties relations in nuclear graphite [6] and cement paste [7].

This work has three aims. Firstly, we will present a novel development of the discrete calculus, or analysis on graphs [8], for the solution of 3D deformation-damage problems. The extension offers an elegant, more efficient and exact way of solving discrete lattice problems compared to classical finite element method with spring elements. Moreover, the discrete calculus apparatus provides insights into the link between the continuum and discrete representation of the material in terms of local topology and metric, and from there the notions of length, area and volume in the two systems. This is discussed and used for the calibration of stiffness coefficients of spring bundles, as well as for the definition of area elements associated with springs.

Secondly, we will present a method for generation of microstructure-informed site-bond models for materials which can be idealised as three-phase media: stiff inclusions in a compliant matrix containing pores. The experimental data required for such correspondence are the size distribution and volume densities of inclusions and pores. The former is used to

calculate the cell size and from there the spring elastic behaviour. The latter is used to define the failure behaviour of individual springs together with the associated area elements.

Thirdly, we will present results of the application of the proposed methodology for model generation and analysis to nuclear graphite and cement. For the former, the emphasis is on the effects of irradiation on the deformation and failure behaviour, including fracture energy changes. Such effects are emergent from the underlying changes of pore system characteristics, as illustrated in Fig. 1(a). For the latter, the emphasis is on the effect of cement aging on the behaviour, which is also communicated to the macroscopic level through changes in the pore system, albeit differently from the graphite case, see Fig. 1(b).

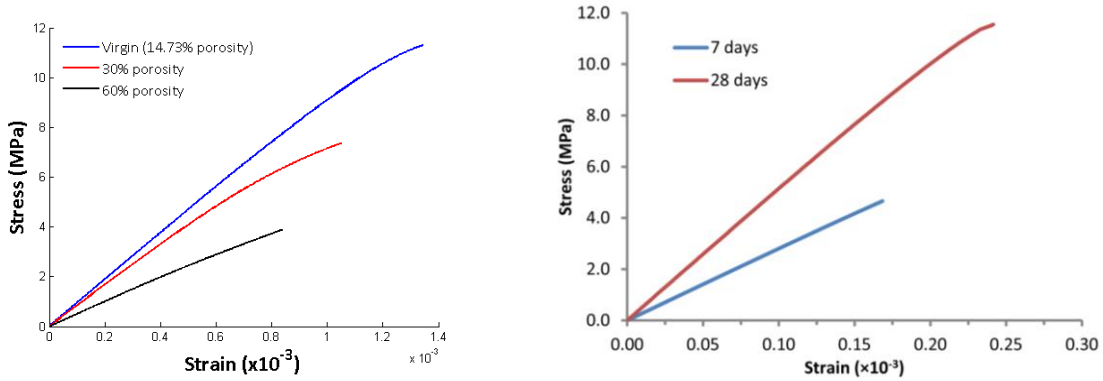

Figure 1. Predicted uniaxial stress-strain response of: IG110 graphite after different irradiation times (left); and cement paste at different curing ages (right).

The results of the work are in very good agreement with experimentally observed behaviours, which supports the realism of the proposed methodology. Requirements and options for further development of the methodology, in theoretical and microstructure representation aspects, are discussed.

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