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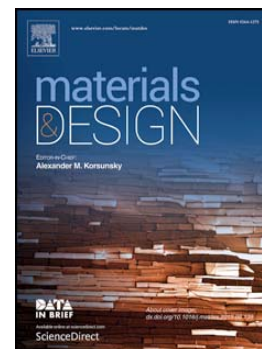
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Macro- and micro-modeling of crack propagation in encapsulation-based self-healing materials: application of XFEM and cohesive surface techniques

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Abstract

Encapsulation-based materials are produced introducing some small healing fluid-filled capsules in a matrix. These materials can self-heal when internal cracks intercept and break the capsules. If the healing agent is released, the crack can be sealed. However, this is not always the case. These capsules need to be designed with the adequate shape and material to be properly broken. This paper presents two application models based on the combination of eXtended Finite Element Method (XFEM) elements and Cohesive Surfaces technique (CS) to predict crack propagation. Two types of encapsulated systems are considered: a concrete beam in a three-point bending test, and a micro-scale model of a representative volume element of a polymer subjected to a uniaxial tensile test. Despite both systems rely on different capsule shapes and different constituent materials, the models predict a similar non-linear response of the overall material strength governed by the coupled effect of the interface strength and the capsule radii-to-thickness ratio. Furthermore, even if an inadequate material and geometry combination is used, it is found that the mere presence of capsules might achieve, under certain conditions, an interesting overall reinforcement effect. This effect is discussed in terms of clustering and volume fraction of capsules.

Keywords: self-healing materials, micro-capsules, crack propagation, debonding, cohesive zone, extended finite element method

1. Introduction

The fundamental feature of any encapsulation-based self-healing material relies on inserting small fluid-filled capsules in a matrix [1–5]. When the matrix is internally damaged, cracks can intercept these capsules and transfer the stresses at the their propagating fronts to the capsules. In that sense, three basic scenarios can be produced: (i) the capsules are not able to withstand the stress concentration and they break, releasing in this way the healing fluid content inside the crack space, (ii) the constitution of the capsules is robust enough as to withstand comfortably much higher stresses, whilst the interface with the the matrix fails, and (iii) the level of transferred stresses are not sufficient either to break the capsule nor the interface with the matrix. Naturally, (i) represents the desired scenario for this self-healing strategy. In this case, the healing agent can spread into the crack space via capillarity. To complete the healing process, this initially-fluid agent can cure after some reaction, in such a way that the crack path becomes sealed and the final internal structure is partially repaired [6]. If the scenarios (ii) or (iii) occur, it is clear that this self-healing strategy cannot be carried out successfully. In particular, (ii) involves that an incoming crack will simply trigger a premature debonding, similarly to what happens when a solid inclusion is weakly bonded to a matrix [7, 8]. Also, even if premature capsule debonding

takes place before the crack interception, a hole-like region could be created and therefore additional nearby cracks would be attracted. These cracks would simply pass along the capsule perimeter and continue their path again through the matrix [9, 10]. This situation would not only result in an intact capsule preventing the internal repairing, but it might also accelerate the level of damage in the matrix. Regarding scenario (iii), albeit no healing effect would be triggered a priori, it might still produce some beneficial aspects in terms of mechanical reinforcement. Nevertheless, this reinforcement effect would naturally depend on the characteristics and properties of each constituent, as well as on the mechanical performance of the interface.

In terms of designing a predictive tool, the interest in encapsulation-based self-healing strategy is currently leading to an increase of theoretical and numerical works with the aim of getting a better understanding of its mechanisms and determining the key factors to improve efficiency and feasibility [11–15]. In spite of this, most models deal with very specific application-oriented materials and also assume specific geometries, boundary conditions and loading configuration. Moreover, the mere presence of the capsule-matrix interface has received less attention, when not neglected. As an example, within the context of cementitious materials, even when the interface has been accounted for, these models often assume a certain range of typical values of the interface properties, which are selected as a function of mechanical similarities given by composition or the degree of brittleness [16, 17].

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