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A semi-concurrent multiscale approach for modeling damage in nanocomposites

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ABSTRACT

The paper presents an effective implementation of a semi-concurrent multiscale method in the commercial finite element software package ABAQUS. The method is applied to the pre-localized damage initiation and propagation in the fully exfoliated clay/epoxy nanocomposite. The obtained results of the proposed method is also compared with the hierarchical multiscale approach. This method can be easily used to get a better understanding of damage mechanism in the nanocomposite materials in order to improve the constitutive models and to support the future design of those materials.

1. Introduction

In computational material design, the multiscale methods are powerful tools to extract the material parameters based on the fine scale details. While numerous multiscale methods (see for example [1–3]) were developed for intact materials, far less methods are applicable for fracture and damage simulations.

Multiscale methods can be categorized into hierarchical, semi-concurrent and concurrent methods [4], Fig. 1. In hierarchical multiscale methods, the information are passed from the fine scale to the coarse scale but not vice versa. Computational homogenization [5] is then a classical upscaling technique. Hierarchical multiscale approaches are very efficient to extract material properties.

In concurrent multiscale methods, there is not an information transfer between fine- and coarse-scale and both scales are solved simultaneously. A compatibility condition enforces the displacement gap between the fine- and coarse-scale to be zero. Numerous concurrent multiscale methods [7–10] have been developed that can be classified into 'Interface' coupling methods and 'Handshake' coupling methods. Interface coupling methods seem to be less effective for dynamic applications as avoiding spurious wave reflections at the 'artificial' interface seem to be more problematic. Some of the concurrent multiscale methods have been extended to modeling fracture [4,11,12]. More detailed discussion on the different aspects of multiscale methods can be found in Refs. [11,13–15].

The basic idea of semi-concurrent multiscale method is illustrated in Fig. 1(b). In semi-concurrent multiscale methods, information are passed from the fine scale to the coarse scale and vice versa. Semi-concurrent methods are of the same computational efficiency as concurrent multiscale methods. The key advantage of the semi-concurrent multiscale methods over the concurrent multiscale methods is their flexibility, i.e. their ability to couple two different software packages, e.g. MD software to FE software [16,17]. Parallelization is generally simple in this approach. A classical semi-concurrent multiscale method is the FE^2 by [18] originally developed for intact materials. Kouznetsova [5] was the first who extended this method for problems involving material failure, see also Kouznetsova et al. [19] or the recent contribution by Nguyen et al. [20]. Verhoosel et al. derived a homogenization procedure for both adhesive and cohesive failure on the macro-scale in FE^2-setting [21].

Based on the FE^2 multiscale method, Belytschko et al. [22] developed a semi-concurrent multiscale method wherein the material instability in the fine scale is circumvented by introducing discontinuities at the coarser scale. In this method that is called multiscale aggregating discontinuities (MAD), the unit cell dimensions should be close to the characteristic element size in the coarse scale which makes the method computationally expensive.

Extensive studies have been done to model nanocomposite material behavior [23,24]. These research were mainly based on hierarchical multiscale concepts. For example for the clay/epoxy nanocomposites, Sheng et al. [25] defined the concept of 'effective particle' and modeled the discrete structure of intercalated nanoclay (For a brief introduction on different categories of clay

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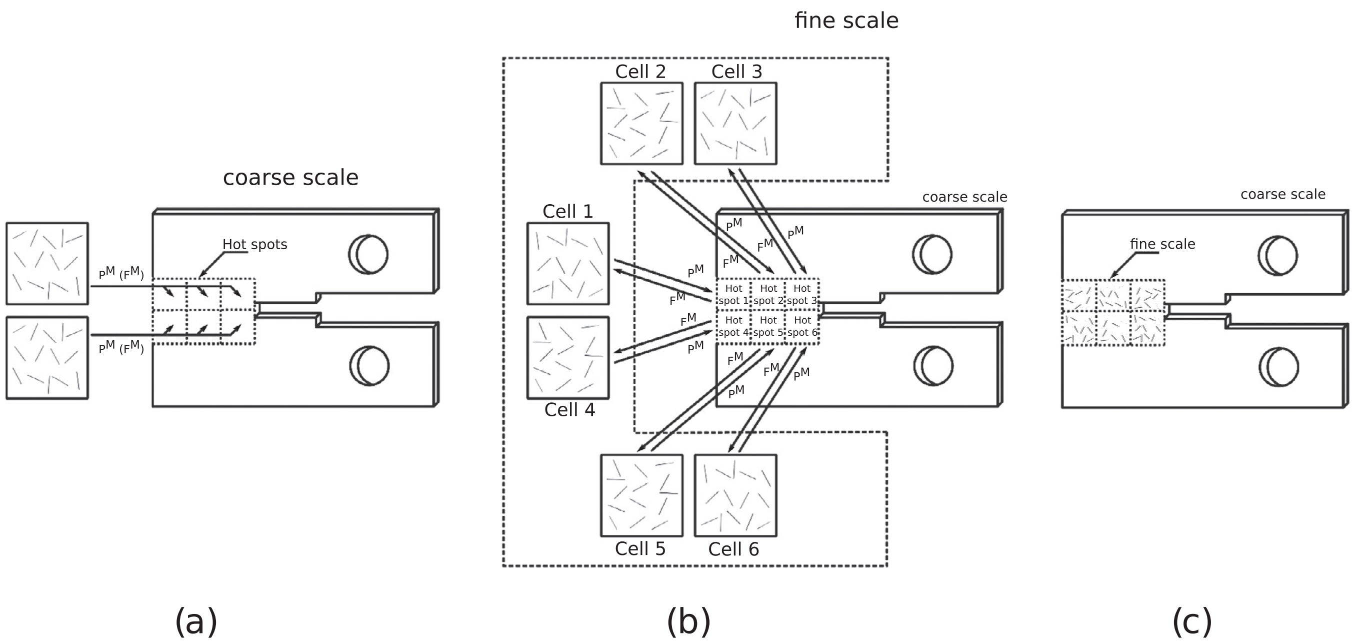

Fig. 1. Schematic of a (a) hierarchical, (b) semi-concurrent and (c) concurrent multiscale methods adopted from [6].

nanocomposites see Refs. [26,27]). Scocchi et al. [28–30] presented a bottom-up computational multiscale approach to investigate the behavior of the polymer/clay nanocomposites. Their method is based on quantum/force-field-based atomistic simulation in nano-scale and the mapping of these values into mesoscopic beadfield hybrid method. They used mesoscopic simulations to determine density and morphology of clay/polymer nanocomposites. Zappalorto et al. [31] presented a multiscale modeling techniques to assess the effect of plastic yielding of nanovoids on the toughening of nanocomposites. Salviato et al. [32] provided a multiscale analytical model to study the toughening improvements in nano-particle filled polymers.

Beside numerical investigations, there are some analytical models to predict polymeric composite materials behaviors. Using different debonding criteria, Lauke [33,34] studied the effect of particle size on the fracture toughness of particle reinforced polymers. Williams [35] proposed a model to describe the toughening of particle filled polymers based on the plastic void growth. Hsieh et al. [36] performed a series of experimental and analytical studies to investigate the toughening mechanisms in epoxy polymers and fiber composites.

There are also some analytical micromechanical approaches to deal with debonding phenomena in nanocomposites, e.g. [37] in carbon nanotube (CNT)-reinforced composites and nano-clay/epoxy nanocomposites [38]. Sevostianov et al. [39] studied the effect of interphase layers on the overall elastic properties of composites. They concluded that if the interface layers between inclusions and matrix are thin, the effective elastic properties are almost unaffected by the interfaces. Some models also consider the effect of the interface on the elastic properties of nanocomposites, both analytically and numerically [40–42]. The authors in [43] accounted for the effects due to debonding.

Although there are many experimental and numerical studies to investigate the mechanical properties of clay nanocomposites [44–47], there is still not a clear understanding about how the clays affect the toughness and damage in nanocomposites.

In this paper, a semi-concurrent approach for modeling damage in the clay nanocomposites is presented. This method bridges the meso-scale to the macro-scale. Based on the micromechanical approach, a homogenized damage parameter is calculated in meso-scale and send back to the next higher level (macro-scale). This damage parameter is then used in the macroscopic constitutive equation of the material in macro-scale. In this approach, the RVE boundary conditions comes from macro-scale deformation state which is more realistic than other conventional methods such as periodic boundary conditions. To implement this multiscale method, we use ABAQUS–ABAQUS coupling in meso and macro scales. We apply this multiscale approach to simulate the fully exfoliated clay/epoxy nanocomposite behavior and compare the results with hierarchical approach.

This paper is organized as follows. The proposed semi-concurrent multiscale method is described in Section 2. Section 3 outlines the implementation details in ABAQUS package. Section 4 presents the numerical results of proposed multiscale method on fully exfoliated clay/epoxy nanocomposite. The discussion on the results and validation of the proposed method is discussed in Section 5. Finally, the conclusion of this research is presented in Section 6.

2. Upscaling method

In this section, the proposed semi-concurrent multiscale approach is described and discussed in details. Fig. 2 shows the schematic representation of this multiscale approach.

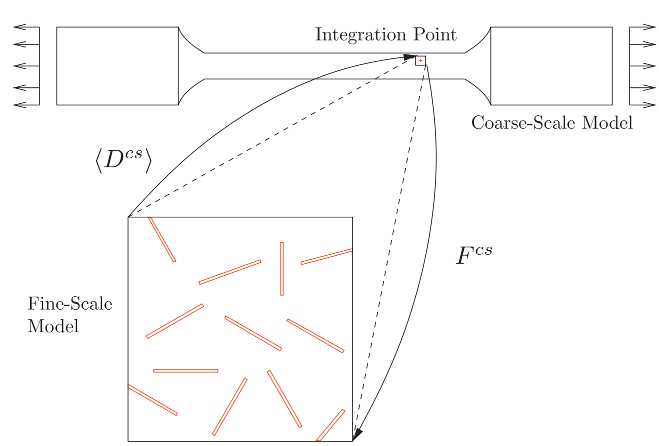

Fig. 2. The schematic representation of proposed semi-concurrent multiscale method.