Computation of effective nonlinear coupled electro-mechanical properties of graphene-reinforced nanocomposites

Xiaoxin LU*†, Julien Yvonnet†, Fabrice Detrez† and Jinbo Bai*

* Mechanics, Structures and Materials (MSSMat)
Centrale Supelec, University Paris Sacley
Grande Voie des Vignes, 92295 Chatenay-Malabry, France
e-mail: {xiaoxin.lu, jinbo.bai}@ecp.fr

† Laboratoire Modélisation et Simulation Multi-Echelle (MSME)
University Paris-Est
5 Bd Descartes 77454 Marne-la-Vallée Cedex 2, France
Email: {julien.yvonnet, fabrice detrez}@u-pem.fr

ABSTRACT

Tunnel effect is a possible mechanism to explain the apparent large electric conductivity and nonlinear electric behavior of graphene-reinforced nanocomposites with polymer matrix[1,2]. In this work, a numerical modeling framework is proposed to evaluate the effective electric conductivity in polymer composites reinforced with graphene sheets, taking into account the electrical tunneling effect, which allows conduction between graphene sheets at small nanometric distances. A nonlinear Finite Element formulation with a distance function field is introduced to model the nonlocal and nonlinear effects introduced by the tunnelling effect conduction model within the polymer matrix between close graphene sheets. In addition, to avoid meshing the thickness of the graphene sheets and in view of their very high aspect ratio, a highly conducting surface model is employed[3]. The computed effective conductivity is evaluated over representative volumes containing arbitrary distributed graphene sheets. To evaluate the degradation of electrical performances with decohesion of graphene sheets under mechanical stress, a nonlinear cohesive model [4] is introduced to describe the mechanic property of the interphase between graphene and matrix. The parameters for the cohesive zone are identified by molecular dynamics. The proposed model is demonstrated to predict the variation of percolation threshold under mechanical stress.

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