Multiscale Mechanical Modelling of Plasmonic Polymeric Microcapsules: Role of Nanoparticle Assembly in Local Stress and Strain Sensing

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EXTENDED ABSTRACT

Quantifying local strains and stresses in soft and heterogeneous materials, such as biological tissues, is essential for understanding complex biomechanical interactions within the human body (Arms et al., 1984; Boccafoschi et al., 2013; Zavatsky and Wright, 2001). However, this remains a major challenge in experimental mechanics, particularly at the nano- and microscale, where conventional sensors lack the spatial resolution and minimal invasiveness required for accurate local measurements.

In this context, we investigate the mechanical response of plasmonic polymeric microcapsules designed as optomechanical stress and strain sensors (Burel et al., 2017; Kim et al., 2023). These microcapsules consist of a soft elastic polymer shell made of plasticised polystyrene, in which high-purity gold nanoparticles are densely embedded. This structure forms a complex core-shell architecture whose deformation governs both mechanical integrity and sensing performance (Burel et al., 2022).

The mechanical parameters of the plasticised polystyrene embedding gold nanoparticles are first identified experimentally through uniaxial tensile tests performed on macroscopic specimens composed of plasticized polystyrene both without and with embedded gold nanoparticles. These experiments provide the mechanical response used as input for the numerical modelling.

The mechanical response of individual microcapsules is then characterised numerically using finite element simulations based on representative volume elements, designed to capture the heterogenous nanostructure induced by the assembly of gold nanoparticles. This approach enables the establishment of constitutive mechanical laws linking applied displacements to local stress and strain fields within the microcapsules.

A two-dimensional model has been firstly investigated to study the influence of matrix stiffness and matrix size on the mechanical response of the microcapsule and on its morphology after deformation. Subsequently, a full three-dimensional model is developed to account for geometrical effects and to analyse the spatial redistribution of nanoparticles during the deformation of the microcapsules.

Numerical results show that stress and strain concentrations are localised within the plasticised polystyrene layer near the symmetry axis of the microcapsules when the surrounding matrix is not stiffer than the plasticised polystyrene shell. In contrast, when the matrix stiffness exceeds that of the plasticized polystyrene layer, stress and strain concentrations predominantly develop within the matrix material. The microcapsule morphology and the redistribution of embedded gold nanoparticles are strongly influenced by the mechanical properties of both the plasticised polystyrene shell and the surrounding matrix, as well as by the matrix size.

The numerical results obtained from 2D and 3D simulations during periodic stretching —including microcapsule morphology, nanoparticle redistribution, and local stress and strain fields—will be discussed in detail.

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