ABSTRACT:

Finite Element Modelling of Plasmonic Polymeric Microcapsules: Nanoparticle Assembly and Strain-Sensing Mechanisms

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Quantifying local strains in soft and heterogeneous materials, such as biological tissues, is critical for understanding complex biomechanical interactions within the human body [1]. However, this remains a significant challenge in experimental mechanics, especially at the nano- and microscales, where conventional sensors fail to provide the spatial resolution and minimal invasiveness required for precise local measurements.

In this context, we investigate the mechanical response of plasmonic polymeric microcapsules (MC), designed as optomechanical strain sensors [2]. These MCs comprise a soft elastic polymer shell–composed of plasticised polystyrene–within which high-purity gold nanoparticles (NP) are densely embedded. As the MCs elongate, the interparticle distance increases, shifting the plasmonic absorption frequency towards shorter wavelength, away from the excitation and fluorescence emission wavelengths of the dye. Consequently, the dye inside the capsules can be more efficiently excited and re-emits more light in the infrared, compared to their resting state. Thus, these microcapsules function as deformation-sensitive sensors, emitting fluorescent light whose intensity varies as they are deformed.

The mechanical response of individual microcapsules was investigated numerically using finite element simulations, based on representative volume elements designed to capture the heterogeneous nanostructure arising from the assembly of gold nanoparticles. Initially, a two-dimensional model was employed to assess the influence of matrix stiffness and matrix size on both the mechanical response of the microcapsule and its post-deformation morphology.

Following this, a fully three-dimensional model was developed to account for geometric effects and to analyse the spatial redistribution of nanoparticles during microcapsule deformation.

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.

[1] Arms, S.W., Pope, M.H., Johnson, R.J., Fischer, R.A., Arvidsson, I., Eriksson, E., 1984. The biomechanics of anterior cruciate ligament rehabilitation and reconstruction. Am. J. Sports Med. 12, 8–18.
[2] Burel, C.A.S., Alsayed, A., Malassis, L., Murray, C.B., Donnio, B., Dreyfus, R., 2017. Plasmonic-Based Mechanochromic Microcapsules as Strain Sensors. Small 13.