Modelling the dynamics of graphene encapsulation with application for atom probe tomography

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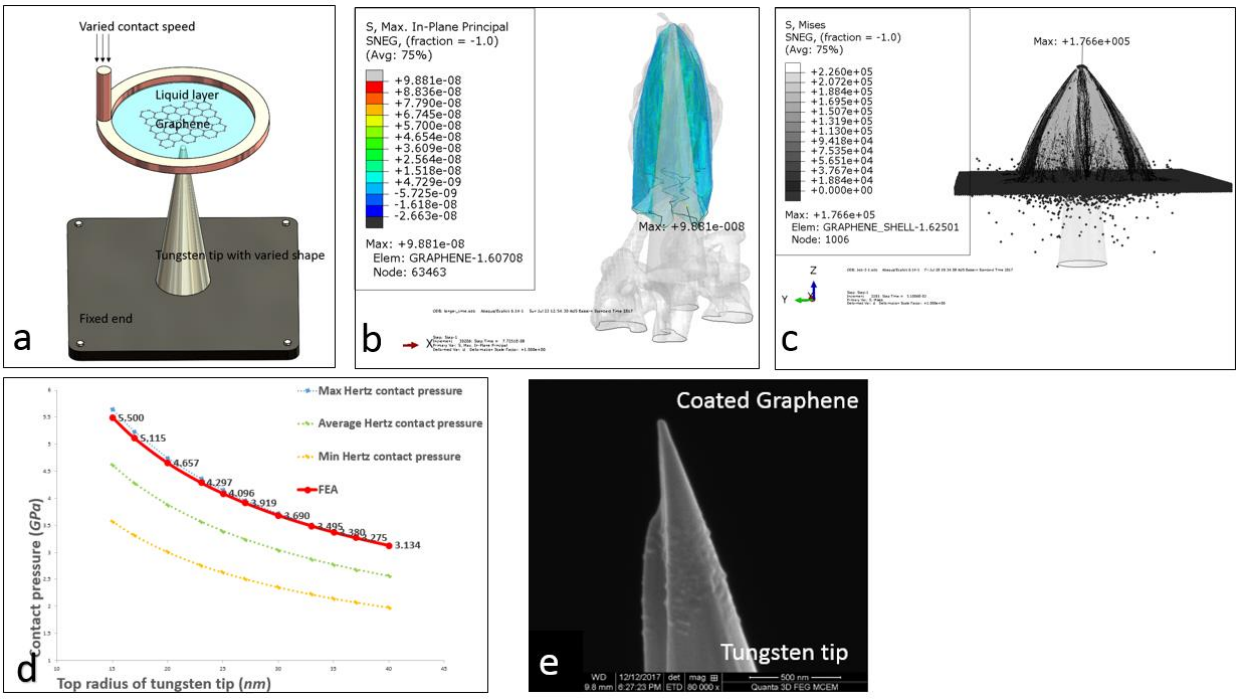
Atom probe tomography (APT) has recently demonstrated its unique capability as an imaging tool to achieve near-atomic 3D chemical mapping of mammalian and bacterial cells [1, 2]. We propose a novel approach for APT imaging of electrically insulated samples by introducing a graphene encapsulation approach to 'disguise' the low-conductivity barrier. In this study, we aim to investigate the dynamic process of graphene membrane encapsulation as it contacts the nanoscale specimen tip geometry required by APT, and to optimise the physical parameters with particular focus on contact speed. A computational framework is first established that provides various insights including the distribution of stress and strain during graphene encapsulation. A schematic diagram of the process is shown in figure (a), with the graphene membrane initially floating on a water membrane layer. Dropping the graphene layer at controlled speed to contact the APT tip is simulated by Coupled Eulerian-Lagrangian (CEL) and Smoother Particle Hydrodynamics (SPH) methods, figure (b) and (c). The computational model is also validated by Hertz contact theory and further confirmed by experimental study. The successful establishment of this modelling framework is expected to provide suggested optimal contact speed given the radius of the APT tip (figure (d)), in order to perform optimal coating and encapsulation towards APT imaging of insulated and hydrated samples.

Figure. (a) Schematic diagram of the proposed graphene encapsulating process. FEA simulation results with the water membrane modelled by (b) CEL (c) SPH. (d) Maximum contact pressure vs tip radius at a specific contact speed < 1 mm/s. (e) APT tip sample (Tungsten) is coated with graphene using the recommended contact speed from simulation.



References:

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