Computational characterization of nanowire network electrodes

Davide Grazioli*†[1], Matteo Ferliga[1], Lucia Nicola[1], and Angelo Simone[1]

[1]University of Padova – Italy

Abstract

Transparent electrodes find applications in optoelectronic devices, solar cells, light emitting diodes, and transparent heaters. Indium tin oxide (ITO) is currently the most widely employed material for producing transparent electrodes due to its low sheet resistance and high transparency. Unfortunately, the scarcity of indium is making ITO too expensive to meet commercial requirements. Furthermore, ITO is intrinsically brittle and therefore inappropriate for deformable electronic devices. Electrodes based on metallic nanowire (NW) networks are nowadays the best alternative to ITO electrodes in terms of electrical conductivity and transparency, and their intrinsic mechanical flexibility makes them suitable for deformable electronic devices too.
Metal NW electrodes are planar arrangements of interconnected NWs that form a network capable of withstanding mechanical deformations and ensure electric current conduction. The electrode production process involves the synthesis, deposition, and welding of NWs. These steps affect network features at different characteristic lengths that range from tens of nanometers (nanowire scale) to hundreds of micrometers and above (network scale). More specifically, the synthesis process determines the crystallographic structure of the NWs, the welding process the morphological characteristic of the junctions (nanowire scale), whereas the deposition strategy determines nanowire density and arrangement (network scale). As the deposition process results in the random positioning of the NWs, the overall network properties are spatially not uniform (1). Consequently, mechanical stress and current density localizations take place causing NW and junctions breakages (local damage) (2). These occurrences negatively affect the macroscopic response of the network, eventually leading to failure.

To characterize these failure phenomena, we present a multiscale computational strategy that involves electrical and mechanical processes taking place in metallic nanowire networks. Molecular dynamics simulations are employed to identify the dependence of junction structure and properties on welding conditions, i.e., sintering temperature, time, and NWs relative orientation. Two-dimensional synthetic representations of electrode microstructures are converted into networks of beam and resistor elements to analyze the mechanical and electrical network responses, respectively.

We observe that the sintering process and the relative orientations between nanowires determines the microstructure of the junctions and their mechanical and electrical properties. Recommendations on welding parameters, nanowire arrangement and density are identified

*Speaker
†Corresponding author: davide.grazioli@unipd.it

to limit the failure of electrodes based on metallic nanowire networks.

References

(1) D. Grazioli, A.C. Dadduzio, M. Roso, A. Simone, Quantitative electrical homogeneity assessment of nanowire transparent electrodes, Nanoscale, 15: 6770-6784, 2023.
(2) D. Grazioli, G. Gangi, L. Nicola, A. Simone, Predicting mechanical and electrical failure of nanowire networks in flexible transparent electrodes, Composites Science and Technology, 245: 110304, 2024.