MULTISCALE MATERIALS MODELLING OF NANOTUBE-BASED DEVICES

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Carbon nanotubes (CNT) arranged in thin films have many interesting properties that make them a focus of research in a wide range of technological applications, including resistance switching and neuromorphic devices. While a single nanotube demonstrates certain desirable properties, a CNT film exhibits complex features that do not necessarily correlate to the individual tube's properties. Nevertheless, experiments show that current through a CNT film flows primarily through percolation pathways which are dependent on the structure of the film.
To model the complex behaviour of CNT films, we have taken a multi-scale approach to describe the various elements involved. Electronic structure simulations were used to calculate the current across a wide range of representative junctions between nanotubes. This data allowed us to develop simple models capable of predicting current based on the geometric properties of a nanotube pair, e.g. the minimum distance between them. On a larger scale, the film itself is treated using a mesoscopic potential, where the nanotubes are coarse-grained into connected cylindrical segments. This allows us to make representative models of CNT films with dimensions relevant to experimental devices. The current through these mesoscopic structures can be evaluated using our previously parameterized current models and compared to electrical measurements of typical devices.
The model presented here is a proof of concept, showing that the current can be directly calculated in physics-based models of CNT films. Dynamical effects can also be also included, as the films' force field allows for time-dependent evolution of the structure. Therefore, mechanisms determining device properties such as resistance switching can be identified within this model. Finally, we demonstrate how structural information and physical parameters can be extracted to be employed in statistical device simulations.