Scienza Computazionale

Computational Science

DII research group
COMS - Computational Materials Science

Angelo Simone
angelo.simone@unipd.it
Phone: +39 049 827 6808

Lucia Nicola
lucia.nicola@unipd.it
Phone: +39 049 827 6769

http://coms.dii.unipd.it

The study was conducted in the framework of the ERC Consolidator grant 'Computational Modelling of Structural Batteries'.

Researchers: Mingzhao Zhou (TU Delft) and dr. Davide Grazioli (TU Delft)

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Main research topics
- Computational Methods
- Multi-scale Modeling
- Mechanics of Materials
- Modeling of Failure for Brittle and Ductile Materials
- Micromechanics of Defects
- Phase Transformations
- Contact and Friction
- Structural Batteries

Computational Modelling and Simulation of Fiber-Based Electrodes

A structural battery is a novel design concept for an energy storage device. By endowing the battery components with a structural function, it is conceptually possible to eliminate the rigid casing of traditional batteries. Such an approach would immediately reduce weight and size of portable devices and make room for radically different form factors in consumer electronics. This concept is also being investigated by Volvo (composite battery-in-body-panel technology) and NASA (structural battery walls to power CubeSats).
A structural Li-ion battery can be devised using a fiber-reinforced composite material in which active and conductive material fibers are randomly dispersed in a solid polymer electrolyte matrix. The optimal mixture of active and conductive inclusions is a compromise between electrochemical and mechanical requirements: conductive fibers have to form a uniformly distributed conductive network leaving enough room for active fibers to guarantee a reasonable energy storage capacity; at the same time, mechanics requires fibers stiff enough to guarantee the load bearing capacity of the composite without electrochemically-inactive (additional) reinforcement.
One of the studies conducted in the context of the ERC project 'Computational Modelling of Structural Batteries' regards the determination of the effective conductivity and capacity of fiber-based electrodes. As in any composite, the overall response depends on its fiber content and orientation if all other characteristics are kept unchanged. As a way of example, the figure below shows the electric potential field when the carbon nanofibers are (a) distributed in an isotropic manner, (b) aligned, or (c) perpendicular with respect to the direction along which the voltage is applied. The figures at the bottom show that the conductivity in the isotropic case increases exponentially with the fiber volume fraction, whereas the electrode capacity is maximized for a specific carbon nanofiber content that does not depend on the active material. The optimal composition of structural battery electrodes should balance these findings against the requirements of the target application.