

Multiscale modelling at NPL

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Abstract

NPL is the UK's National Measurement Institute, and has a long history of characterisation and measurement of material properties, including structural, thermal, and electromagnetic behaviour. Materials modelling is used at NPL to understand quantitatively the nature of processes in materials at various scales, to help design experiments, and to simulate the phenomena that are often challenging to investigate in the lab, whether due to thermodynamic conditions (temperatures and pressures, harsh or dangerous environments) or the nature of the material (toxic or radioactive elements).

The capability to develop and manufacture new materials with tailored properties underpins innovation and competitiveness of many industrial and technology sectors. Increasing miniaturization requires an understanding of processes that occur at the nanoscale (such as mass transport, charge transport, lattice distortion, and diffusion) and of how these processes affect bulk scale behaviour. Although traditional materials design provides improvements, the demand is for new avenues in simulation and modelling capable of delivering significant technological advances. NPL's strategy in materials modelling and simulation is the development of multiscale multiphysics models with better predictive power to meet industrial and metrological needs. The key in this synergistic approach is to formulate all models within a sound thermodynamic framework to ensure consistency and well-defined parameterisations.

The poster gives an overview of our recent work on multiscale models and describes some future directions where a combination of measurement and modelling can create industrial impact.