Seminar

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Online

# Engineering models for microscopically driven materials


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## Speaker introduction

Graduated from the Moscow Engineering Physics Institute in 1983, received PhD and DSc degrees at the same institution. Continued the career development at Oxford, where is presently a Fellow of Linacre College.

Research interests:

- Multiscale mathematical models for fusion and fission nuclear materials.
- Density functional and electronic-structure based methods for modelling defect structures in metals and alloys.
- Langevin dynamics and dislocation dynamics models, models for radiation induced microstructures and effects of irradiation on physical properties of materials.
- Spin-lattice dynamics, magnetic potentials, effects of magnetism on mechanical properties of alloys and steels.

## Seminar abstract


Multiscale modelling aims at deriving macroscopic solutions from first principles using a hierarchical approach, based on a concept where lower-level models feed their output into higher-level coarse-grained descriptions, typically culminating with a finite element continuum treatment, compatible with macroscopic observations and applications. Whereas this seemingly plausible approach offers the advantage of conceptual simplicity, its practical realization often proves difficult as the data transferred upwards across the mathematical “interfaces” appear not necessarily compatible between the models operating on different length and time scales.

I shall explore solutions developed using a self-consistent semi-hierarchical approach where appropriately chosen parameters characterizing defects and dislocations formed in microscopically driven materials, and modelled using ab initio simulations, act as sources providing a direct input for a finite element model. Another example illustrating the apparent failure of multiscale hierarchy is magnetism, where sub-atomic effects of electron correlations control not only the relative free energies of phases in magnetic iron and its alloys but also affect the self-energies of defects and dislocations, producing some remarkable macroscale effects.


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