Atomistic modelling of metals: Introduction and Applications

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Atomistic simulation can provide kinetic and dynamical insight into the fundamental component processes underlying both mass-transport and plasticity within a solid. To directly extrapolate atomistic simulation results to the experimental time-scale is however difficult and remains a general challenge to the atomistic modelling community. This is particularly the case when performing simulations that investigate the plastic response of a material, where strain rates are generally 8-10 orders of magnitude faster than that seen in experiments. The present series of lectures gives an introduction to the basics of atomistic modelling methods and case-studies a number of examples that demonstrate both the power of the technique and its corresponding caveats.

The first lecture will give an introduction to the atomistic method covering the molecular dynamics method, structural relaxation, reaction path calculation methods and semi-empirical potential development. The second lecture will give a number of atomistic simulation examples that exist in the published literature concentrating on point-like defects and their diffusion, and atomic scale plastic processes such as dislocations and their interaction with structural defects. How such information can be used in higher length- and time-scale modelling methods will also be addressed. In both lectures the time-scale problem inherent to the molecular dynamics technique will be discussed and the atomistic acceleration techniques that have attempted to overcome this will be reviewed.