Multiscale computer modelling and experimental investigation of diffusion and segregation in metal alloys

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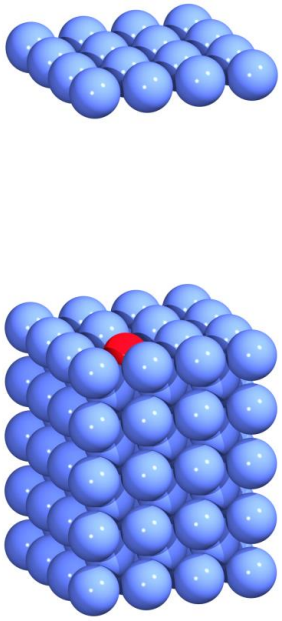
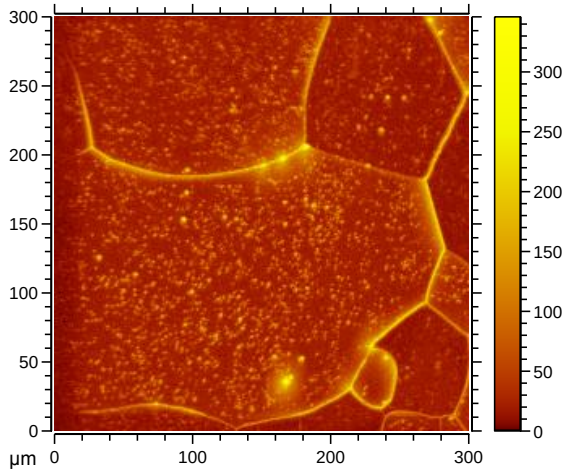
How do atoms move and why? The answer to this question is important for materials which are being used as catalysts, turbine engines, metals in the manufacturing of vehicles etc. Computational modelling is performed from the atomic to the macroscopic scale to investigate the properties of the material. Density functional theory (DFT) modelling allows for an atomistic description of the system taking the electron interactions into account. This allows for properties such as the magnetic, charge, thermodynamic and kinetic properties to be determined from first principles. For a macroscopic description these properties are then used in rate equation models to describe the macroscopic process of diffusion. To confirm the computer simulations, experimental measurements are performed with electron and ion scattering spectroscopy techniques. The combination of experiment and computer modelling allows for a unique and complete view of the system under study, describing the system from the atomistic to the macroscopic scale.

Atomistic description using DFT



Sulfur atom (red) which have diffused to the surface layer of Fe(100)

Macroscopic view as determined by TOF-SIMS experiments



Sulfur (yellow) diffusing via the grain boundaries in bcc Fe (orange) at a temperature of 743 K