Modelling of Nitrogen and Carbon Transport in Metals with Crystal Defects

Studentship: PhD, 3 years duration
Funding: £14,000 per annum
Start Date: October 2016
Supervisors: Dr Michael Auinger and Professor Claire Davis

Project overview
Steel hardening techniques are important methods to obtain very stable and wear-resistant materials, for example for tool steels and cutting blades.

This project aims to deliver a profound understanding and modelling capability for the nitrogen/carbon transport behaviour in bcc and fcc metals on an atomistic level, and its dependence on temperature and local thermochemical activity. Results will be compared with published experimental studies, and will be capable of providing sound descriptions of nitrogen/carbon transport related problem in the temperature and nitrogen/carbon-activity range under investigation. The model can be used for understanding high temperature reaction kinetics, such as nitrogen and carbon transport during hardening processes and many more.

Background
Besides experimental knowledge, largely based on the experiences of the hardening manufacturers, relatively little is known on the fundamentals of nitrogen and carbon diffusion in polycrystalline metals. Whereas solubility and diffusion coefficients of carbon and nitrogen in an ideal metal lattice are well-known, interactions with defects such as vacancies, grain boundaries etc are often neglected. Consequently, theoretical models may fail to provide sufficient information that would help optimising a hardening process for a material.

The surface hardness value is increased by the transport of nitrogen and/or carbon into the material. Whereas the workpiece interior remains almost the same, a proper design of the hardness transition zone is vitally important. If the transition zone is too small, the material suffers from a so-called “egg-shell effect” (hard but brittle surface and soft interior). This leads to the loss of the hardened surface area during use and would require the expensive hardening process to be continuously redone. If the transition zone is too large, the entire material would be brittle, which drastically decreases lifetime of the workpiece.

The project will primarily involve atomistic modelling, although there will be the opportunity to carry out experimental work for model verification if desired. The candidate will join a large dynamic Steel Processing group within WMG that currently comprises 5 academic staff and around 10 research fellows / visiting scientist and 20 PhD students.

Eligibility:
The ideal candidate should have an interest in steel-related topics and modelling. They should be willing to work both individually and as part of a team. The candidate should also be self-motivated and possess sufficient programming skills.

Previous knowledge of atomistic simulation techniques is preferred, although not strictly required.

For funding requirements, applications will only be accepted from UK/EU residents.

Application: Applicants with a degree in any of the physical sciences (chemistry, physics, engineering, materials and mathematics) are encouraged to contact Dr. Michael Auinger (m.auinger@warwick.ac.uk) for further information on the project. For applications, please complete our online enquiry form.