Project title: Kinetic Blockages in the Steam-Iron Reaction using Bragg Coherent X-ray Imaging

UCL Lead department: London Centre for Nanotechnology

Lead Supervisor: Ian Robinson

Project Summary: This PhD project will use Bragg coherent diffraction imaging (BCDI) to investigate diffusion barriers forming during the hydrogen gas reduction of small crystals of hematite and magnetite undergoing the "Steam-Iron" reaction. Hydrogen is generated by oxidizing iron with steam at high temperatures, reversibly converting oxides to iron for safe storage of its chemical energy. We will use the strain sensitivity of BCDI to obtain 3D images of strain in situ during the reaction.

You will be supervised by Professor Ian Robinson in the London Centre for Nanotechnology. Your project will start by examining how the structure of nanometre-sized crystals of hematite (Fe_2O_3) and magnetite (Fe_3O_4) change in response to hydrogen gas exposure, or water for the reverse reaction. It is known that both directions of the reaction show kinetic blockages in the reaction rate, attributed to the formation of defects of unknown nature.

Impact: By understanding the role of crystal defects in the reaction rate and cycling stability of the reaction, the interconversion of iron oxides and iron metal by hydrogen and gaseous water, we can design better storage materials. We will address two overlapping environmental planet-care goals, hydrogen storage and carbon-free steelmaking, achieving either of which will significantly reduce global CO_2 emissions.

Who we are looking for: This project suits a talented and ambitious student with an interest in experimental condensed matter and materials physics. You will be trained in coherent X-ray diffraction imaging of nanocrystalline materials and will interact with the doctoral training cohort at UCL. You will use and help develop software, including Machine Learning methods, for the analysis of BCDI data. You will learn to use national central facilities, such as the Diamond Light Source, where there are also opportunities for training placements. You will publish your work and present it at conferences.

References:

"Coherent Diffraction Imaging of Strains on the Nanoscale" Nature Materials (2009)
DOI: 10.1038/nmat2400
"Anisotropy of Antiferromagnetic Domains in a Spin-orbit Mott Insulator" PRB (2023)
DOI: 10.1103/PhysRevB.108.L020403