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Multi-scale investigation of dislocation-assisted carbon migration in ferrite

Tigany Zarrouk

SPEAKER / LEAD AUTHOR:
Tigany Zarrouk

INSTITUTION:
King's College London

ABSTRACT:
Martensitic bearing steels undergo subsurface microstructural decay, forming Dark Etching Regions, which promote failure through rolling contact fatigue.

Dislocation-assisted carbon migration is thought to be the underlying mechanism, yet empirical studies have been inconclusive as to how dislocations move carbon and where excess carbon from martensite migrates to upon transformation to ferrite. We detail a multi-scale modelling approach to elucidate carbon transport by dislocations.

Quantum-mechanical tight-binding simulations found that carbon stabilises the 1/2<111> hard screw dislocation core in agreement with ab-initio calculations. Equilibrium carbon concentrations, estimated from solute-dislocation interaction energies, suggest all dislocations are pinned in this hard-core configuration, under typical conditions. A dislocation line tension model found kink-pair formation enthalpies to decrease with both carbon content and stress. Kinetic Monte Carlo simulations incorporating solute diffusion will complete the multi-scale description, showing potential mechanisms for dislocation-assisted carbon migration.