

# Multi-scale investigation of dislocation mediated carbon migration in iron

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\*Abstract\*

We investigate the validity of a dislocation-assisted carbon migration mechanism underpinning the formation of dark etching regions in bearing steels undergoing high-cycle fatigue through use of a multi-scale approach: from quantum mechanics, to stochastic simulations. We start from tight binding simulations of  $1/3\langle 111 \rangle$  screw dislocations to obtain

the 2-d Peierls potential and Fe-C binding energies. These become ingredients for a line-tension model of the  $1/3\langle 111 \rangle$  screw dislocation to obtain the kink-pair formation energy as a function of stress and carbon concentration. Finally, 3-d kinetic Monte-Carlo simulations of dislocations in an environment of carbon are used to ascertain which temperature and stress regimes dislocation-assisted carbon migration is a valid mechanism.

### Bibliography

References