MULTI-SCALE INVESTIGATION OF DISLOCATION ASSISTED CARBON MIGRATION IN FERRITE

Tigany Zarrouk

tigany.zarrouk@kcl.ac.uk

Tony Paxton

tony.paxton@kcl.ac.uk

Sebastián Echeverri Restrepo

sebastian.echeverri.restrepo@skf.com

23.02.2021

SKF®

Materials Processing Institute

KING'S College LONDON

INTRODUCTION

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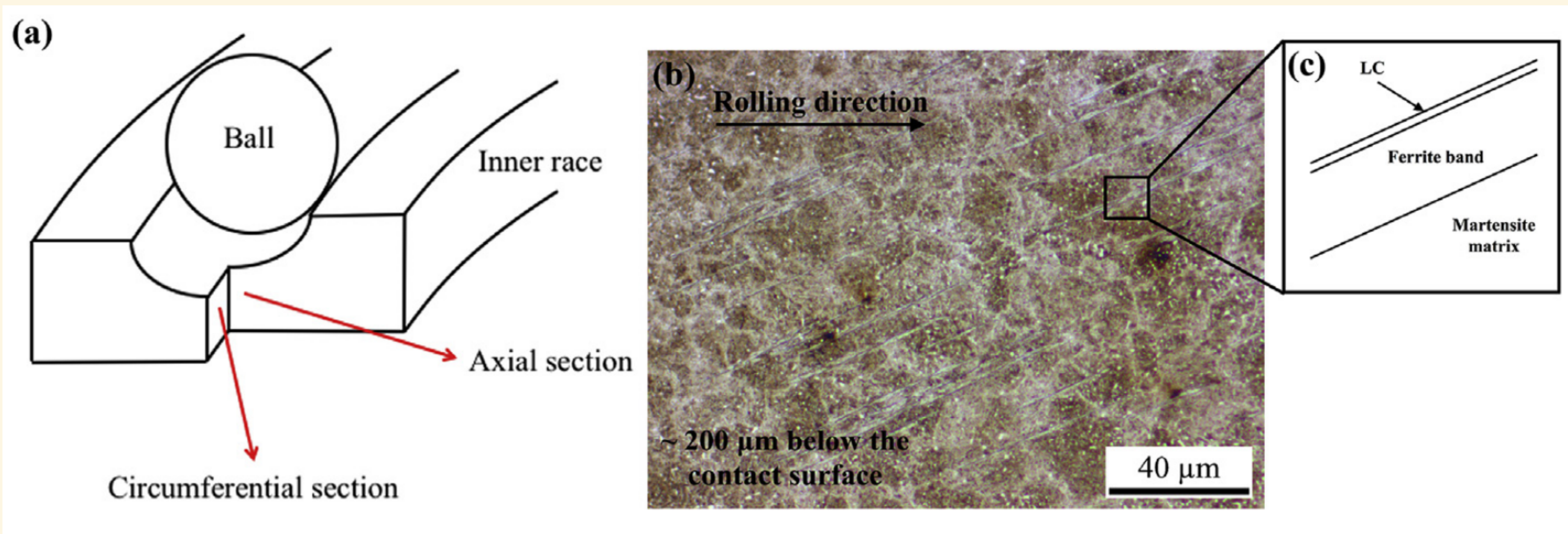
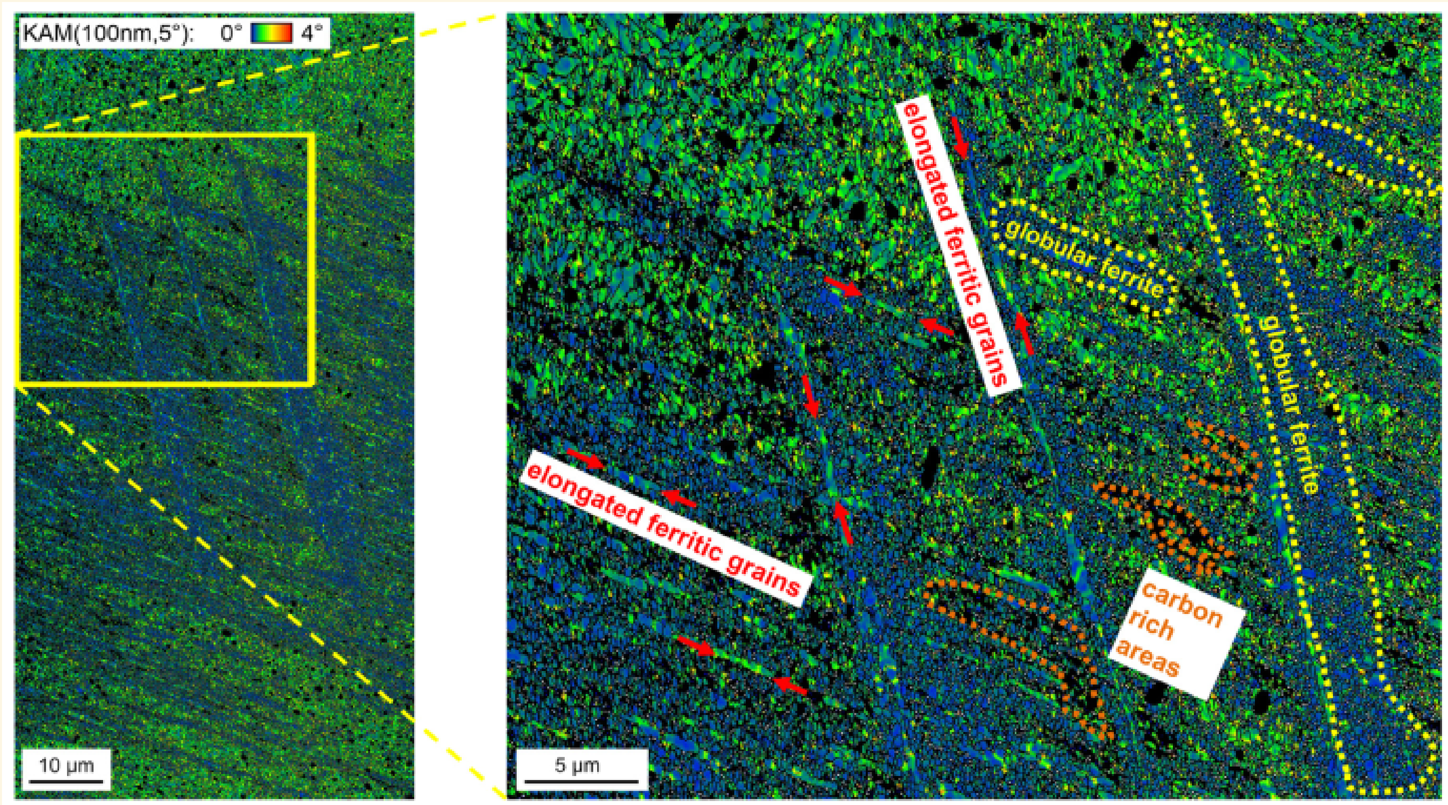
- Rolling contact on bearing raceways causes *degradation in subsurface* microstructure.
- Plays role in Rolling Contact Fatigue (RCF).
- Degradation arises in form of *Dark Etching Regions* (DERs).
- DERs characterised by development of ferrite and carbide features with patches of unaltered martensitic matrix.



Circumferential section showing DER [Fu2017].

FEATURES OF DER

1. Martensite → ferrite microbands (from strain localisation).
2. Residual carbides gradually dissolve.
3. 30° and 80° ferrite features form: White Etching Bands (WEBs).
4. Lenticular carbides precipitate at ferrite band boundaries.
5. These carbides thicken during DER development; correlated with WEB growth.



EBSD Kernel Average Misorientation (KAM) map showing 30° & 80° WEBs and carbide features in circumferential section [Smelova2017].

UNANSWERED QUESTIONS

1. Where does excess carbon from the martensitic matrix find itself when the structure decays to low C solubility (0.02 wt%) ferrite?

2. How is carbon transported, given its low diffusivity in martensite/DER phases?

3. Do pre-existing carbides dissolve or thicken?

Dislocation-assisted carbon migration has been suggested as fundamental mechanism, but no proof/consensus.

DISLOCATION-ASSISTED CARBON MIGRATION

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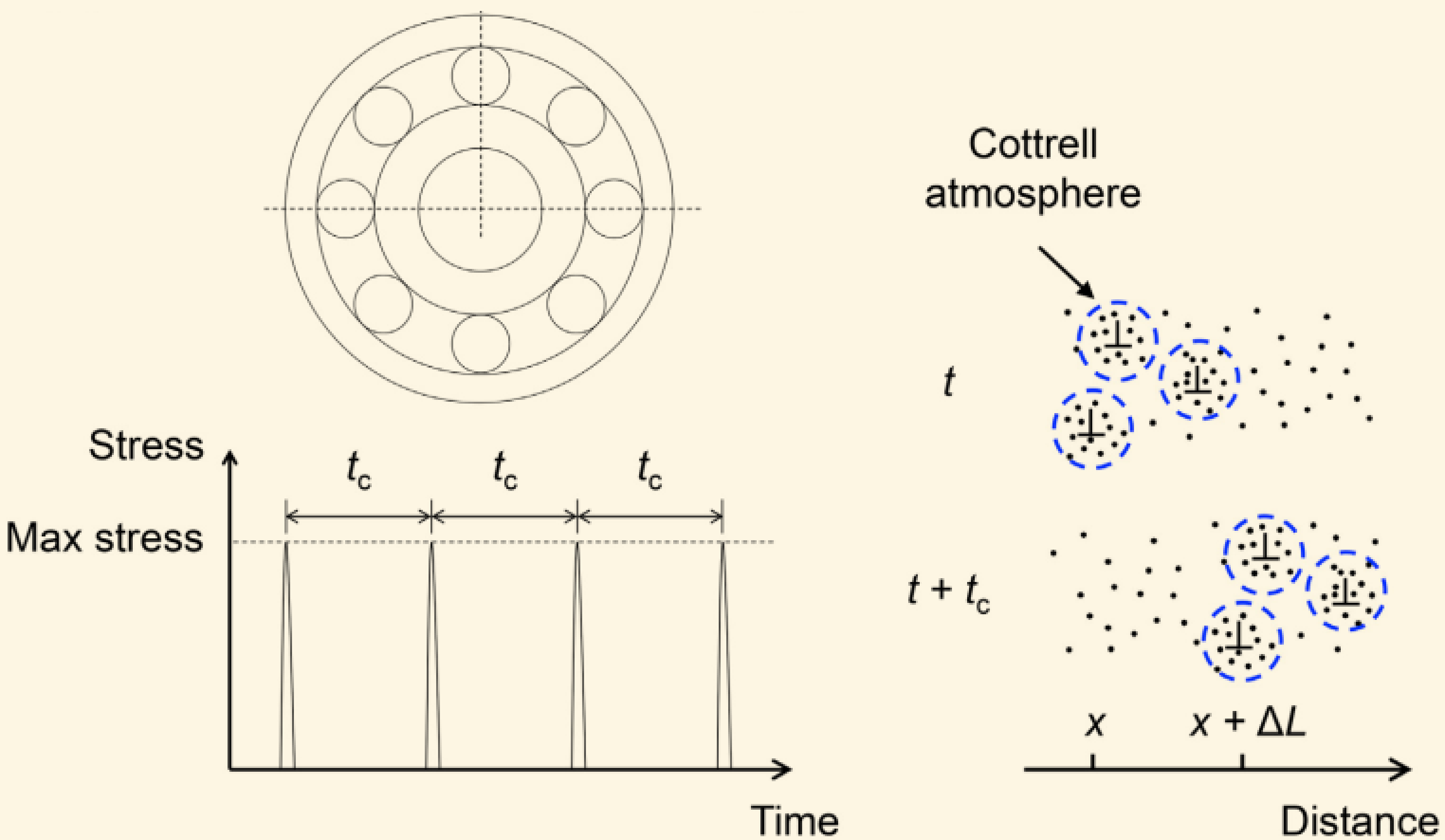


Cyclic stresses caused by bearing use causes dislocations to drag carbon [Fu2017].

- Carbon segregated to dislocations.
- Cyclic stresses cause dislocations to break away from carbon environment.
- Carbon re-attracted to dislocation, causing carbon flux.
- Modelling can find regimes of stress/temperature/carbon concentration/dislocation density in which this is feasible.

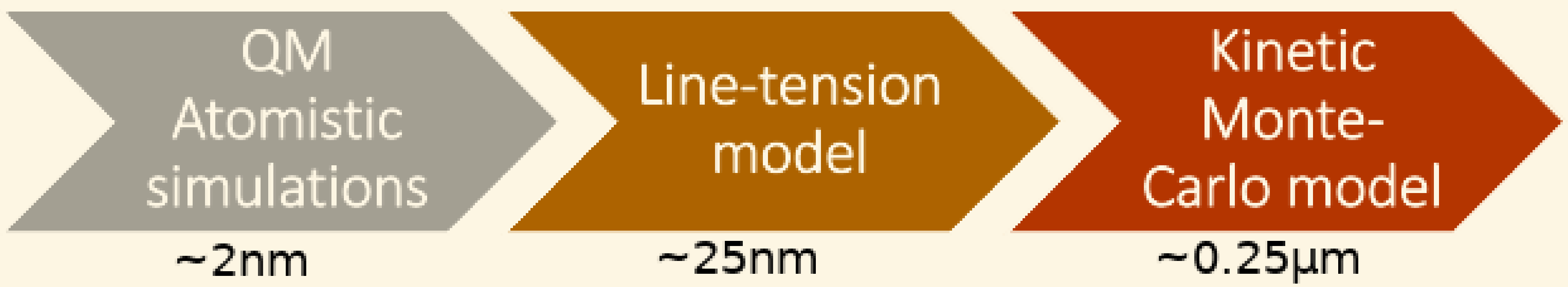
WHY IS IT PLAUSIBLE?

- Explains:
  - Martensite to ferrite transformation.
  - Carbon transport.
  - Lenticular carbide growth.
  - Pre-existing carbide dissolution.
- Can use multi-scale modelling to ascertain if mechanism of dislocation-assisted carbon migration is valid.

MULTI-SCALE MODELLING

METHODS

- Quantum-mechanical, atomistic (tight-binding/TB) simulations used to see how solutes interact with dislocations.
  - Tight-binding is more accurate than empirical potentials, with better scaling than DFT.
- Line tension model of dislocations used to ascertain how carbon interactions modify thermally-activated dislocation movement (kink-pair formation).
- SCkMC model to simulate dislocation dynamics and measure effects on dislocation velocity and loop debris in carbon environment. [Katzarov2017]



ATOMISTIC RESULTS

EASY AND HARD CORE SCREW DISLOCATIONS

- Two types of dislocation core found in bcc iron.
- Ground state dislocation core in pure iron is easy core.
- The hard core is a higher energy, unstable state.

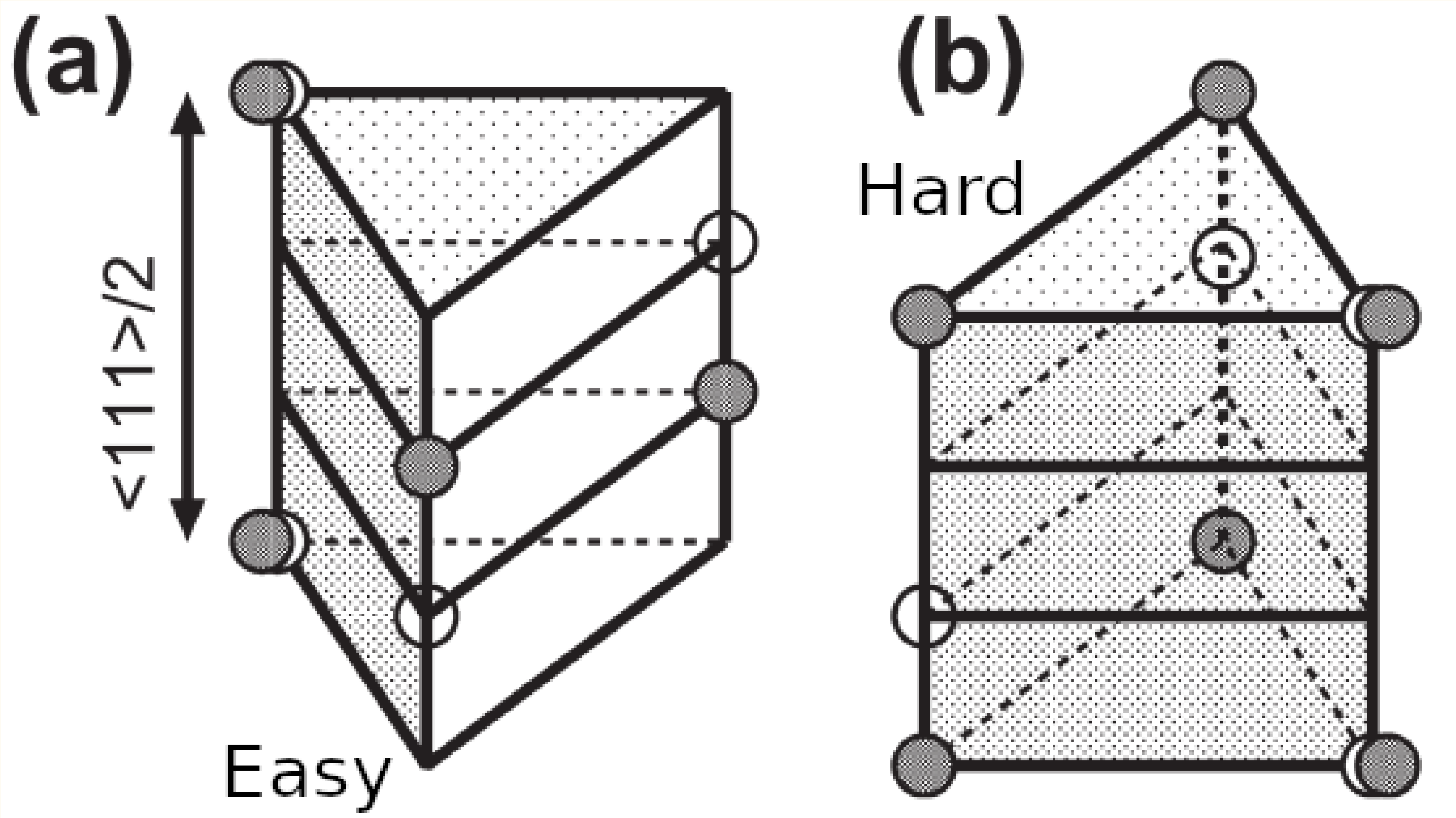
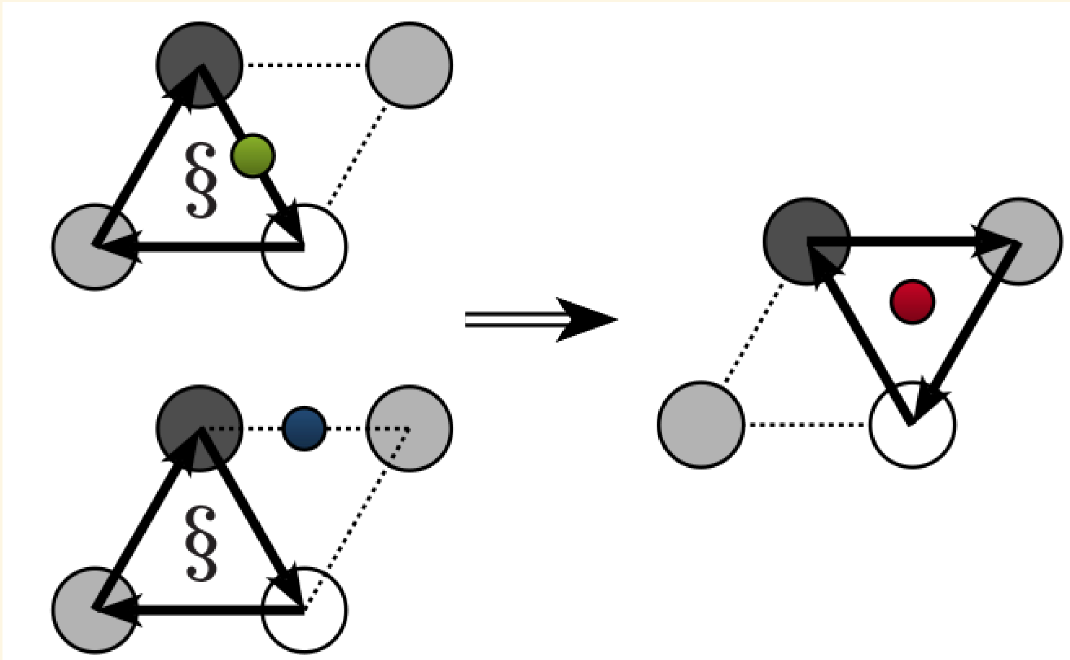


Diagram of displaced atoms (grey) compared to perfect lattice (white) for both easy (a) and hard (b) dislocation cores [Itakura2012].

CORE RECONSTRUCTION



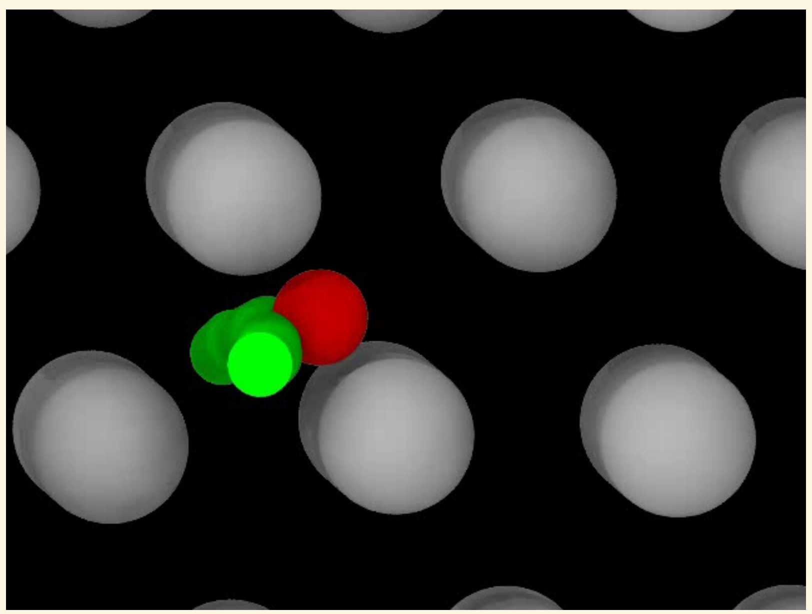
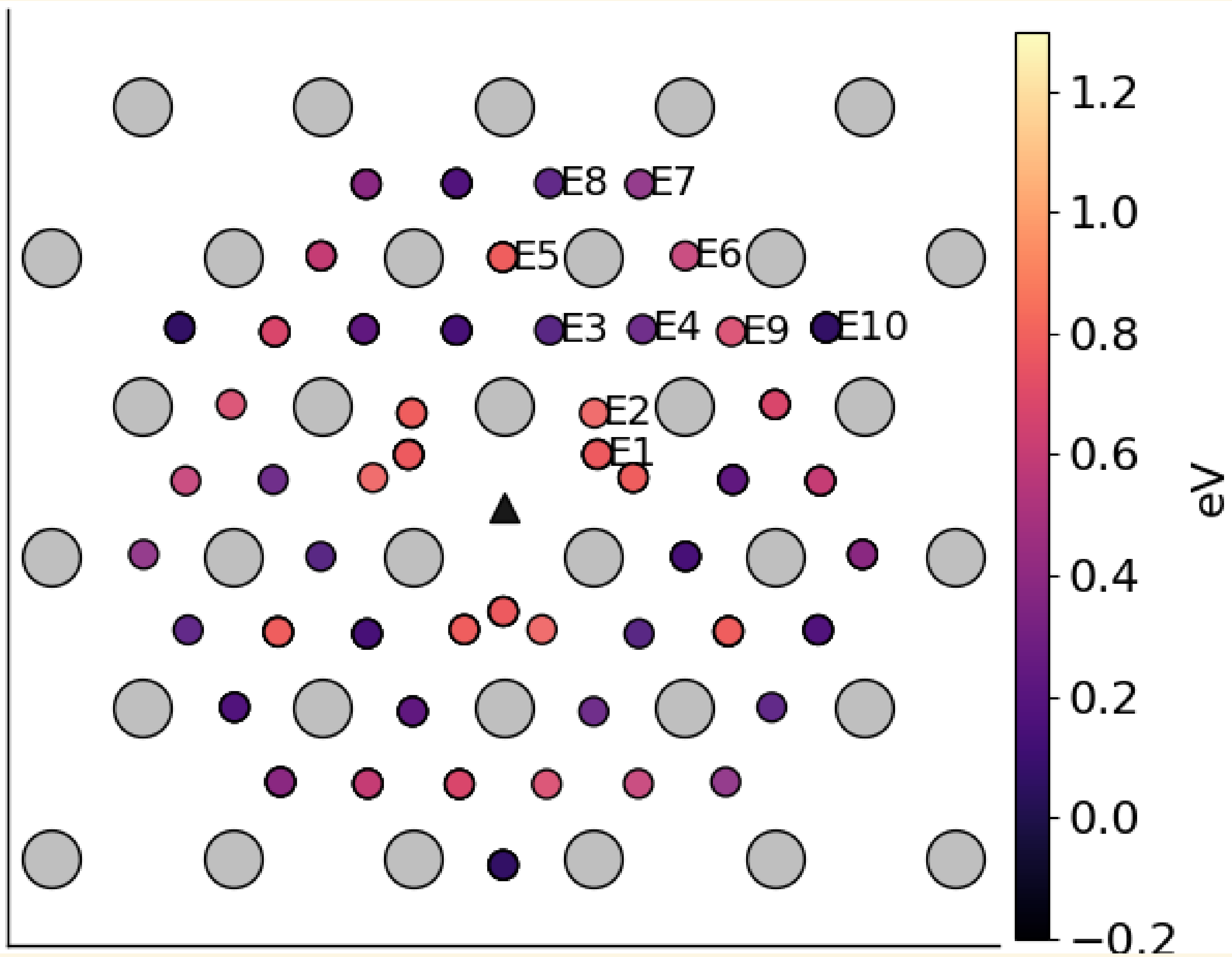


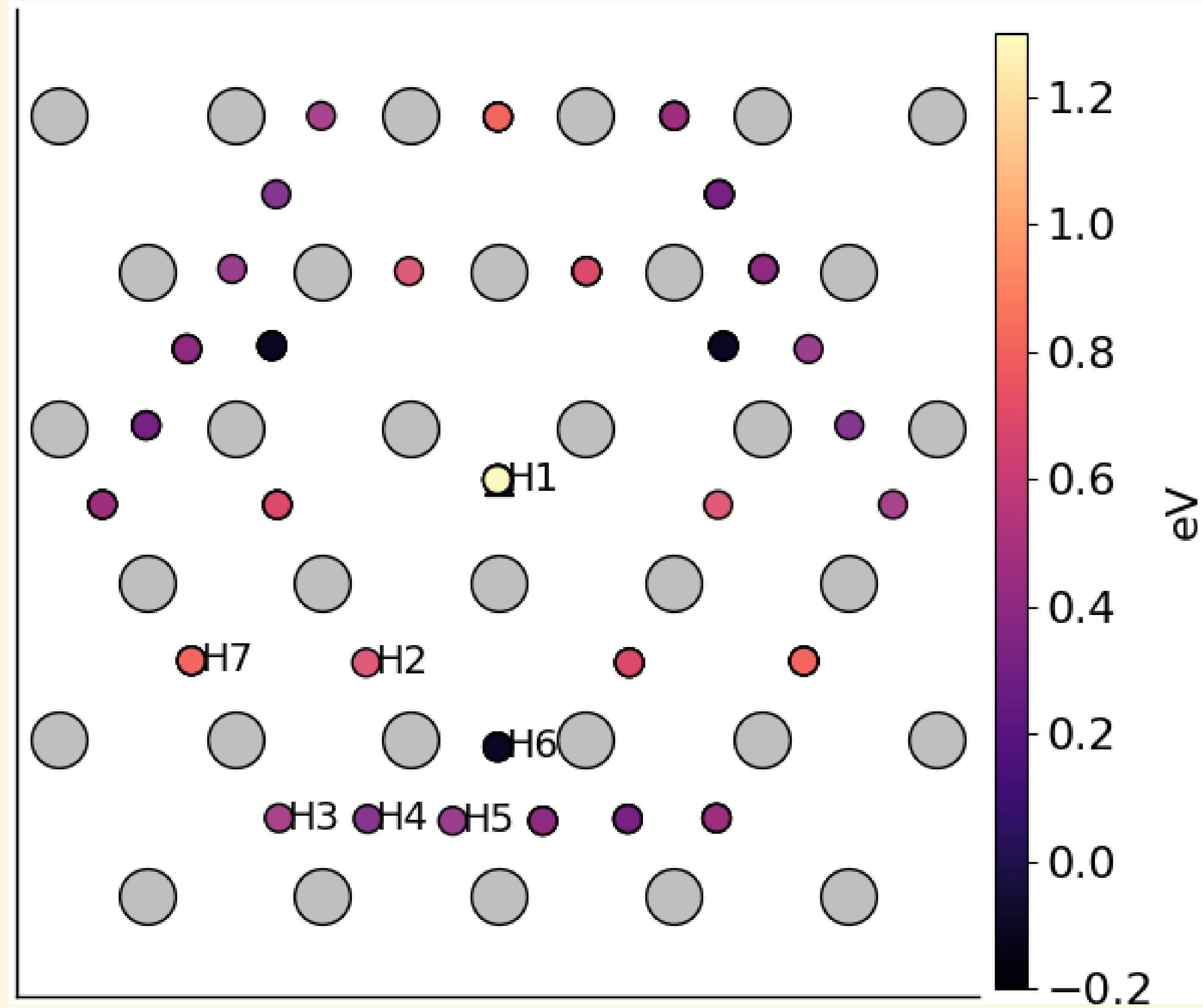
Diagram: C reconstruction of easy screw core § to hard [Ventelon2015]. Video: Tight-binding simulation of reconstruction.

- C transforms the easy screw core, the ground-state core structure in pure Fe, to hard core.
- *The hard screw core is the ground-state dislocation configuration when carbon is dissolved in ferrite.*
- Empirical potentials only predict core spreading, *no* spontaneous reconstruction to hard core.

BINDING OF C TO SCREW CORE



Carbon binding sites/energies around <u>easy core</u> dislocation in TB.



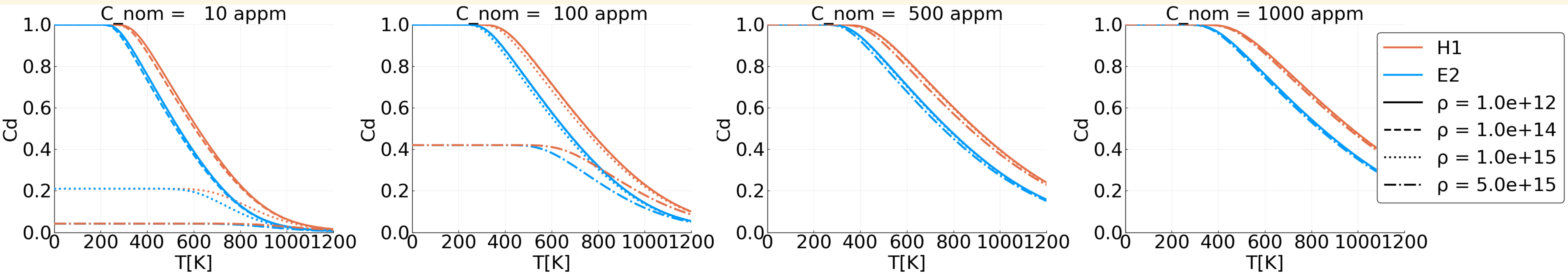
Carbon binding sites/energies around <u>hard core</u> dislocation in TB.

- Highest binding energy found inside hard core.
- Cores fixed in position, such that reconstruction does not occur.
- Binding to both cores important for further modelling.

CONCENTRATION ANALYSIS

CARBON CONCENTRATION ON DISLOCATION LINE

- We can calculate the carbon concentration on dislocation line, C_d, where carbon atoms are at equilibrium with the matrix.
- We link the nominal concentration of carbon atoms per iron atom C_{nom}, to the carbon concentration in the matrix, C_{bulk}.
- Included the effect of the C-C first-neighbour repulsive energy of carbon within hard-core prismatic site, with atomistics.
- Used dislocation densities up to maximum found in martensite.



C_nom = 10 appm
C_nom = 100 appm
C_nom = 500 appm
C_nom = 1000 appm
Cd
T[K]
H1
E2
ρ = 1.0e+12
ρ = 1.0e+14
ρ = 1.0e+15
ρ = 5.0e+15

WHAT DOES THIS TELL US?

- All dislocations are decorated with carbon around normal operating temperature (320° K), carbon concentrations and dislocation densities.
- We predict that all dislocations are reconstructed to the hard core in typical conditions, even in high-purity iron.
- How does carbon affect thermally-activated dislocation movement?

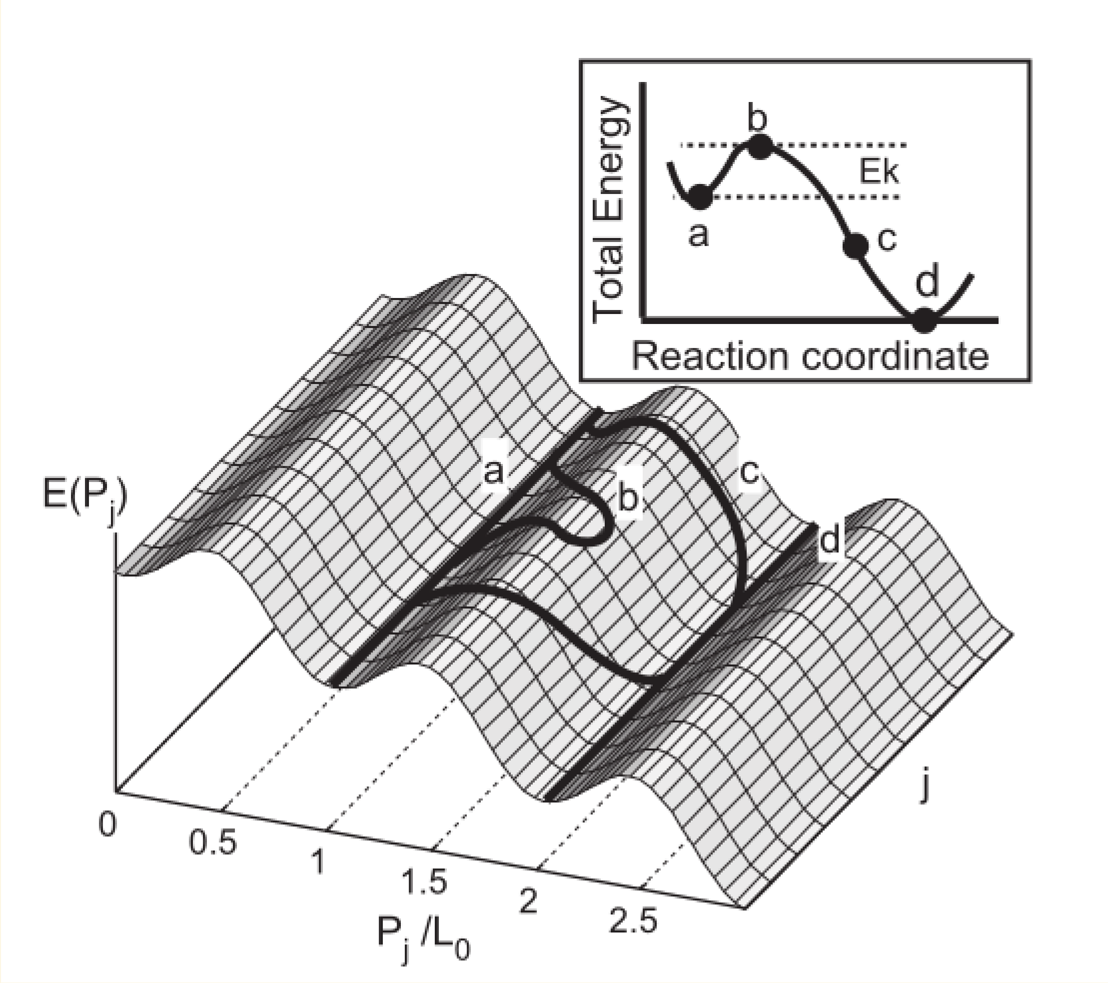
LINE-TENSION RESULTS

LINE-TENSION MODEL OF DISLOCATION

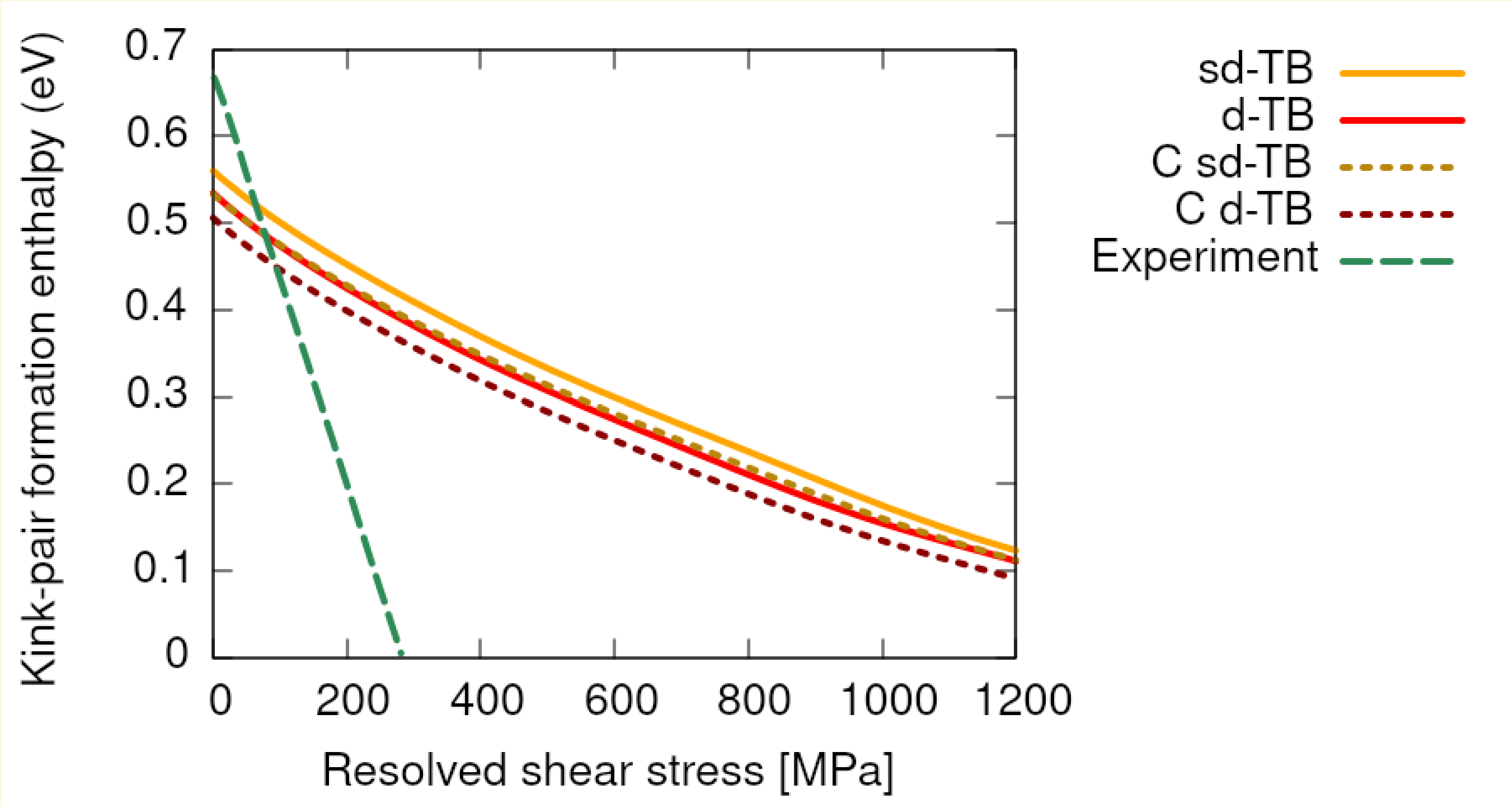
$$E_{\mathrm{LT}} = \underbrace{\underbrace{\frac{K}{2}\sum_j (\vec{P}_j - \vec{P}_{j+1})^2}_{\text{Spring term}} + \underbrace{\sum_j \Delta E_{\mathrm{P}}(\vec{P}_j)}_{\text{Peierls Potential}} - \underbrace{\sum_{j,k} E_{\mathrm{C}}(|\vec{P}_j - \vec{P}^{\mathrm{C}}_k|)}_{\text{C Interaction}}}_{\textbf{From Atomistics}} + (\sigma \cdot \vec{b}) \times \vec{l} \cdot \vec{P}_j$$

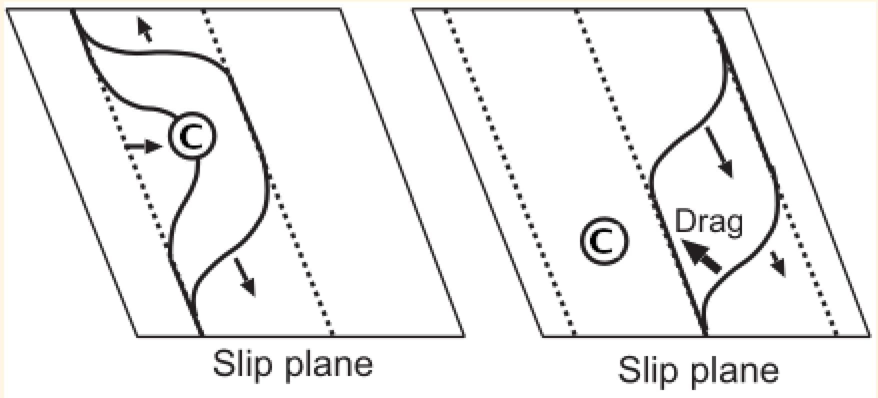
- We can obtain the kink-pair formation enthalpy as a function of stress, temperature and carbon concentration.
- All terms from atomistic data, apart from Peach-Kohler term.
- The interaction between solutes is parameterised with a lorentzian.

Figure: Kink-pair formation in Peierls landscape [Itakura2012].



KINK-PAIR FORMATION ENTHALPIES



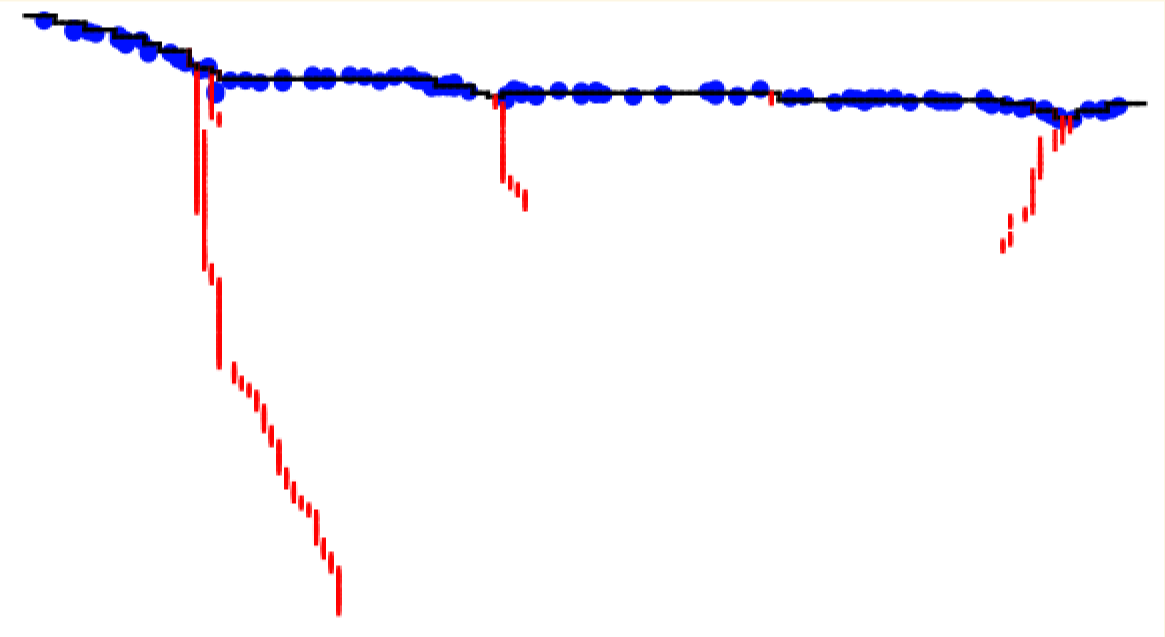


- Carbon decreases the kink-pair formation enthalpy, when the carbon is ahead of the dislocation.
- Carbon will reduce dislocation velocity, if behind.

SCKMC (FUTURE WORK)

SCKMC SIMULATIONS

- Kinetic Monte Carlo simulations incorporating carbon diffusion will complete the description of how carbon can move with dislocations.
- Dislocation moves through thermally-activated kink-pair formation.



- Figure of kMC work with hydrogen (blue), showing dislocation line (black) with generated debris loops (red) during movement of dislocation line [Katzarov2017b].

SUMMARY

- Dark Etching Regions are formed during Rolling Cycle Fatigue of bearing steels, but no consensus on mechanism.
- Multi-scale modelling can shed light on the validity of dislocation-assisted carbon migration.
- Atomistics finds the hard screw core to be ground-state due to carbon interaction.
- **All** dislocations are decorated with carbon, during martensite → ferrite transition, due to large binding energy of C.
- Therefore, initial assumption of ***dislocation-driven carbon migration*** is correct.
- Dislocations, even in high-purity iron, are pinned with carbon in a hard core configuration (up to 400° K).
- Line-tension model shows amount by which carbon decreases kink-pair formation enthalpy if ahead of dislocation. Drag if behind.
- Further work, through SCkMC model will ascertain regimes in which dislocation-assisted carbon migration is valid.

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