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Atomistic Simulation of Oxygen-Dislocation interaction in Ti alloys. Tigany Zarrouk King's College London

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Introduction?

columns 0.4 * Main question

- How does oxygen play a role in solution hardening in Ti alloys? - Dislocations are defects that have an atomistic origin. They are line defects. - How does atomic oxygen interfere with dislocations which in turn changes how the plasticity of titanium as a whole? - Screw dislocations are the most important as they have the least mobility in hcp.

0.6 * Method

- Need quantum mechanical method such that we can describe the directionality of the bonding sufficiently and obtain accurate forces in the core of the dislocation (which determines how the dislocation moves). - Also this means that the energy orderng of the polymorphs of Ti are reproduced. - Use TB as quicker than DFT - Can simulate extended defects due to larger cells, thus mitigating finite size effects of simulation due to insufficent relaxation of the dislocation core. - Built model with optimisation algorithm 4cm [targetoffsetx=-9cm, targetoffsety=-6.5cm, width=0.5] e-mail tigany.zarrouk@kcl.ac.uk