

## Discovering atomic scale mechanisms of stress corrosion cracking in aerospace titanium alloys.

Tigany Zarrouk<sup>1</sup>

<sup>1</sup>Department of Physics  
King's College London

<sup>2</sup>Rolls-Royce plc.

R-R Ti Fundamentals Review, 24 October 2018



# Overview

1 Motivation

2 Quantum Methods

3 Titanium Model

4 Future Work

5 Summary

# Table of Contents

## 1 Motivation

# Motivation

- Titanium alloys are used in highly demanding circumstances.
- Brittle oxide layer can crack.
- Solutes affect dislocation mobility and hardening.
- Interactions between oxygen and dislocation cores are not clear.
- Need for atomistic modelling.

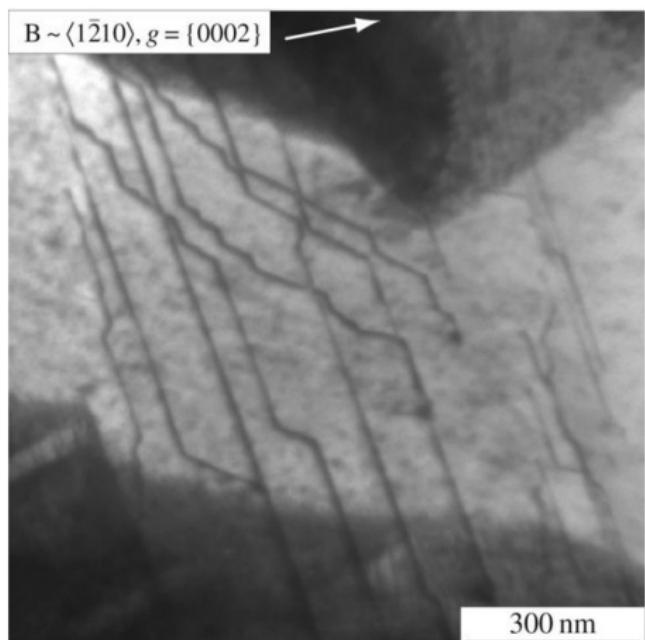


Figure: Dislocations in Ti-6246  
[Chapman, Dye and Rugg, 2017]

# Motivation

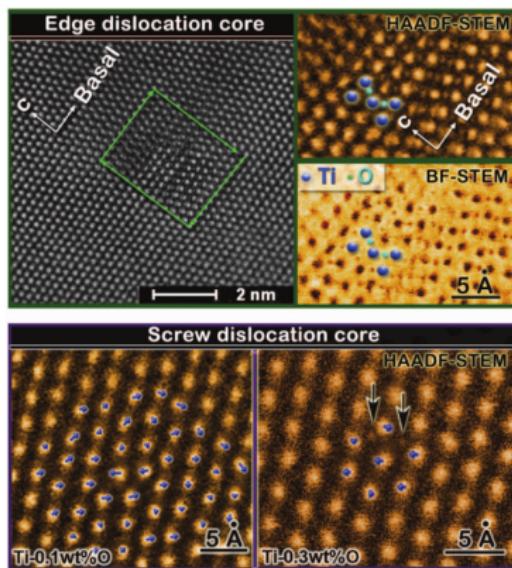


Figure: Dislocation cores in Ti with oxygen [Yu, Qi *et al.*, 2015]

- Core controls properties such as:
  - Selection of glide planes
  - Cross-slip
  - Mobility
- Core of dislocation has non-linear stresses.
- Core spreading causes loss of ductility.

# Table of Contents

## 2 Quantum Methods

# Quantum Methods

- Density Functional Theory is not feasible for molecular dynamics.
- System size is limited due to cost of computation ( $\sim 1000$  atoms max).
- Boundaries of a smaller cell affect relaxation of core.
- Problems in convergence lead to inexact calculation of forces.

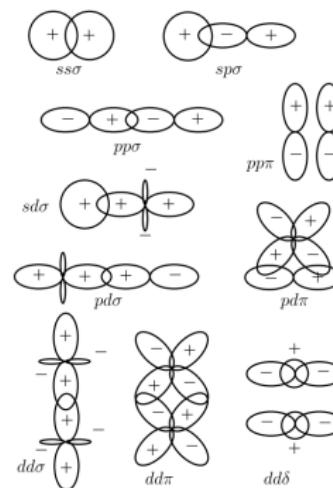
# Quantum Methods

Method	QM Accuracy	Comp. Cost	$N_{\max}$ atoms
DFT	Most accurate	$\mathcal{O}(N^3)$	$\sim 10^3$
TB	Accurate	$\mathcal{O}(N^3)$	$\sim 10^4$
BOP	Approximate	$\mathcal{O}(N)$	$\sim 10^5$
Interatomic Pot.	$\sim$ Classical	$\mathcal{O}(N)$	$\sim 10^6$

Figure: Comparison of methods for atomistic simulation.

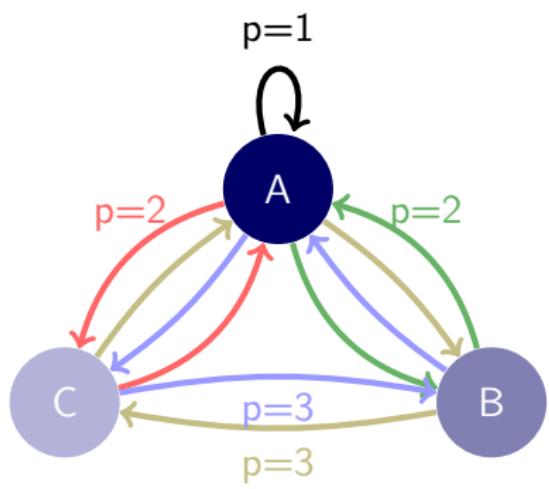
# Tight Binding

- Tight binding (TB) is a QM method; where bond integrals between atomic orbitals are parameters.
- Parameters can be fitted to reproduce experimental data.



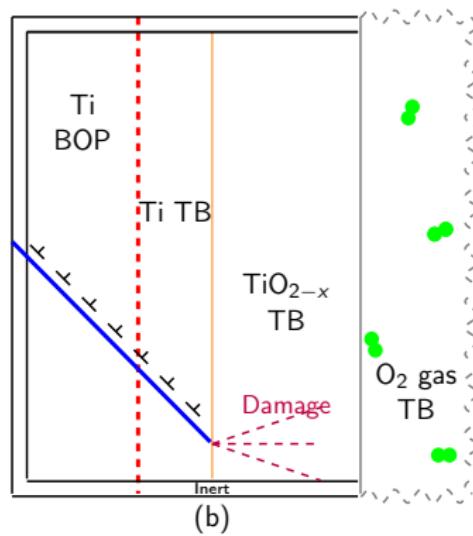
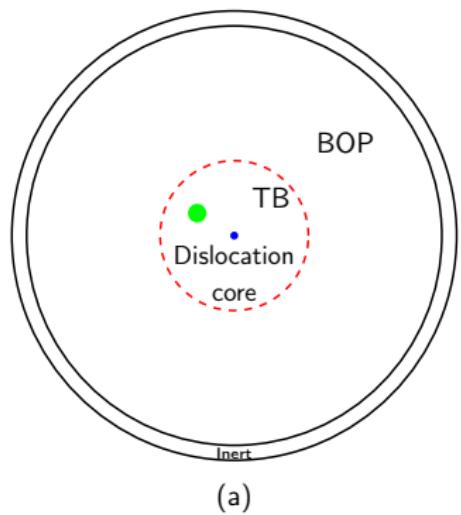
## Bond Order Potentials

The bond order potentials (BOP) method is a faster, but less accurate, method for calculation of interatomic forces within tight binding.



- Density of states is constructed from a number of moments, giving electronic structure information.
- "Intelligent" potential, as considers local environment of atoms, and knows how electrons move.
- Better scaling than TB ( $\sim \mathcal{O}(N)$  to  $\sim \mathcal{O}(N^3)$ )

## Embedding of TB and BOP



(a) Oxygen interaction with dislocation core. (b) Dislocation pile-up at  $\text{Ti}/\text{TiO}_{2-x}$  interface with partial pressure O<sub>2</sub> environment.

# Table of Contents

## 3 Titanium Model

## Parameter Fitting

Used a global fitting scheme (genetic algorithm) to find parameters

- Bond integrals and pair potential fitted such that empirical quantities are reproduced, such as the:
  - elastic constants
  - equilibrium lattice parameters:  $a$  and  $c$ .
  - bulk modulus
  - correct energetic ordering of polymorphs.
- Thus a simple model of Ti with only 5 parameters captures the physics.

# Comparison of Ti TB and BOP with experiment

Fit Quantities	DD	BOP	exp.
$a_{\text{hcp}}$	5.51	5.48	5.58
$c_{\text{hcp}}$	8.80	8.84	8.85
$a_{\text{omega}}$	8.66	8.96	8.74
$c_{\text{omega}}$	5.35	5.51	5.32
$u_{\text{omega}}$	0.98	0.90	1.00
$C_{11}$	184.2	179.1	176.1
$C_{12}$	63.0	63.0	86.8
$C_{13}$	67.6	72.7	68.2
$C_{33}$	190.9	178.8	190.5
$C_{44}$	53.1	44.4	50.8
Bulk Modulus	108.5	106.0	110.0

Figure: Fit quantities in TB and BOP. DD refers to the direct diagonalisation of the TB hamiltonian.  $a_*$  and  $c_*$  are in bohr. The elastic constants are in GPa.

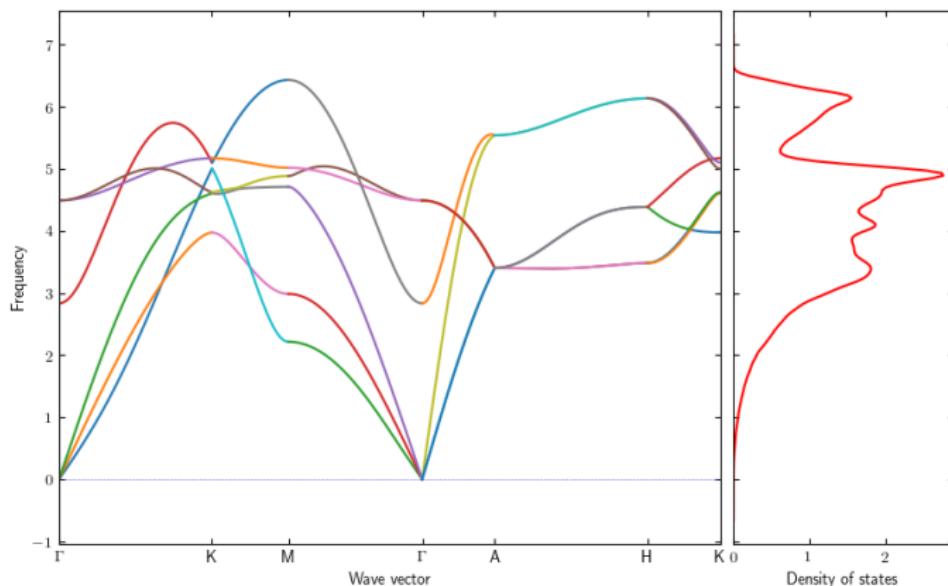


Figure: Phonon bands for hcp phase in TB.

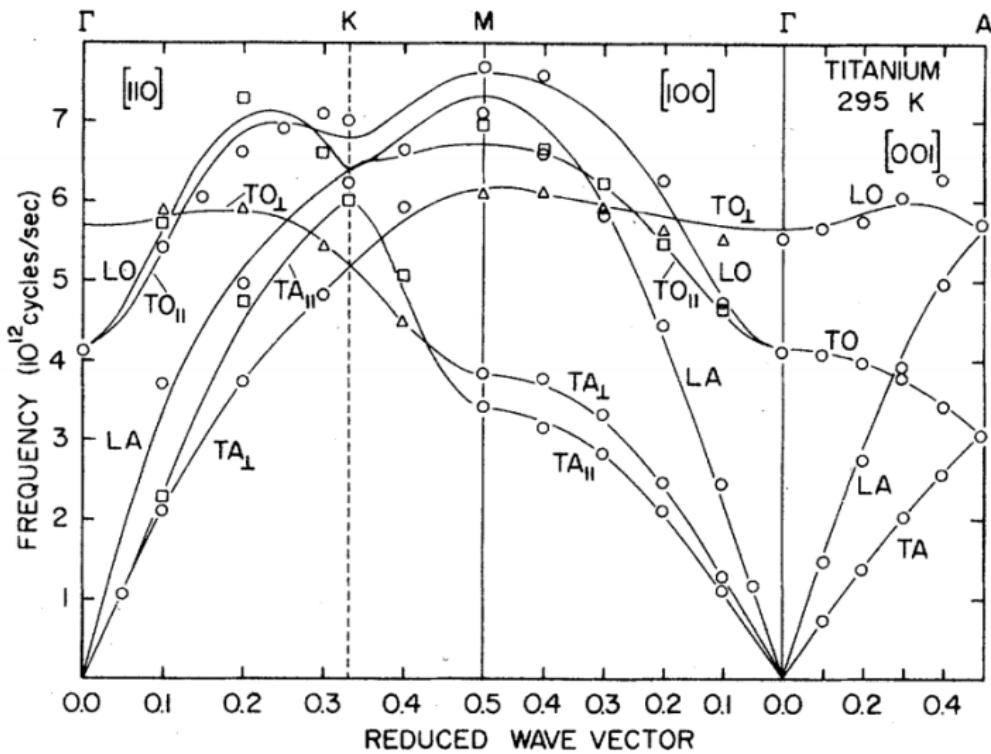


Figure: Phonon bands of hcp Ti from experiment. [C. Stassis, et al. 1979]

## Other computational structures.

- New Ti model integrated with previous TB TiO<sub>2</sub> model.
- Compatible with water on interface.
- Additional parameters fitted for oxygen and nitrogen, for air mixtures.
- Ti-H parameters also added.

# Table of Contents

## 4 Future Work

## Future Work

- Embed TB in BOP region and investigate O interaction with dislocation.
- Obtain peierls barrier as a function of O.
- Investigate double kink migration with and without O.
- Simulate titanium/titania interface.
- Add alloying elements (e.g. vanadium and aluminium).

# Supercell of Ti with prismatic dislocation.

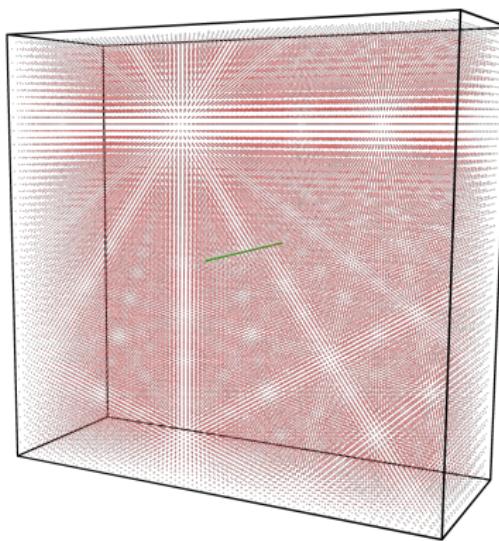


Figure: Supercell of Ti with  $\mathbf{b} = \frac{1}{3}[11\bar{2}0]$  prismatic screw dislocation.

## Supercell of Ti and H<sub>2</sub>O

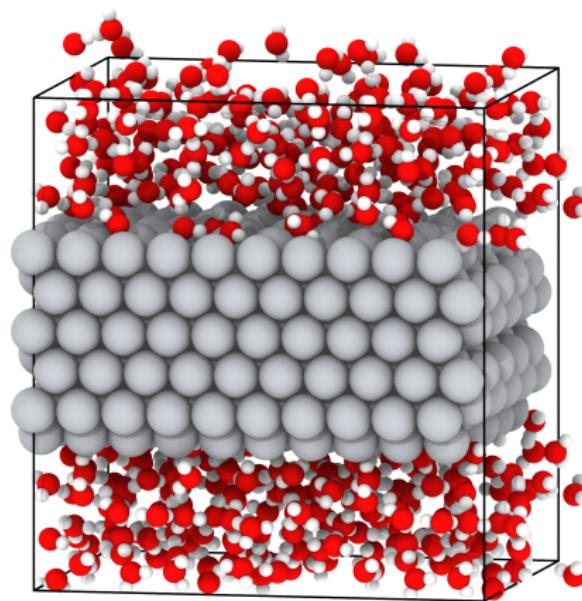


Figure: Supercell of Ti and H<sub>2</sub>O.

## Supercell of Ti and air.

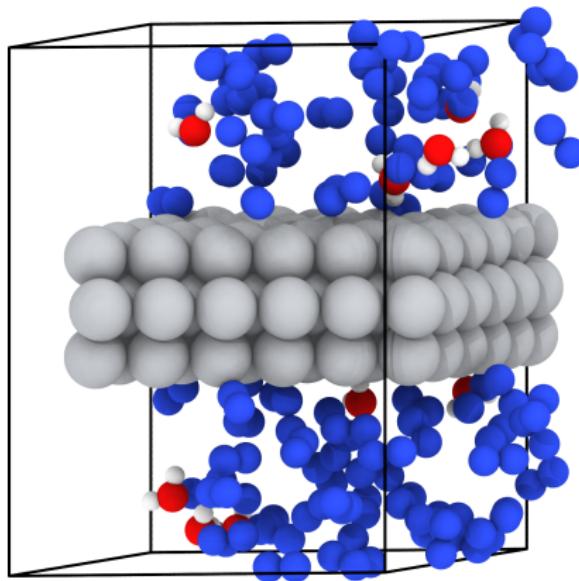


Figure: Supercell of Ti, N<sub>2</sub> and water for simulation of air.

# Table of Contents

## 5 Summary

## Summary

- Described embedding models combining TB and BOP, which has sufficient scaling for elucidation of dislocation kinematics.
- These models allow for atomistic simulation of dislocation interaction with interstitials and interfaces in Ti.
- Simulation of oxygen-dislocation interactions will provide insight into how oxygen affects dislocation core structures, which modify plasticity.
- This will shed light on mechanisms behind stress corrosion cracking.
- Can investigate other related areas, such as water/high pressure steam on Ti interface and H/N/O diffusion.

Thank you for listening.