Elasto-plastic evolution of single crystals driven by dislocation flow

Tom Hudson & Filip Rindler (Warwick)

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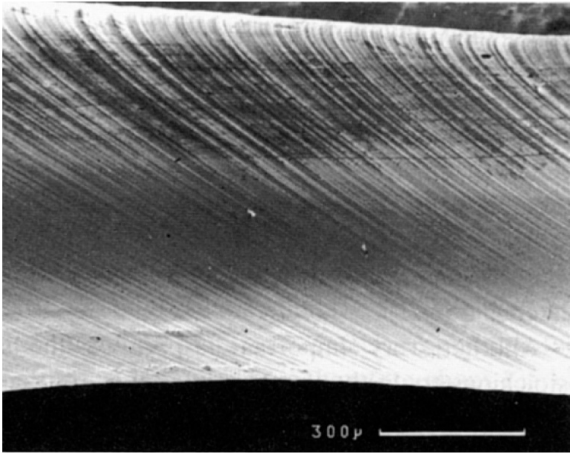
Crystal plasticity and dislocations

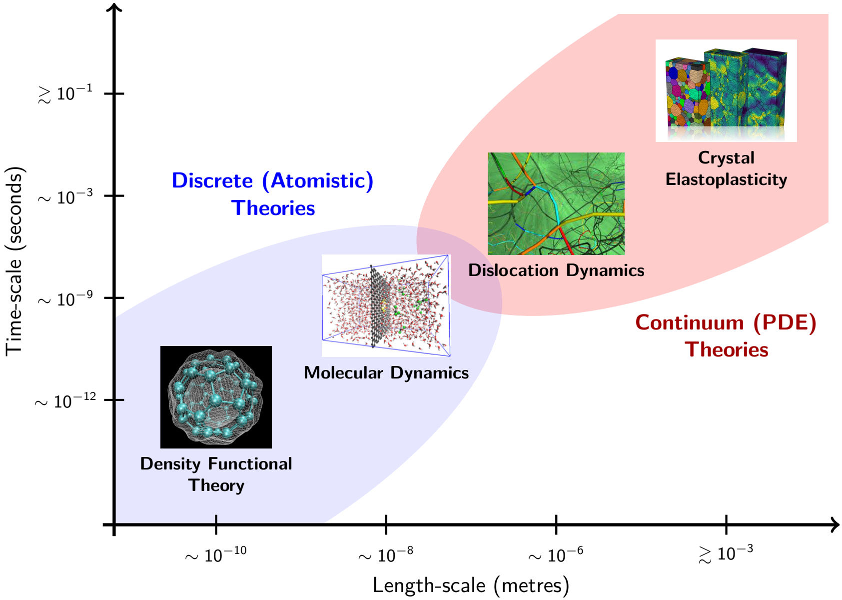
Crystal Plasticity = **'slip'** of crystallographic planes.

Orowan/Polanyi/Taylor '34: Slip propagates by motion of **dislocations**.



http://www.doitpoms.ac.uk/tlplib/miller_indices/uses.php

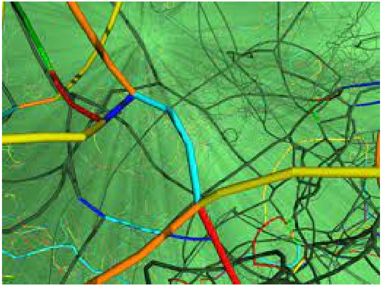
Dislocation modelling approaches



Dislocation Dynamics

Advantages:

- Discretise only dislocations: better **numerical** complexity.
- Allows mechanism identification: better **human** complexity.
- Acts as a **bridge** between discrete and continuum.



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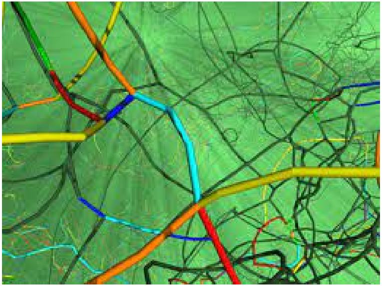

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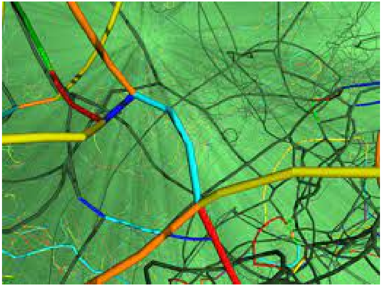

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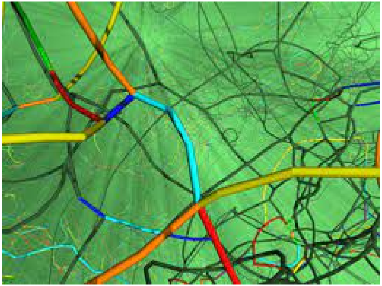

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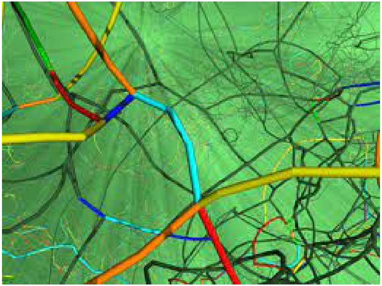

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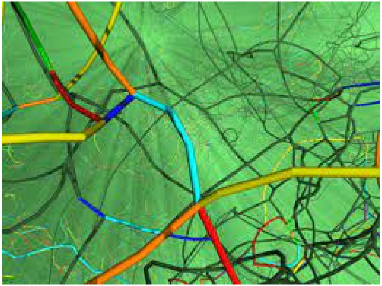

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This talk: Towards a formulation resolving Problem 1.

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- **Deformation gradient:** $\nabla y(t,x) \in \mathbb{R}^{3\times 3}$.
- **Plastic distortion:** $P(t,x) \in \mathcal{L}(T_x\Omega; S_x\Omega) \simeq \mathbb{R}^{3\times 3}$.
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Or, equivalently:

- Crystal 'scaffold': $Q(t,x) = P^{-1}(t,x)$.
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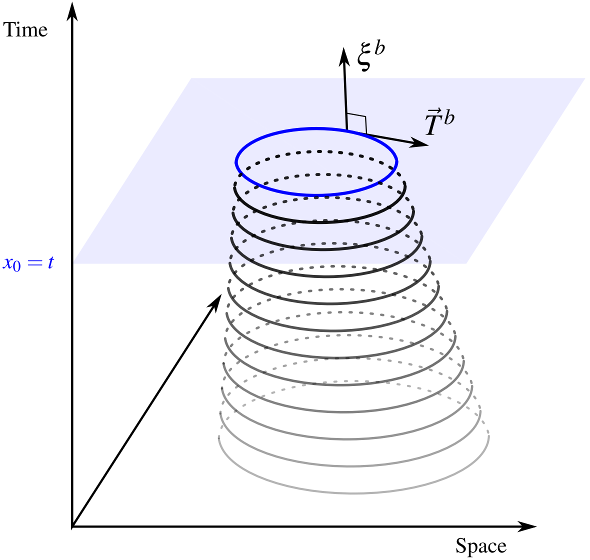
In particular, want something like

$$\frac{d}{dt} P(t) = D\left(T^b(t), \frac{d}{dt} T^b(t) \right).$$

However: $\frac{d}{dt} T^b$ is a time-derivative of a current and should depend in a coupled way on the stress, so is a nasty object!

Dislocation velocities and slicing

- Treat trajectories as 2-currents in 4-dimensional space-time.



Geometric slip rate

We argue that the rate of plastic distortion should be written as

$$\frac{d}{dt}P = \sum_b b \otimes g^b \in \mathcal{L}(T_x\Omega, S_x\Omega)$$

where the **geometric slip rate** g^b is of the form

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- γ^b is the equivalent two-vector slip rate at (t, x).

Energetic considerations

$E = \nabla y\, P^{-1}$, so assuming hyperelasticity, internal energy is:

$$\mathcal{W}_e(y, P) = \int_\Omega W_e(E)dx = \int_\Omega W_e(\nabla y\, P^{-1})dx$$

Rate of doing internal work is

$$\mathcal{I}(\Omega) = \int_\Omega \frac{d}{dt} W_e(\nabla y\, P^{-1}) + \sum_b X^b \cdot g^b\, dx.$$

Differentiating in time, we find that

$$\frac{d}{dt} W_e(\nabla y\, P^{-1}) = T : \nabla \dot{y} - M : L$$

where

- T is the **Piola-Kirchoff stress**, $T = DW_e(\nabla y\, P^{-1})P^{-T}$,
- M is the **Mandel stress**, $M = P^{-T} \nabla y^T DW_e(\nabla y\, P^{-1})$, and
- L is the **structural plastic flow rate**, $L = \dot{P} P^{-1} = -Q^{-1} \dot{Q}$.

Energetic considerations

By standard arguments, we can deduce:

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To close the system, we propose a **flow rule** of the form

$$PX^b \in \partial R^b (P^{-T} g^b),$$

where:

- R^b is a positive, convex dissipation potential, and
- g^b is the geometric slip rate.

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  $$X^b \cdot g^b = (P^{-1} M^T b) \cdot g^b \approx -v^b \cdot \Big((\mathbb{C}\beta_e) b \times \vec{T}^b \Big).$$

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- Plastic incompressibility arises in a natural way:

$$\frac{d}{dt} \log \det(Q) = \mathrm{tr}(Q^{-1} \dot{Q}) = -\mathrm{tr}(LQ) = -\mathrm{tr}\Big(\sum_b Qb \otimes g^b \Big),$$

  so $\det(Q) = \det(P) = 1$ for all time if Qb is orthogonal to g^b, i.e. only glide motion is allowed.

Conclusions and outlook

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Ongoing and future work:

- A study of Frank-Read sources.
- Further investigation of constitutive relations, linearisation and numerical methods.
- Homogenisation?

Reference: TH, Filip Rindler, Math. Model. Appl. Sci. 2022, 32(5) pp 851–910.