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Motivation And Challenges
Crystalline plasticity is strongly governed by dislocation motion and their interaction with other dislocations, solutes and precipitates.

Challenges in modelling dislocations:
- Physics across disparate length scales from significant electronic-structure perturbations at the dislocation core to long-range elastic fields at macro-scale.
- Limitations of plane-wave based electronic-structure methods in quantifying the core energetics of isolated dislocations whose geometry is not periodic.

Real Space Formulation of Orbital-Free DFT
Orbital-Free Density Functional Theory (OFDFT) is a linear scaling model for electronic structure calculations. The ground state energy of a collection of atoms (located at $R = (R_1, R_2)$) is obtained by minimizing a functional of electron density ($\rho$):

$$E_{\rho}(R) = T(\rho) + E_F(\rho) + J(\rho),$$

subject to the constraint $\int \rho = N$, where $N_{\text{elec}}$ is the number of electrons. $T(\rho)$ is the kinetic energy of non-interacting electrons, which under the WGC[5] approximation, is given by

$$E_{\rho}(R) = \min \left\{ \int \psi^2 + \frac{1}{2} \int \psi \nabla \psi \right\},$$

where $\psi(x) = \sum \phi_k(x - k)$. Finally, the non-local component of $T(\rho)$ is formulated locally through introduction of auxiliary kernel potentials $u_{\alpha}(x)$:

$$T(\rho) = \min \left\{ \int \left( \frac{1}{2} \nabla u_{\alpha} \cdot \nabla u_{\beta} + \frac{1}{2} \int \frac{u_{\alpha}(x) u_{\beta}(y) - u_{\alpha}(x) u_{\beta}(y)}{|x-y|} \right) \right\},$$

Configurational forces (atomic and cell relaxations) given by the Gâteaux derivative of the ground state energy, $E(\psi|\Omega, (\Omega'))$ with respect to the perturbations of the underlying space $\Omega$.

Dirichlet Boundary Conditions
- Mixed boundary conditions: Periodic along $\Omega$ (dislocation line)
- Dirichlet along 2 and 3
- Cauchy-Born hypothesis used to compute electronic fields on Dirichlet boundary
- The local real-space formulation and Finite Element basis are key to consider such boundary conditions.

Acknowledgements
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References

Isolated Edge Dislocation in Aluminum

![Image](image1.png)

Table: Elastic and electronic contributions to the perfect edge screw dislocation formation energy

<table>
<thead>
<tr>
<th>$\rho$</th>
<th>$\rho_{iso}$</th>
<th>$\rho_{EL}$</th>
<th>$\rho_{ec}$</th>
<th>$\rho_{core}$</th>
</tr>
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<tr>
<td>1.0</td>
<td>0.10</td>
<td>0.43</td>
<td>0.76</td>
<td>1.50</td>
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</tbody>
</table>

Isolated Screw Dislocation in Aluminum

![Image](image2.png)

Table: Elastic and electronic contributions to the perfect screw dislocation formation energy

<table>
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<tr>
<th>$\rho$</th>
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Isolated Basal Edge Dislocation in Magnesium (ongoing)

![Image](image3.png)

Table: Elastic and electronic contributions to the perfect basal edge dislocation formation energy

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<th>$\rho$</th>
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Conclusions so far

- Size of dislocation cores are predicted to be 7-10 nm (much larger than previous displacement field based estimates of 1-2 nm) underlining the long-ranged electronic structure perturbations due to the dislocation core.
- Core energy is strongly dependent on the external macroscopic deformations.

Core Forces in Dislocation-Dislocation Interactions

- When dislocation is present in an inhomogeneous strain field, core-energy dependence on applied external macroscopic deformations leads to a configurational force (referred to as core force) on the dislocation given by,

$$\mathbf{f}_{\text{core}}(\rho) = \frac{\partial E_{\text{core}}(\rho)}{\partial \rho},$$

- Developed an energetic model to incorporate the core forces into discrete dislocation dynamics [4].

Figure: Top figures- schematic of the case studies: (a) between a edge dislocation and a circular glide loop (b) two parallel circular glide loops. Bottom figure: contour plot of base 10 logarithm of the ratio of the core force to the elastic Peach-Koehler force on the blue colored dislocation structure as a function of its position ($x$, $y$). The red colored dislocation structure is fixed at the origin. The left and right contour plots correspond the schematics (a) and (b) respectively.

Above case studies suggest that core forces can be significant in comparison to the classical elastic force even up to distances of ~ 10-15 nm between the dislocation structures.

Core forces can potentially influence dislocation enabled hardening during plastic deformation.