Mixed atomistic/continuum modeling of domain wall structure and kinetics

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Multi-scale modeling of domains

- Homogenization
- Relaxation
- Renormalization
- Quasicontinuum
- Molecular Dynamics
- Quantum Mechanics

Scale ranges:
- $10^{-2}$ m
- $10^{-6}$ m
- $10^{-7}$ - $10^{-4}$ m
- $10^{-8}$ - $10^{-6}$ m
- $10^{-10}$ - $10^{-8}$ m
- $10^{-8}$ m
Objectives

- Consideration of both atomistic and continuum (long range) effects is required for understanding:
  - *The structure, kinetics and stability of extended structures such as domain-wall steps, kinks…*
  - *Long-range Interaction between domain walls and lattice defects such as vacancies, crack tips…*

- Basic strategy: Start from a full atomistic description of the material and:
  - *Simplify field equations by recourse to the harmonic approximation, lattice statics*
  - *Quasicontinuum method: Retain full atomistic resolution where needed, coarsen description elsewhere*
Domain-wall structure: Harmonic analysis

- **Objective:** Ascertain analytically
  - *The structure of isolated domain walls, domain-wall steps in infinite bodies (no finite-cell, periodicity, effects)*
  - *The long-range elastic interactions between domain walls and (distant) lattice defects*
  - *Energy barriers to domain-wall, step, mobility, under the action of macroscopic driving forces*

- **Approach:**
  - *Start from an atomistic description of the material based on empirical potentials (e.g., polarizable reactive force field, Goddard et al)*
  - *Linearize field equations about reference configuration (harmonic approximation)*
  - *Solve the resulting field equations analytically by means of DFT, Green’s functions, Wiener-Hopf technique*
Domain-wall structure: Harmonic analysis

- Model energy:

$$E(y, P) = \frac{1}{2} \sum_{j \neq i} \phi(|y^i - y^j|) + \sum_i \psi(P^i) + \sum_{j \neq i} \left\{ \frac{P^i \cdot P^j}{|y^i - y^j|^3} - \frac{3P^i \cdot (y^i - y^j) P^j \cdot (y^i - y^j)}{|y^i - y^j|^5} \right\}$$

- Pair potential:

$$\phi_I(r) = K_I(r - a)^2(r - b)^2$$
$$\phi_{II}(r) = K_{II}(r - \sqrt{a^2 + b^2})^2$$

- Anisotropy energy:

$$\psi(P) = A(P - P_1) \cdot (P - P_1)(P - P_2) \cdot (P - P_2)$$
Domain-wall structure: Harmonic analysis

- Linearized problem: $y = y_0 + u$, $P = P_0 + v$

$$\partial_y \partial_y E(y_0, P_0) \cdot u + \partial_y \partial_P E(y_0, P_0) \cdot v = -\partial_y E(y_0, P_0)$$

$$\partial_P \partial_y E(y_0, P_0) \cdot u + \partial_P \partial_P E(y_0, P_0) \cdot v = -\partial_P E(y_0, P_0)$$

Reference configurations for 180 and 90-degree walls
Domain-wall structure: Harmonic analysis

Relaxed configurations for 180 and 90-degree walls
Domain-wall structure: Harmonic analysis

Relaxed 90-degree wall
Domain-wall structure: Harmonic analysis

Relaxed 90-degree wall

\[ u_{n+1} - u_n \]
Domain-wall structure: Harmonic analysis

Relaxed 90-degree wall
Domain-wall structure: Harmonic analysis

Relaxed 180-degree wall
Harmonic analysis – Work in progress

- Verification of harmonic approximation…
- Modulation of the solution parallel to wall…
- Extensions to complex lattices, charge redistribution…
- Using polarizable reactive force-field potential (Goddard et al)…
- Analysis of domain-wall steps…
- Macroscopic driving forces, energy barriers…
Extended structures: Quasicontinuum analysis

- Need atomistic realism and accounting of long-range interactions simultaneously: mixed atomistic/continuum modeling
Extended structures: Quasicontinuum analysis

- **Objective:** Ascertain
  - Structure of extended domain-wall defects, structures
  - Short and long-range wall-obstacle interactions
  - Energy barriers due to pinning, wall mobility

- **Approach:** Quasicontinuum
  - Start from a full atomistic description of the material
  - Retain full atomistic resolution where needed, coarsen description elsewhere

- **Extensions with respect to previous work**
  - Complex lattices
  - Charge redistribution
  - Finite temperature (e.g., Langevin dynamics)
Extended structures: Quasicontinuum analysis

- **Kinematics:**
  \[ q_h(l) = \sum_{l_h \in \mathcal{L}_h} \phi_h(l|l_h)q_h(l_h) \]

- **Constrained minimization:**
  \[ \min_{q_h \in X_h} E(q_h) \]

- **Cluster summation rules:**
  \[ E(q_h) \approx \sum_{l_h \in \mathcal{L}_h} n_h(l_h) \left( \sum_{l \in C(l_h)} E(l|q_h) \right) \]
Quasicontinuum analysis: Complex lattices
Quasicontinuum analysis: Complex lattices

- Kinematics:

\[ q_h^A(l) = \sum_{l_h \in \mathcal{L}_h^A} \phi_h^A(l|l_h) q_h^A(l_h) \]

\[ q_h^B(l) = \sum_{l_h \in \mathcal{L}_h^B} \phi_h^B(l|l_h) q_h^B(l_h) \]

- Constrained minimization:

\[ \min_{(q_h^A, q_h^B) \in X_h} E(q_h^A, q_h^B) \]

- Cluster summation rules:

\[ E(q_h^A, q_h^B) \approx \sum_{l_h \in \mathcal{L}_h^A \cup \mathcal{L}_h^B} n_h(l_h) \left( \sum_{l \in \mathcal{C}(l_h)} E(l|q_h^A, q_h^B) \right) \]
Quasicontinuum analysis – Charges

• Polarizable reactive force field potential (Goddard et al):
  – Charges distributed over atoms (Gaussians)
  – Includes shielding when charges overlap
  – Shell can move wrt core, atomic polarizability
  – Allows for charge transfer (shell charges)
  – Self-consistent charge equilibration

\[
\rho_i^{\text{core}}(\vec{r}) = \left( \frac{\eta_i^c}{\pi} \right)^{3/2} Q_i^c \exp\left( -\eta_i^c \cdot |\vec{r} - \vec{r}_i^c|^2 \right)
\]

\[
\rho_i^{\text{shell}}(\vec{r}) = \left( \frac{\eta_i^s}{\pi} \right)^{3/2} Q_i^s \exp\left( -\eta_i^s \cdot |\vec{r} - \vec{r}_i^s|^2 \right)
\]
Quasicontinuum analysis – Charges

- Charge interpolation:
  \[ Q_h^A(l) = \sum_{l_h \in \mathcal{L}_h^A} \phi_h^A(l|l_h)Q_h^A(l_h) \]
  \[ Q_h^B(l) = \sum_{l_h \in \mathcal{L}_h^B} \phi_h^B(l|l_h)Q_h^B(l_h) \]

- Constrained minimization:
  \[ \min_{\{(q_h^A, Q_h^A), (q_h^B, Q_h^B)\} \in X_h} E((q_h^A, Q_h^A), (q_h^B, Q_h^B)) \]

Quasicontinuum analysis – Work in progress

- C++ implementation of complex lattice capability done
- Verification tests in progress…
- Implementation of charge redistribution capability in progress…
- Applications:
Extended structures: Quasicontinuum analysis

R. Zhang and G. Ravichandran

• Need atomistic realism and accounting of long-range interactions simultaneously: mixed atomistic/continuum modeling