# Direct Observation of Phonon-Dislocation Scattering in Lithium Fluoride via Molecular Dynamics (MD)

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## Introduction

- High-Entropy Alloys (HEAs) exhibit exceptional mechanical properties and stability under extreme conditions
- During high strain-rate deformation, mobile dislocations interact heavily with lattice vibrations (phonons)
- This interaction creates phonon drag, a resistive force that limits how fast dislocations can move and ultimately dictates the material's yield strength
- To understand this in complex HEAs, we must first isolate and model how a single, directed phonon wavepacket interacts with a stationary edge dislocation

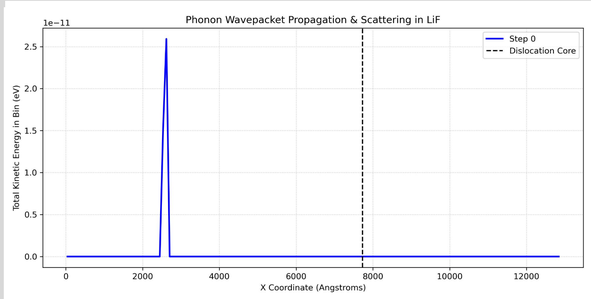
## Objectives

- Construct a stable, noise-free atomic lattice containing a single edge dislocation.
- Inject a localized phonon wavepacket in the linear elastic regime (to avoid catastrophic thermal spikes)
- Track the wave packet propagation and quantify its transmission and reflection as it scatters off the dislocation core.

## Method

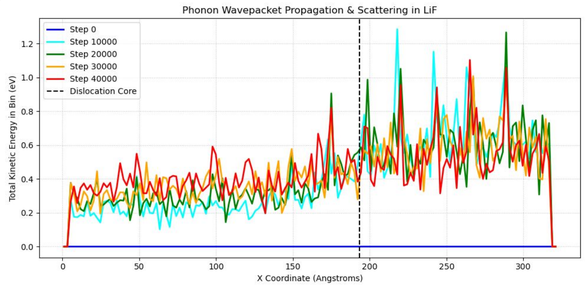
- **Simulation Software:** Molecular Dynamics using LAMMPS
- **System Setup:** A massive simulation box of a 100,000-atoms was constructed using a Buckingham potential to model interatomic forces
- **Relaxation:** The dislocation core was meticulously relaxed using minimization and slowly lowering the temperature to get it as close to absolute zero as possible.
- **Wavepacket Injection:** A Python script applied exact displacements and velocities to create a wavepacket without disturbing the relaxed dislocation core.
- **Boundary Conditions:** Periodic boundaries were utilized to allow dynamic expansion without atom loss during the energy integration

## Results




*Initial State of the phonon being injected*

## Results Cont.

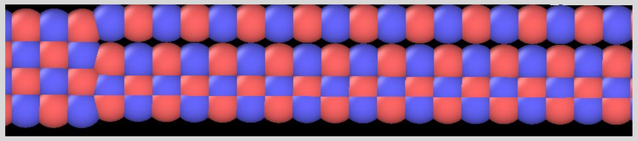



*Phonon packet after 40,000 runs*

- **Wave Propagation:** The phonon wavepacket maintained its shape as it travels towards the core of the dislocation
- **Scattering Event:** Upon striking the dislocation, the wavepacket cleanly split into transmitted and reflected components, demonstrating clear phonon scattering at the defect

- **Energy Scattering:**
  - Post-dislocation (X> 194 Angstroms), there is a significant, highly volatile spike in kinetic energy, reaching peak values between 1.0 and 1.3 eV
  - Pre-dislocation (X<194 Angstroms), a secondary lower-energy background shift develops over later steps (Steps 30,000 and 40,000), indicating backscattering or thermalization of the wavepacket as it hits the defect barrier

- **Spatial Confinement:** Energy peaks remain broadly localized between 170 and 320 Angstroms during the later stages of the simulation, confirming that the dislocation acts as a prominent site for acoustic scattering



*Edge Dislocation of the LiF lattice*

## Conclusions

- By maintaining strict amplitude limits and fine timesteps, 0.00001 and 0.00005 respectively, the Buckingham catastrophe (When two atoms bypass the energy barrier, creating a "black hole" effect in simulation) was bypassed, yielding a stable, dynamically accurate simulation.
- The isolated scattering data provides a pure look at phonon drag mechanics.

## Next Steps

- With the methodology proven on a fundamental lattice, the simulation framework is now ready to be applied to a multi-element HEA matrix.

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