**ABSTRACT**

At the quantum level, experimentalists working on the archetypical bosonic quantum solid 4He have observed unusual material properties such as giant plasticity. Although the theoretical explanation to these observations remains elusive, their interpretation has involved the role of dislocations unquestionably. In this thesis, we aim to fulfill the lack of theoretical support for these experiments through atomistic simulations of dislocations. As a first approach, we have characterized the dislocations under classical conditions for a hep system of Xe with an LJ interatomic potential. Our results reveal the dissociation of the dislocation into two Shockley partial dislocations bounding a wide region of stacking fault. Also, our findings show a very small Peyerls Stress $\tau^*$ which results in an absence of lattice resistance to dislocation motion at finite temperature. To assess the features of the dislocation at the quantum regime, we employ Path Integral Monte Carlo simulations. We have applied on-the-fly and a posteriori methods of analysis to compute the behavior of the dislocation, but none of them have provided conclusive results. Nevertheless, clear evidence for superfluid-like behavior in either the dislocation cores or stacking fault region is not observed in our simulations.

**CLASSICAL SIMULATIONS**

**ZERO TEMPERATURE**

**DISSOCIATION INTO SHOCKLEY PARTIAL DISLOCATIONS**

- The dislocation dissociates into two Shockley partial dislocations (green atoms) when the system is relaxed.
- The partial dislocations bound a region of low energetic stacking fault (blue atoms) where the atoms are arranged in a fcc lattice.

**METHOD 1**

Differential displacement analysis

**METHOD 2**

Common neighbor analysis (CNA)

PEIERLS STRESS

We divide the crystal in three parts along the z axis. Then, follow the next procedure N times:

- we displace the upper part a $\Delta u$ while fixing the lower part.
- relax the middle part of the system to the equilibrium.

The values obtained are:

- $\mathbf{r}_p = 1.7 \pm 0.1667$ MPa (18424 atoms)
- $\mathbf{r}_p = 0.6615$ MPa (354455 atoms)

**FINITE TEMPERATURE**

- NVT, NPT and NVE simulations for two boxes of 2240 atoms and 18424 atoms.
- The dislocations move in absence of external forces due to thermal energy or residual stresses.
- The width of the stacking fault depends on the size of the box but it remains constant throughout the simulation.

**QUANTUM SIMULATIONS**

**INITIAL CONFIGURATION**

Plot of the shear modulus as a function of the temperature for a system of solid 4He. Observe the drop in the shear modulus for $T = 0.2K$, known as Giant plasticity.

**OBJECTIVES**

**CLASSICAL REGIME**

- Comprehension of the behavior of the dislocation at the classical regime, both at zero and finite temperatures.
- Characterization of its features. The aim is to assess the properties of the Peyerls stress $\tau^*$ at $T=0$ K and the motion at finite temperature for a classical system of Xe interacting through a Lennard-Jones potential.

**QUANTUM REGIME**

- Give a theoretical explanation for the observations reported by the experimentalists, such as Giant Plasticity (see Figure in the right).
- Reveal the existence of superfluidity in the dislocation cores [2-3] that could led the system to show unusual properties such as isochoric compressibility or superfluid mass transport.
- Study the interplay between the dislocations and the impurities of 3He. Several experimentalists claim impurities pin the dislocations, disabling them to free glide.

**RESULTS**

- Path Integral Monte Carlo simulations including the Takashi-Imada and the Chin approximations and the Worm algorithm for an effective computation of the superfluidity.
- We have simulated a system containing 1368 atoms of solid 4He at $T=1.5$ K and $T=3$ K.
- The simulation lengths have shown up to be too short to get reliable results.
- Values of zero for the Common Neighbor Parameter refer to a fcc region, and identify the stacking fault region. An hcp region shows values between 2 and 3. Higher values indicate the dislocation core.

**CONCLUSIONS**

- The dislocation of a system of Xe solid arranged in an hcp structure splits up into two Shockley partial dislocations that bound a low energy stacking fault.
- The width of the stacking fault region depends on the size of the box until it reaches a determined value defined by the mechanical properties of the solid.
- There is almost no lattice resistance to motion of the dislocation in the Xe classical system. The Peyerls stress value is in good agreement with these observations.
- We have developed a method to calculate the Peyerls stress that is well behaved for small systems.
- In the quantum simulations, although we have not been able to simulate a long enough simulation to get converged results, we have observed no sign of superfluid-like response.

**REFERENCES**