Simulating Helium Vesicles in Forsterite

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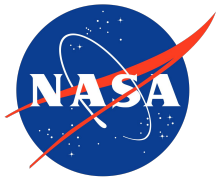
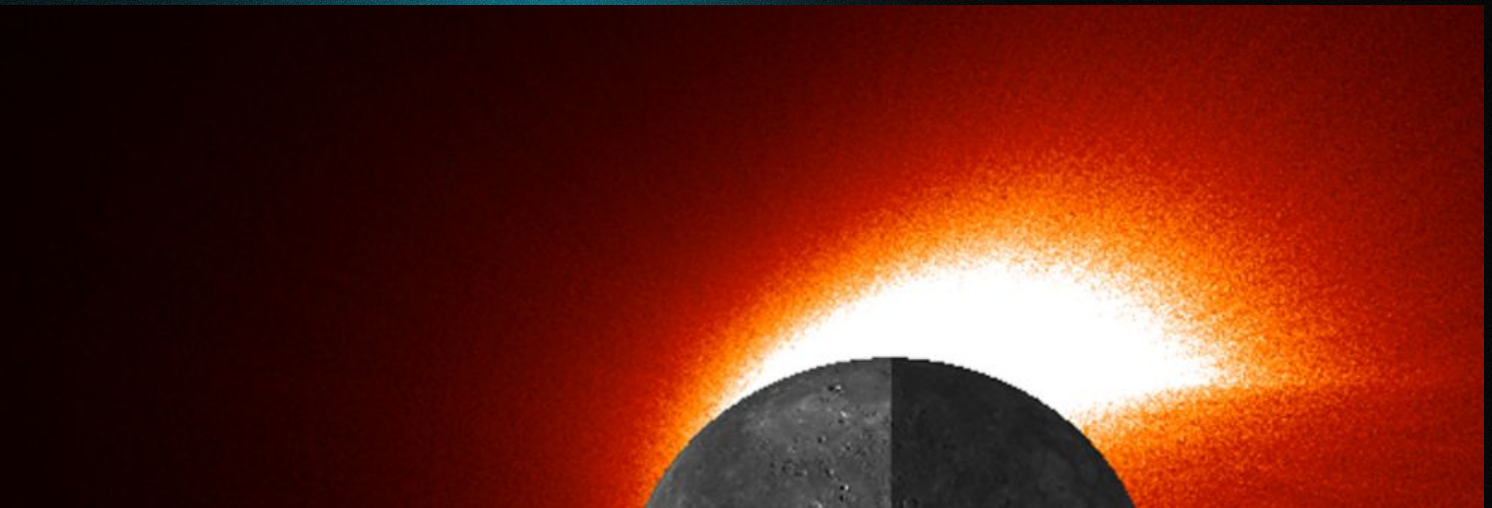
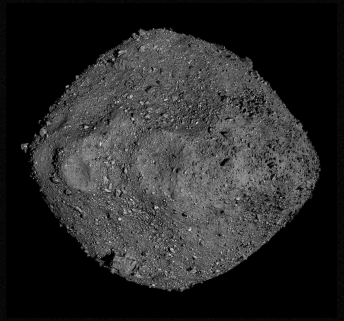


Airless Bodies and Space Weathering

- Planets, moons, and small bodies (asteroids and comets)
- Regolith alteration and exosphere formation
- Solar wind (protons, electrons, He^{2+}, and heavier ions) and micrometeoroids

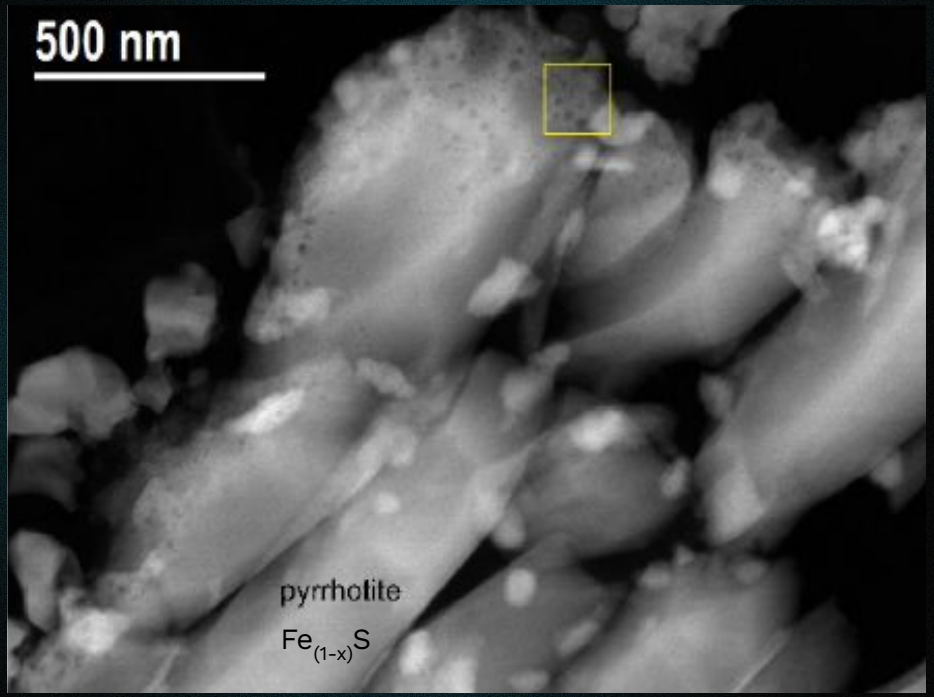


MESSENGER (2009)



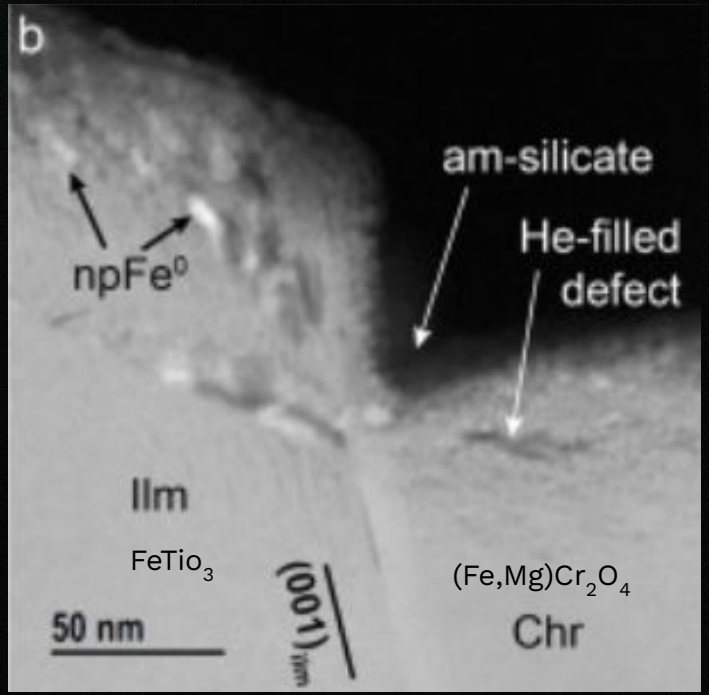
OSIRIS-REx (2021)

VESICLES IN IDP/LUNAR SAMPLES



He-filled vesicles in pyrrhotite IDP grain.
High-angle-annular dark-field (HAADF) image.

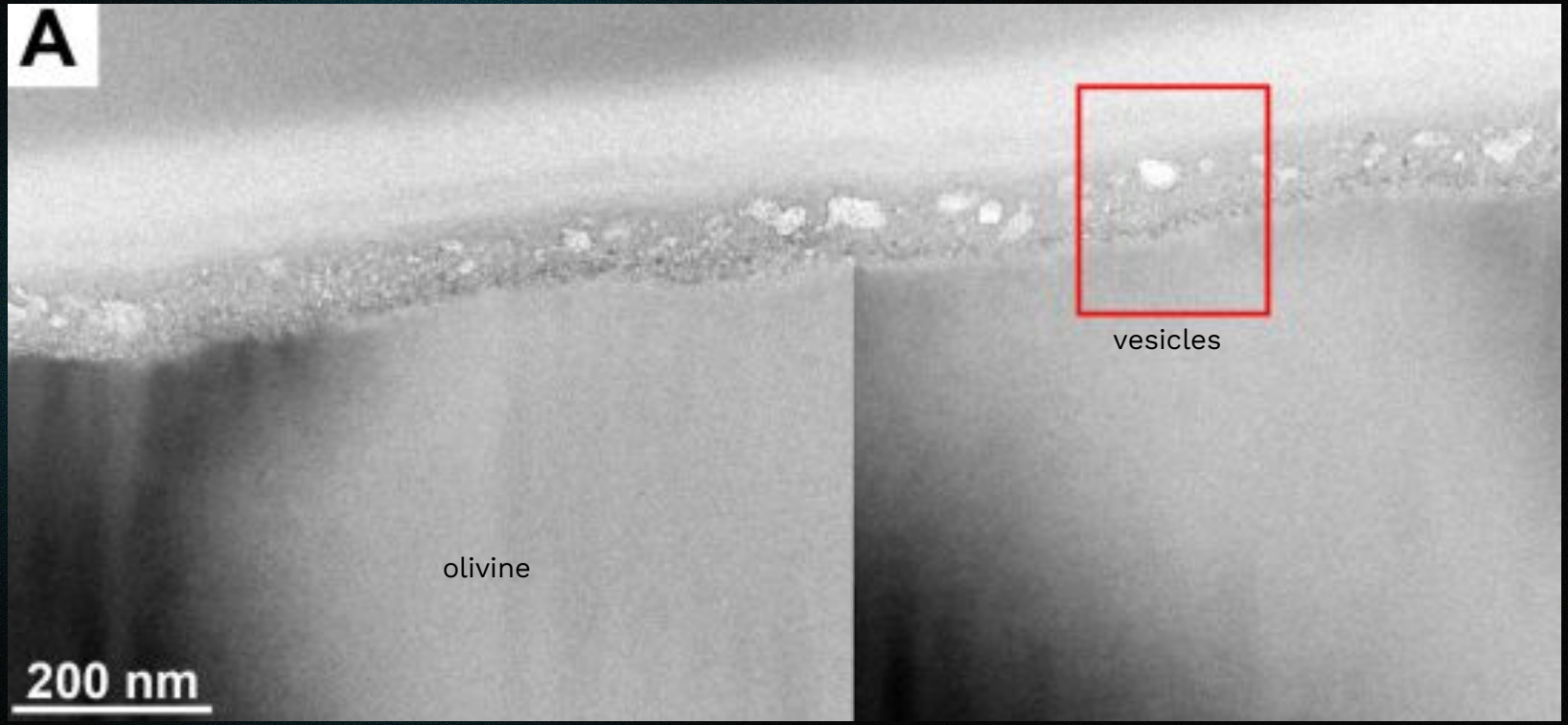
Burgess et al. (2018)



He-filled defect in ilmenite-chromite interface.
HAADF image.

Burgess et al. (2018)

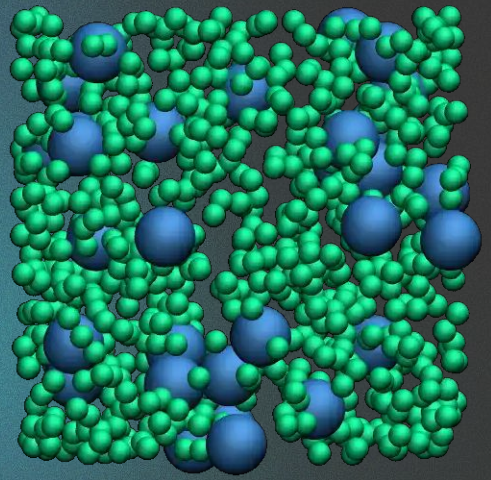
VESICLES IN LABORATORY EXPERIMENTS



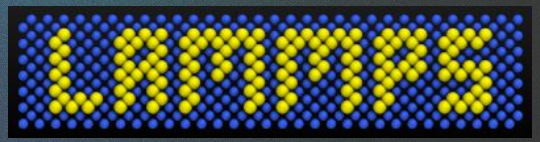
Brightfield TEM image of He+-irradiated Mg-rich olivine sample.

Laczniak et al. (2021)

Large-scale Atomic/Molecular Massively Parallel Simulator



Simon Gravelle

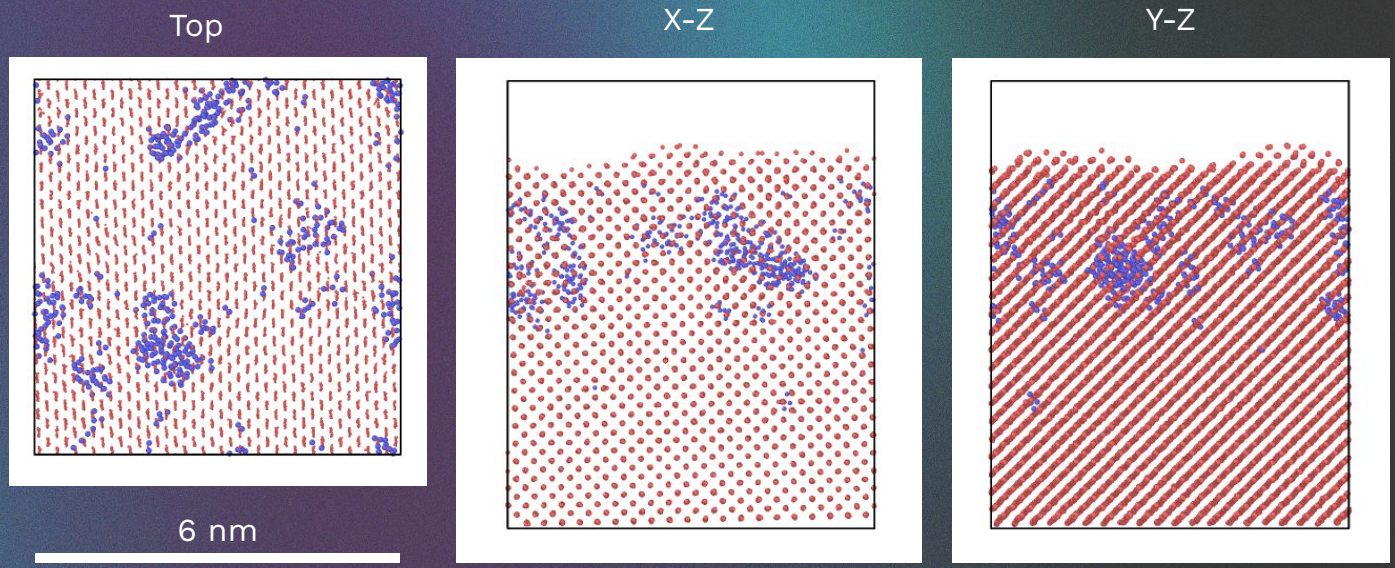


Inspiration: Helium Vesicles in Tungsten

- Reproduced work by Sandoval et al. (2015) to obtain a “jump-off” point
- Nuclear applications, surfaces in contact with slow plasma
- 60 eV incident He into a tungsten block

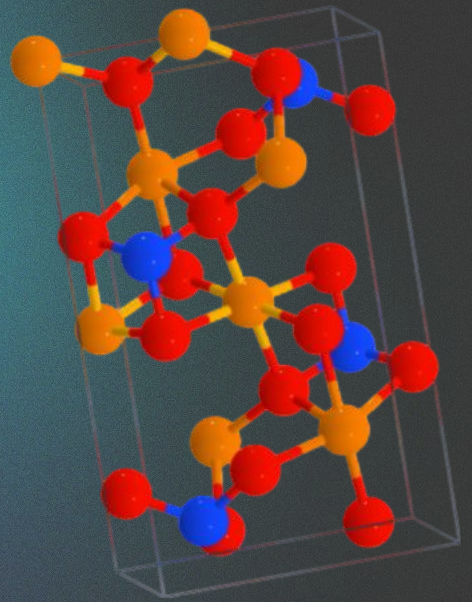
t = 5 ns

522 atoms implanted out of 5000



Our system: Forsterite - Mg_2SiO_4

- Mg-rich end-member of olivine
- Remains crystalline at high temperatures
- Common rocky body analogue
  - Reasonable Fe-free analogue for Mercury
- Experimental precedent (+ in our group)
  - Vesicles have been observed
  - Obtainable at large quantities



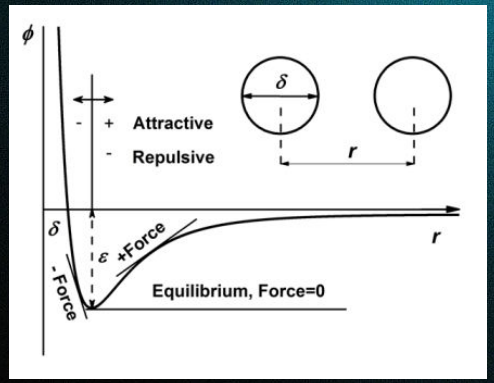
materialsproject.org

INTERATOMIC POTENTIALS

Pedone: modeling the forsterite lattice

- developed for silicates
- bulk interactions (Mg-O, Si-O, and O-O)
- formation energy for Frenkel pairs and Schottky defects

$$U(r) = \frac{z_i z_j e^2}{r} + D_{ij}[\{1 - e^{-a_{ij}\cdot(r-r_0)}\}^2 - 1] + \frac{C_{ij}}{r^{12}}$$

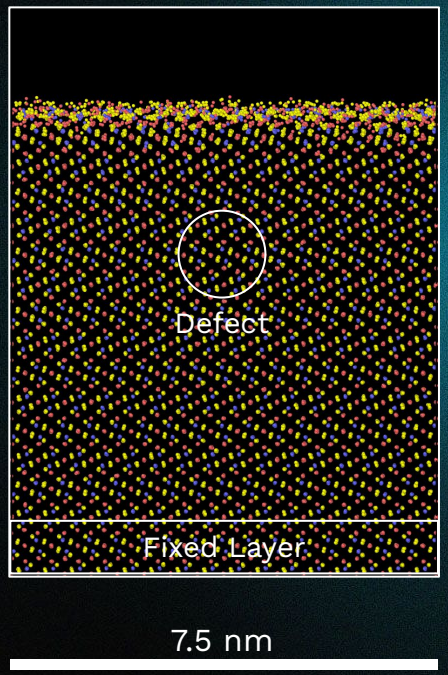


Lennard-Jones: modeling helium interactions

- universal system of potentials
- gas interactions (He-Mg, He-Si, He-O, and He-He)
- parameters epsilon (eV) and sigma (Å)

$$E = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

SIMULATION PARAMETERS



Simulation: Insertion of He into an artificial lattice defect

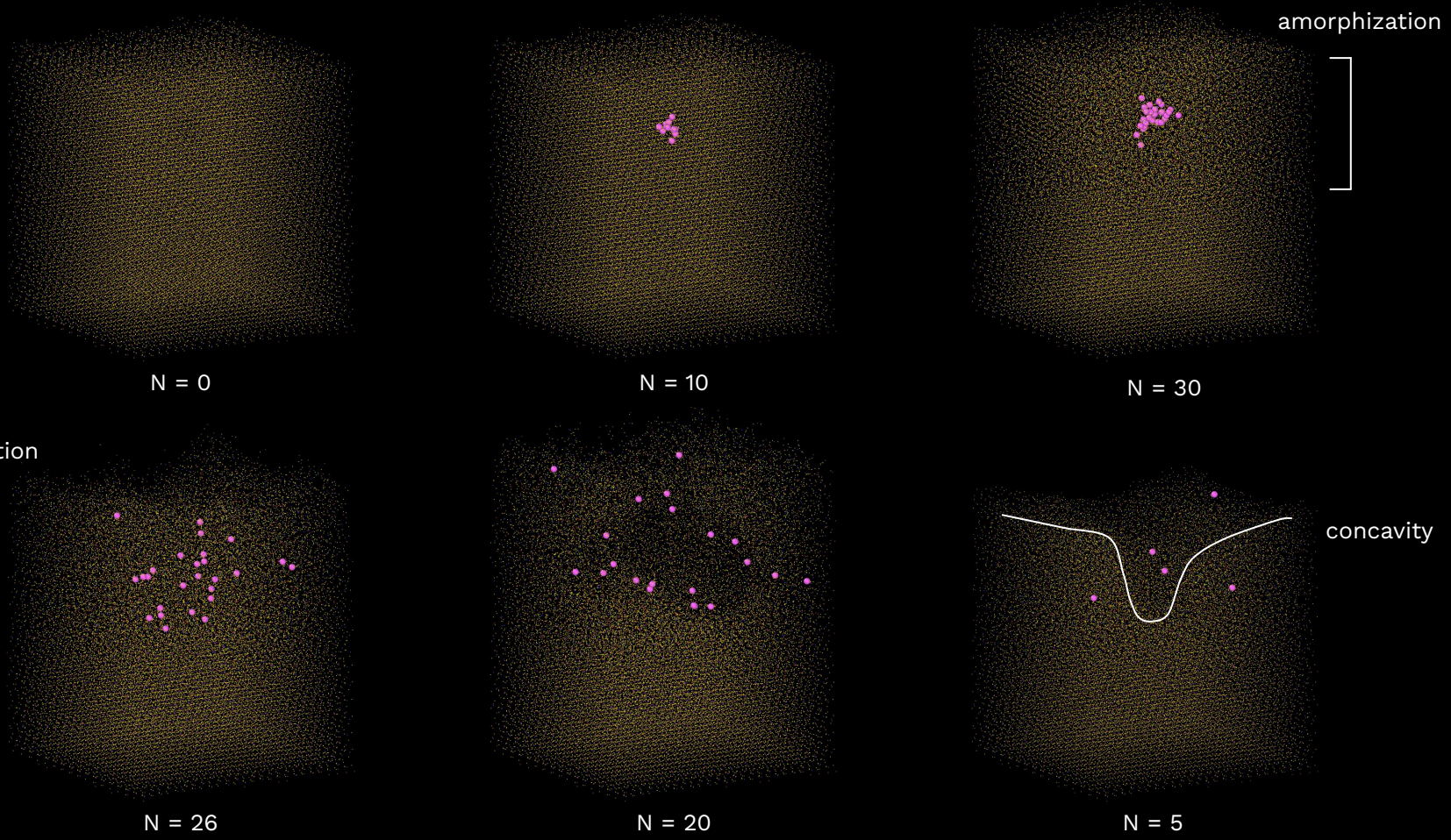
Setup

- 16 x 13 x 8 forsterite supercell (10 nm in height)
- Minimization and equilibration with NPT and NVT
- Bottom layer (1 nm) of fixed atoms
- Spherical defect with 0.5 nm radius
- No He-Mg and He-Si interactions

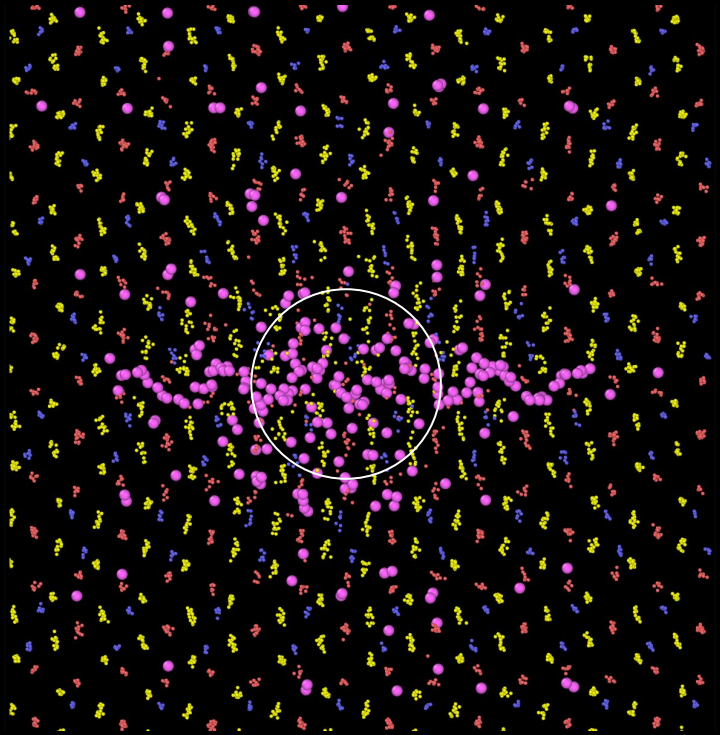
Run

- Langevin thermostat at room temperature (300K)
- Energy conservation with NVE
- Insertion of helium inside defect every 5 picoseconds

Insertion of helium into an artificial lattice defect

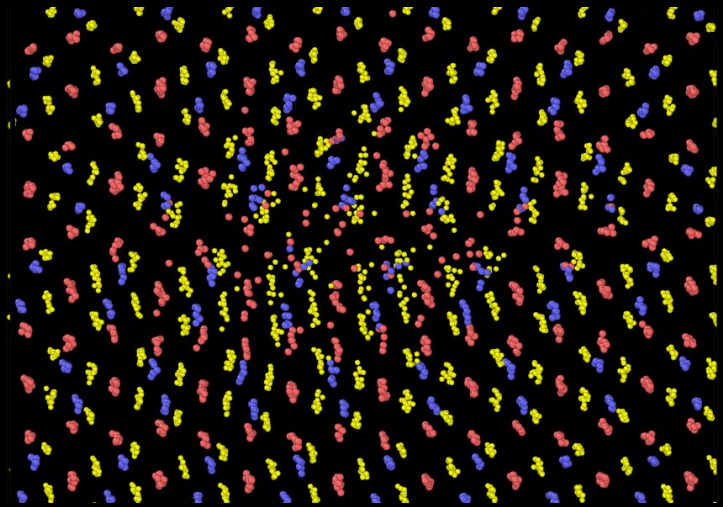


Insertion of helium atoms into a perfect forsterite lattice



Setup

- Similar to previous simulation
- Perfect lattice - no predefined defects
- All helium interactions accounted for



Helium atoms removed. Only magnesium, silicon, and oxygen atoms visible.

Conclusions

- Replication of tungsten irradiation simulations
- Vesicle bursting at forsterite surface
- Formation of defect from perfect lattice

Next Steps

- Density Functional Theory (DFT) fitting
- Machine Learning potentials
- Different bulk materials i.e. enstatite

Acknowledgements

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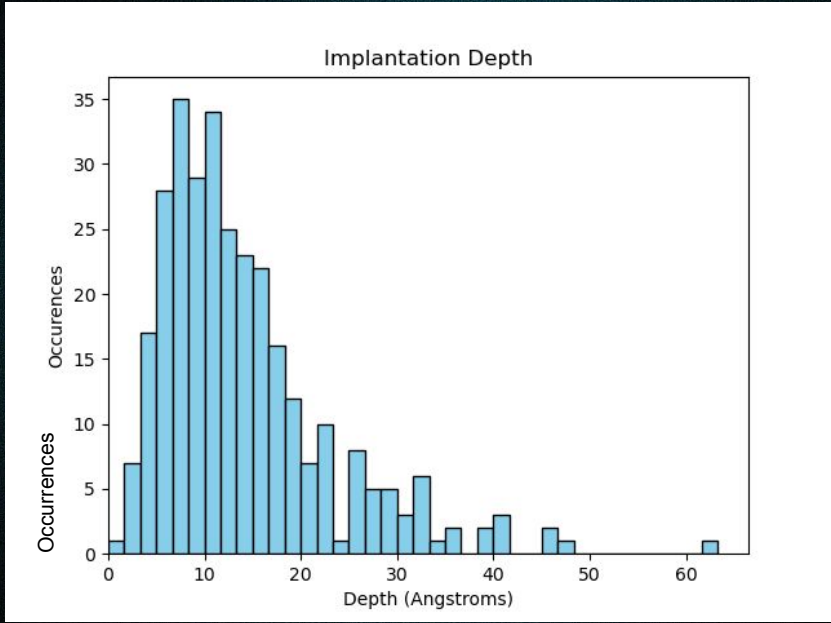
THANK YOU!

Supplementary Materials

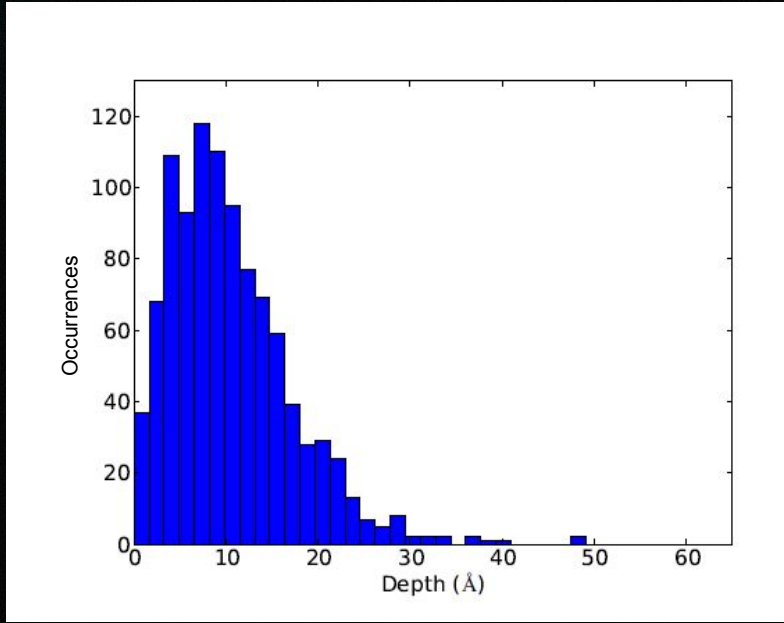
Depth Distribution comparison

our simulation



# of Incident Atoms: 1,046
Implantation: 29.3%
Reflection: 70.7%

Sandoval et al.



# of Incident Atoms: 4,000
Implantation: 28%
Reflection: 72%