Atomistic Modelling of Problems in Materials Science

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EPSRC Engineering and Physical Sciences Research Council

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Overview

- Multiscale Modelling
  - Atomistic Model
  - Multiscale model
  - Results
- Long Timescale Dynamics
- Conclusions

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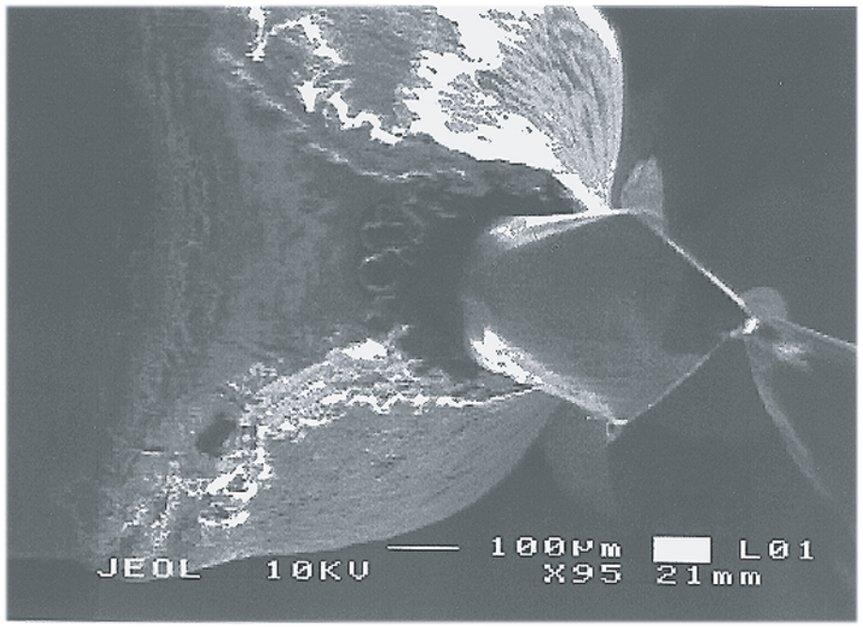
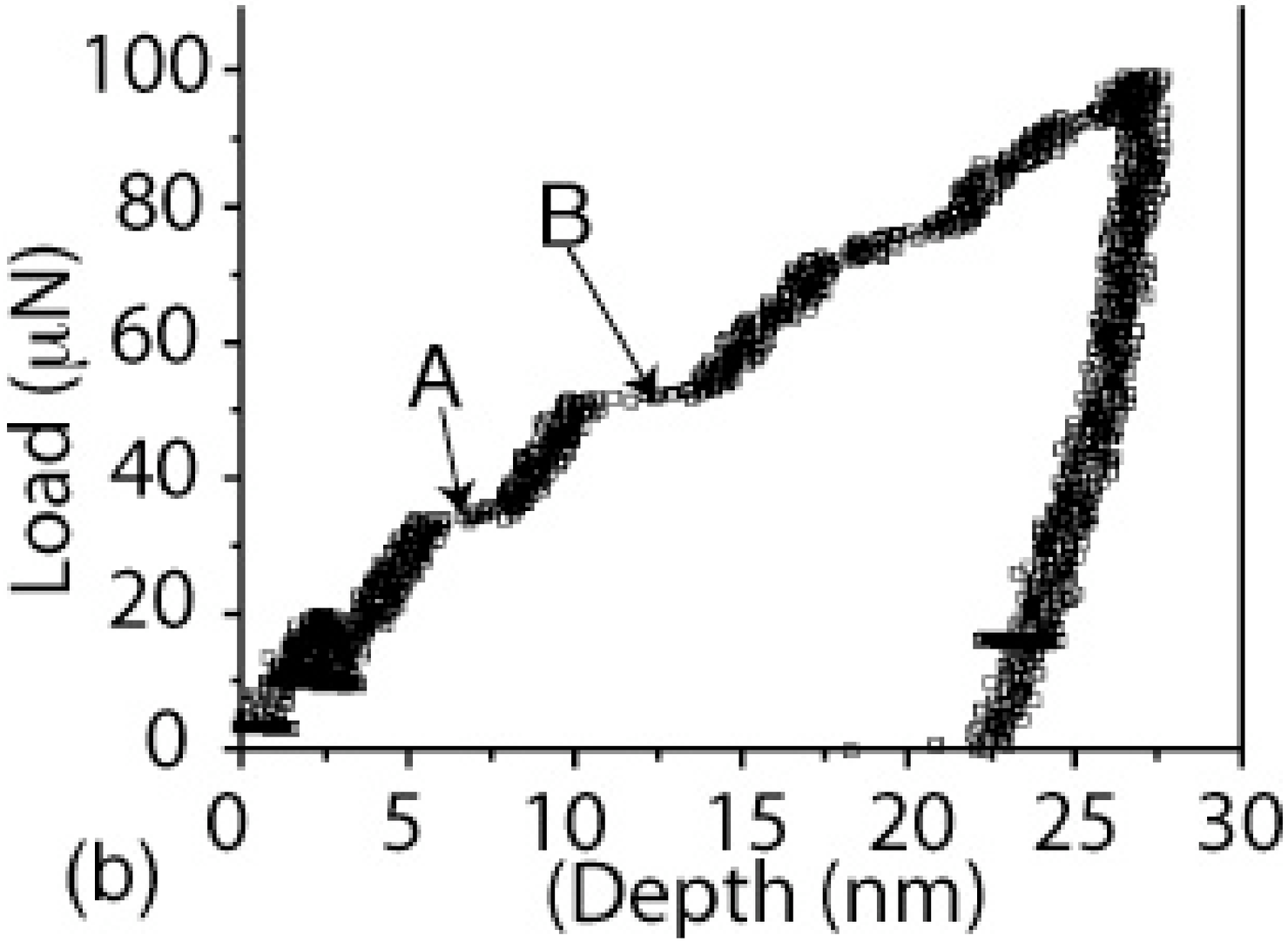
Nanoindentation





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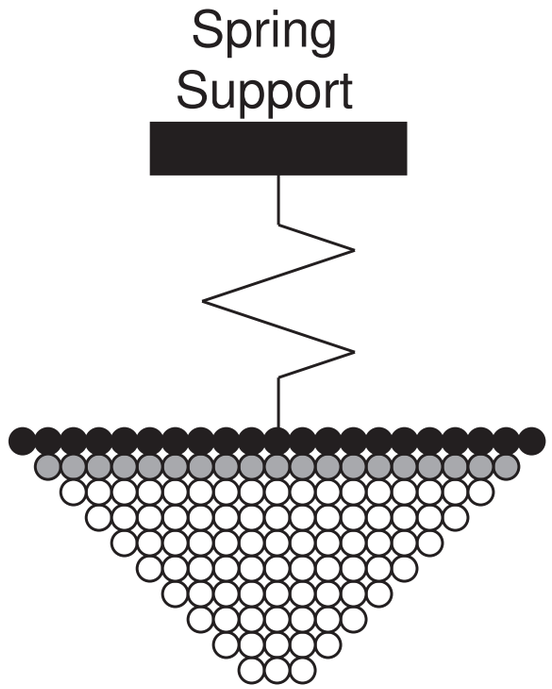
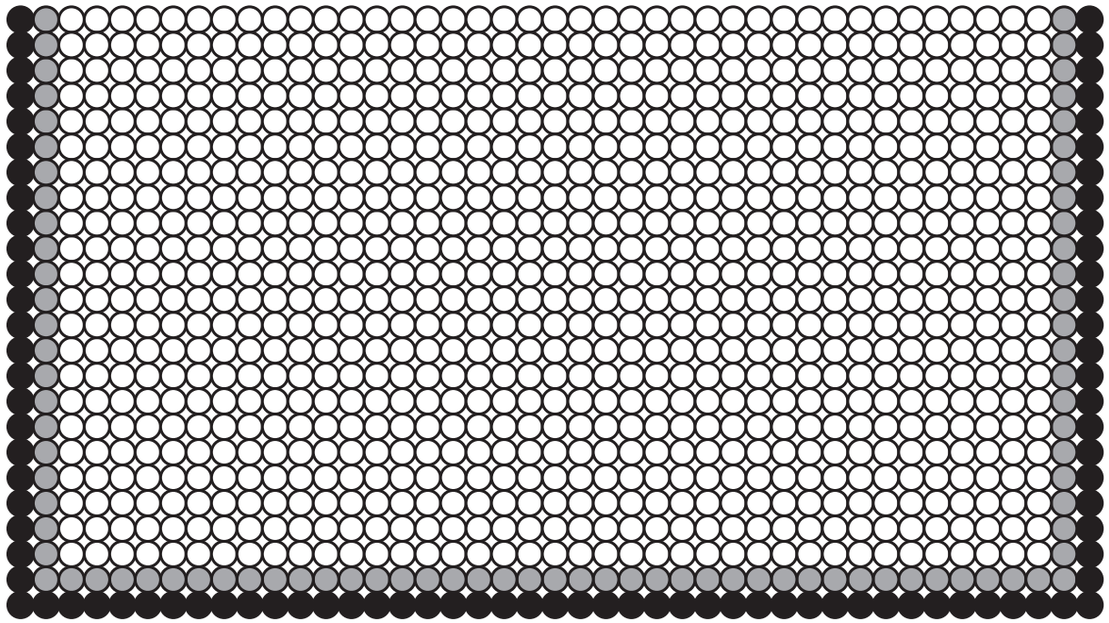
Atomistic Model

- Fixed atom
- Thermostat atom
- Free atom





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Atomistic Model

- A diamond cube corner indenter with the tip rounded is used.
- The C interactions are described by Tersoff potentials.
- The tip-surface interactions are described by the ZBL potential.
- Spring constant taken to be the same as a typical experimental value.

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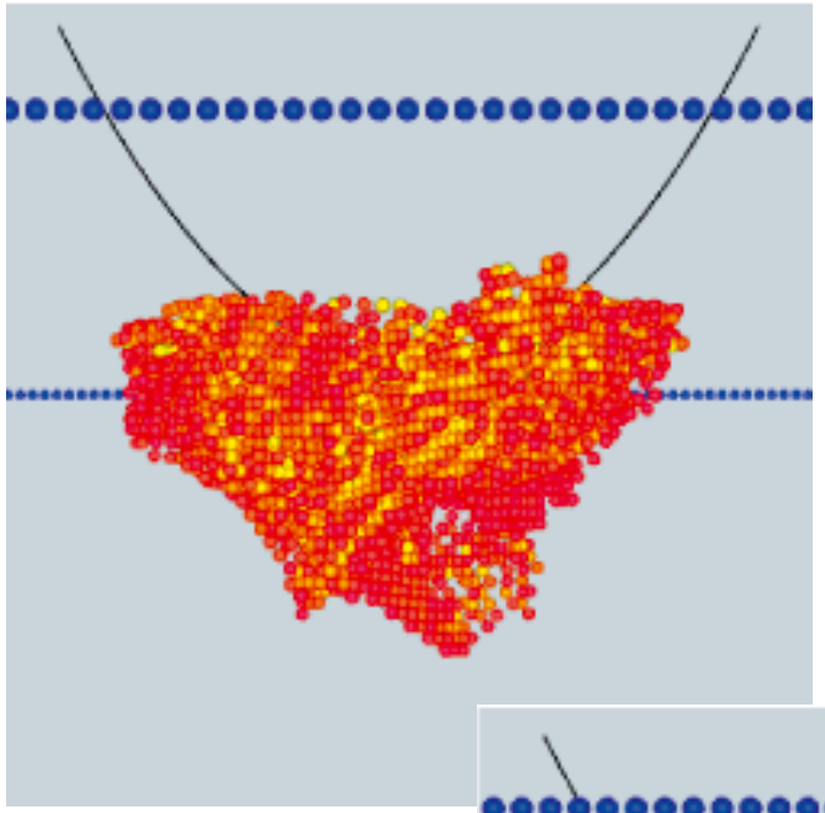
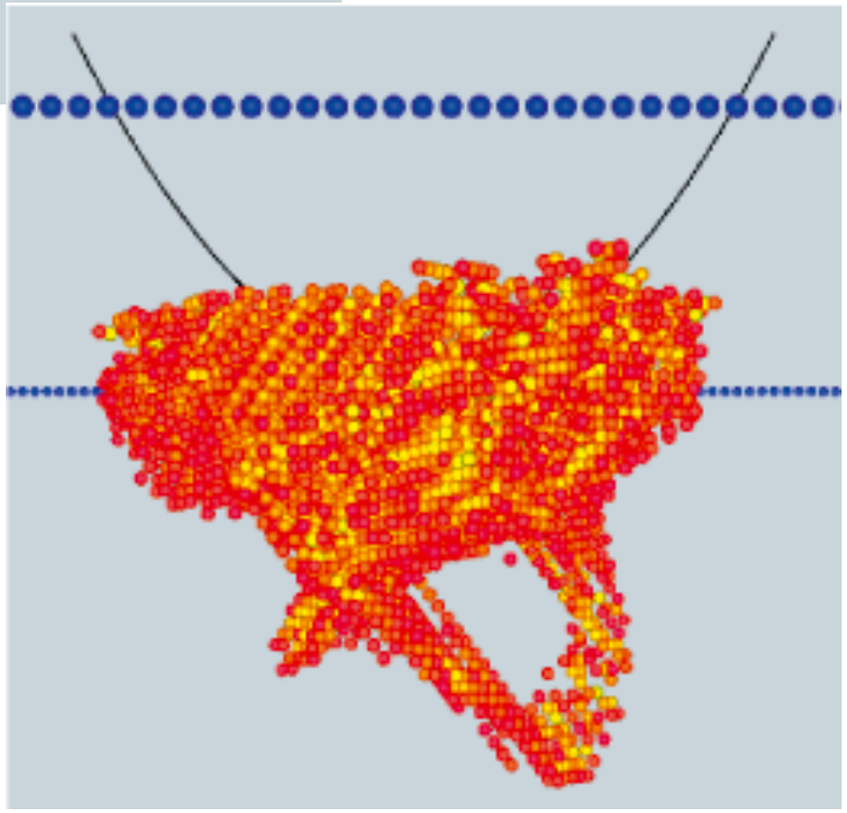
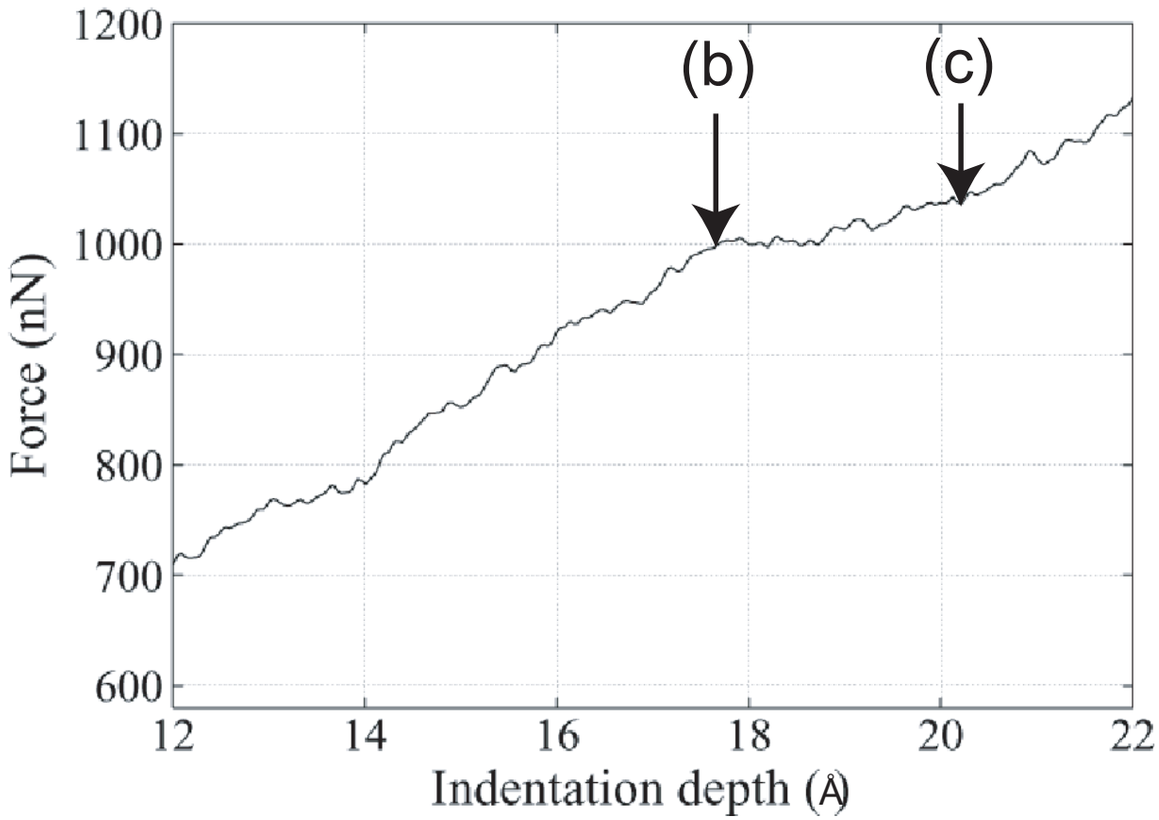
Pop-ins in the Force-Depth Curve







Phys. Rev. B 76 245405 (2003)

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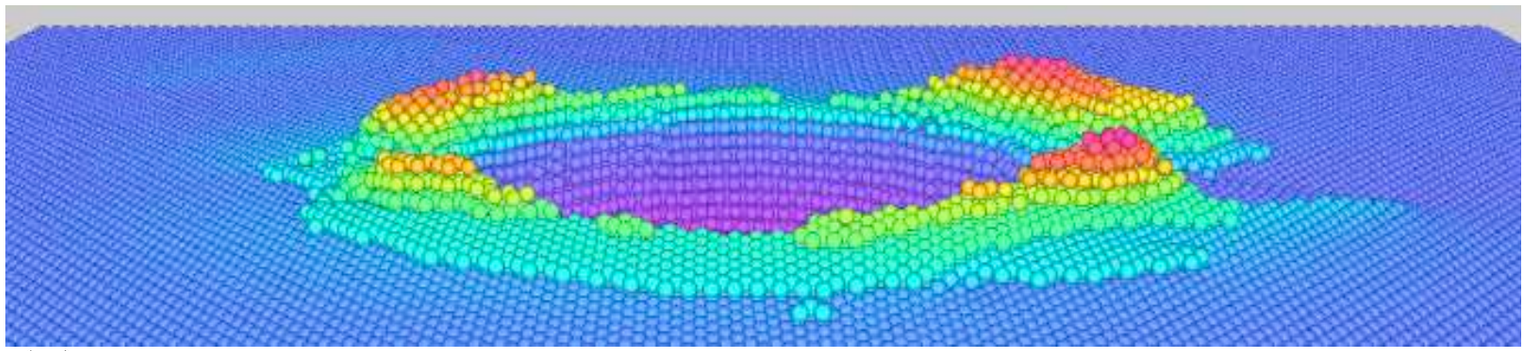
Surface pile-up on (100) Fe



(a)

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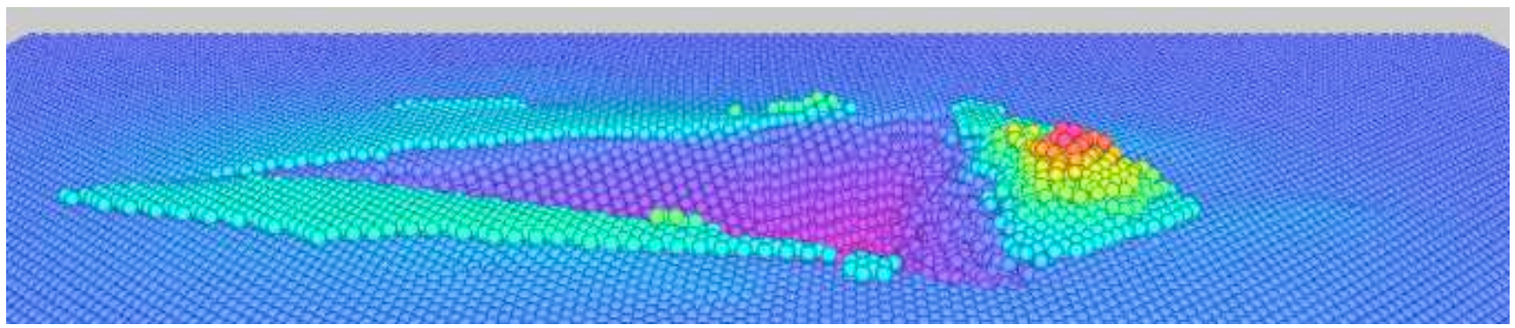

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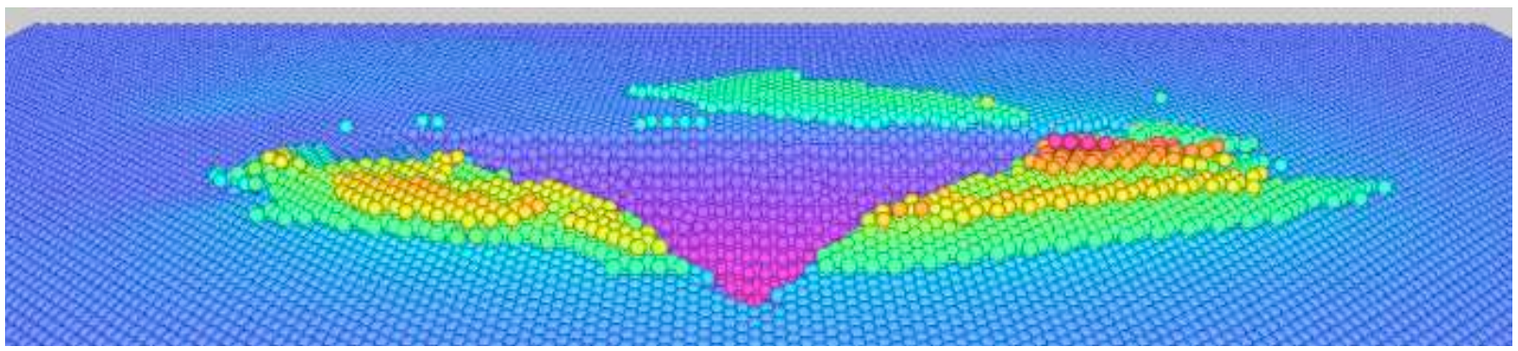

(c)

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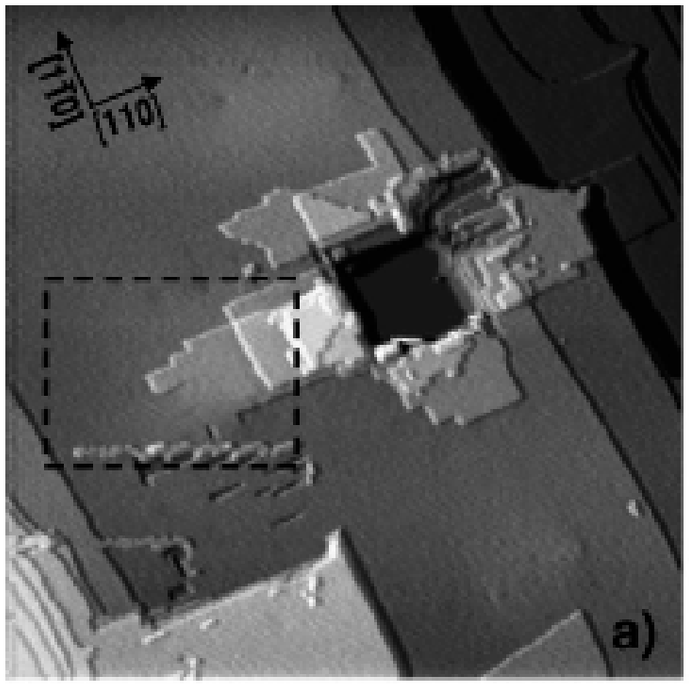
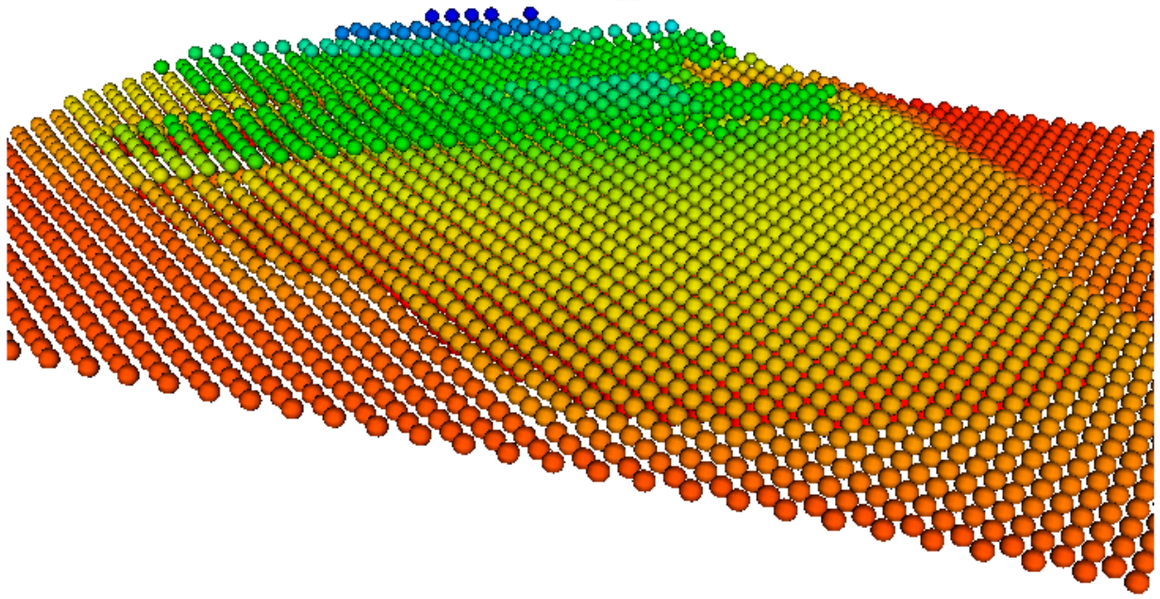
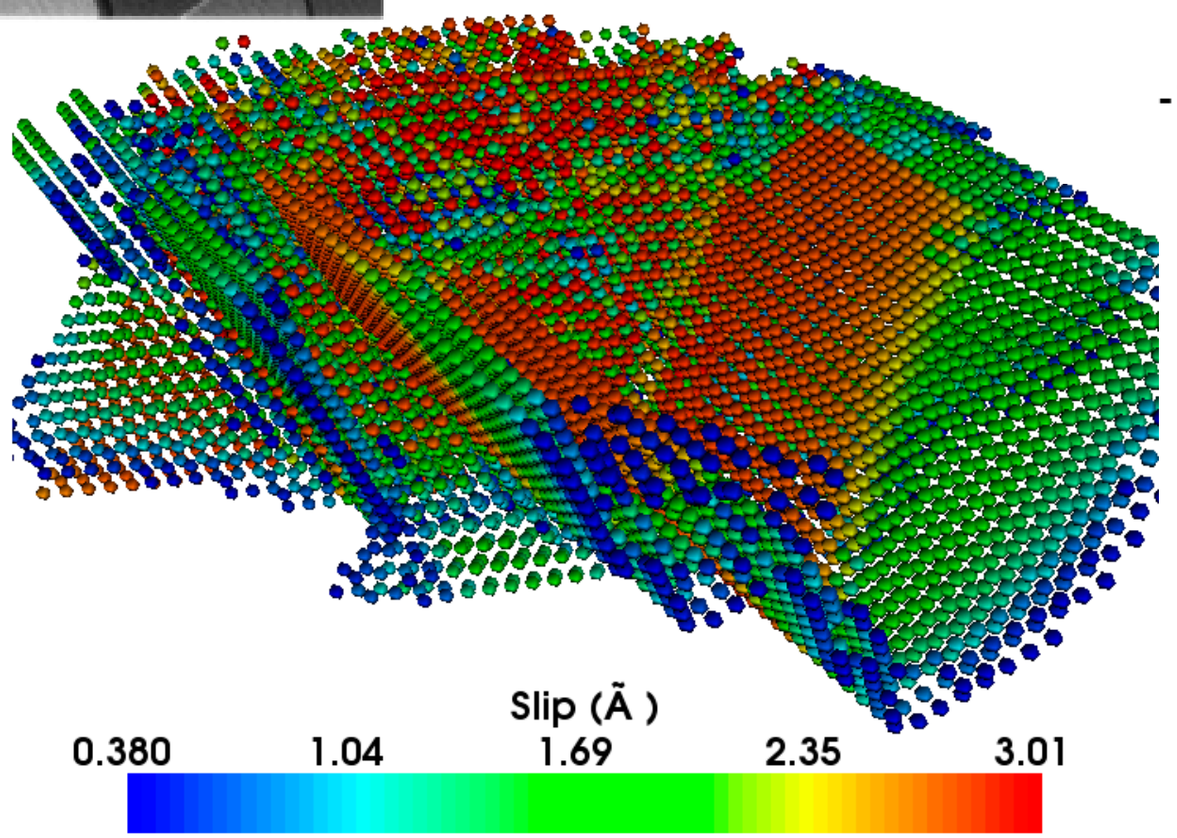
Slip planes in fcc Ag







Phil. Trans. Roy. Soc. A 363
1949-1959 (2005)

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Coupled Model

- Uses atomistic region to describe the material near the indentation site.
- Uses finite elements to describe the long-range elastic fields.
- Both the atoms and the finite element nodes are integrated forward in time using a velocity Verlet algorithm.
- The difficult part is the linking of the two models.

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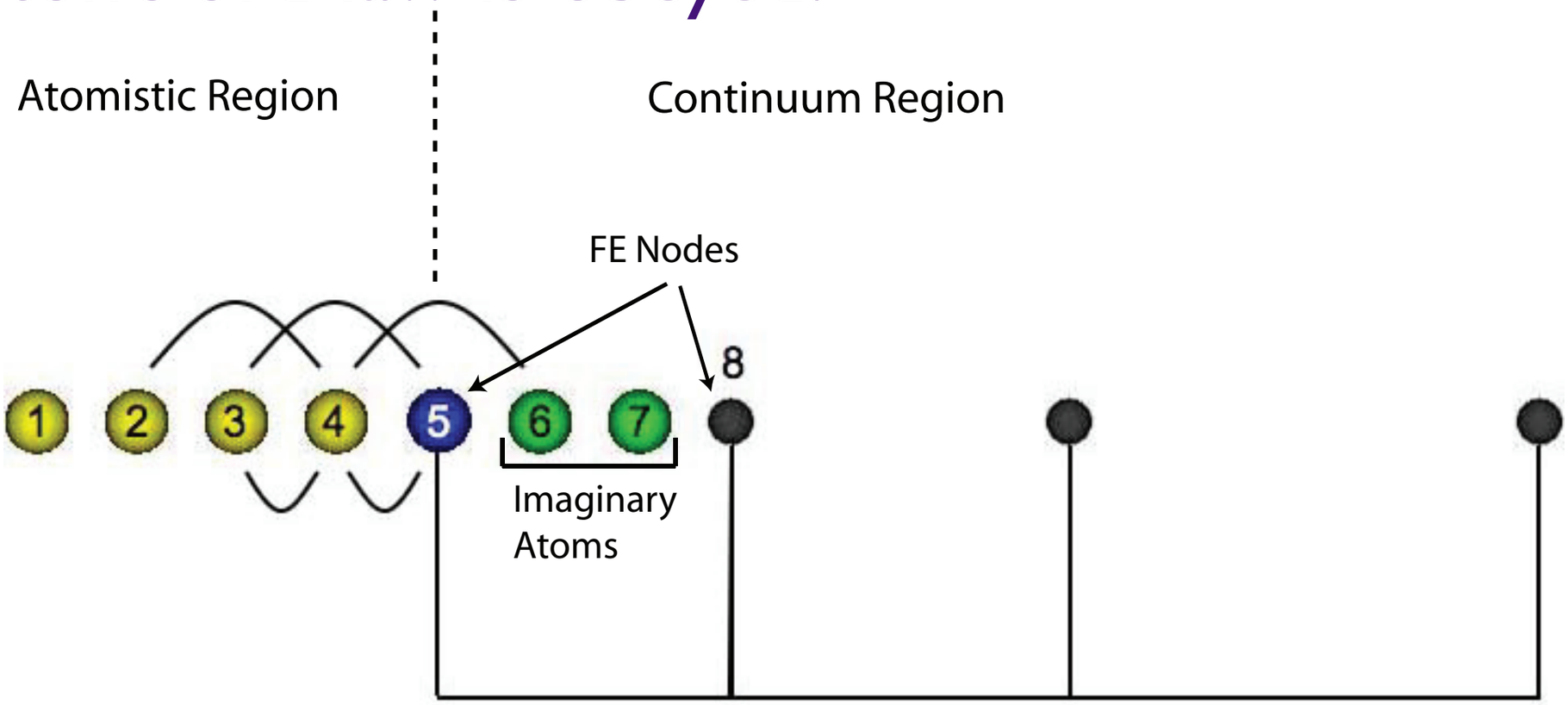
Coupled Model

- Model can deal with any short-ranged potential.
- Forces from the atoms are assigned to the nodes so that Newton's 3rd law is obeyed.



$$F_{nde} = \sum_{i=1}^{n_a} N_{nde} \mid_i F_i$$

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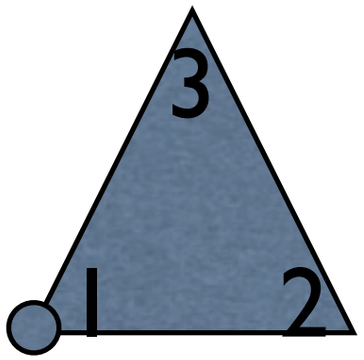
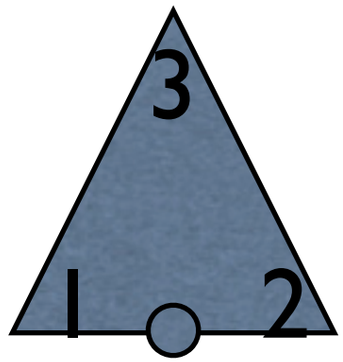
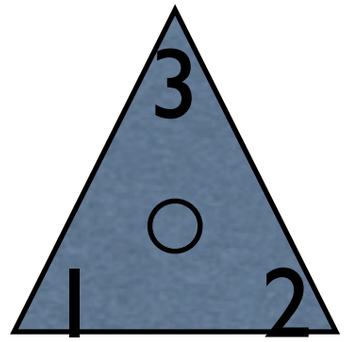
Communication MD to FE



1
2
3



1
0
0



1/2
1/2
0

1/3
1/3
1/3

$$F_{nde} = \sum_{i=1}^{n_a} N_{nde} \mid_i F_i$$

- Forces are present on imaginary atoms due to real atoms.
- The forces are assigned to nodes according to shape function values.
- The nodal force is then used in the dynamical FE update.

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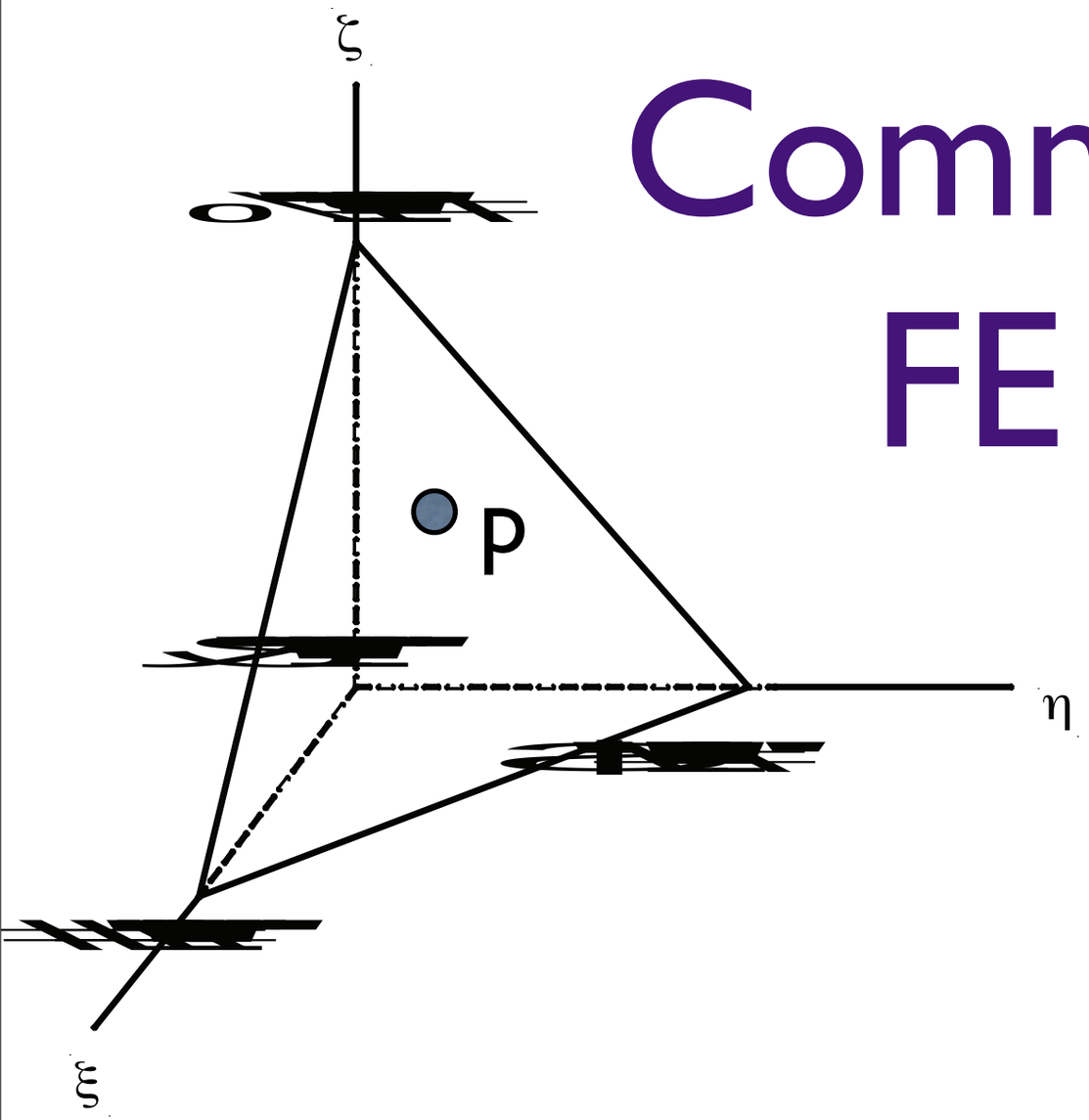
Communication FE to MD



$$u_p = u_{14}\xi_p + u_{24}\eta_p + u_{34}\zeta_p + u_4$$

$$v_p = v_{14}\xi_p + v_{24}\eta_p + v_{34}\zeta_p + v_4$$

$$w_p = w_{14}\xi_p + w_{24}\eta_p + w_{34}\zeta_p + w_4.$$

- Linear interpolation is used to position imaginary atoms according to nodal displacements.
- An atom p with fractional coordinates (ξ_p,η_p,ζ_p) has displacements (u_p,v_p,w_p).
- These equations keep the fractional coordinates constant.
- This provides feedback from the FE model to the MD region.

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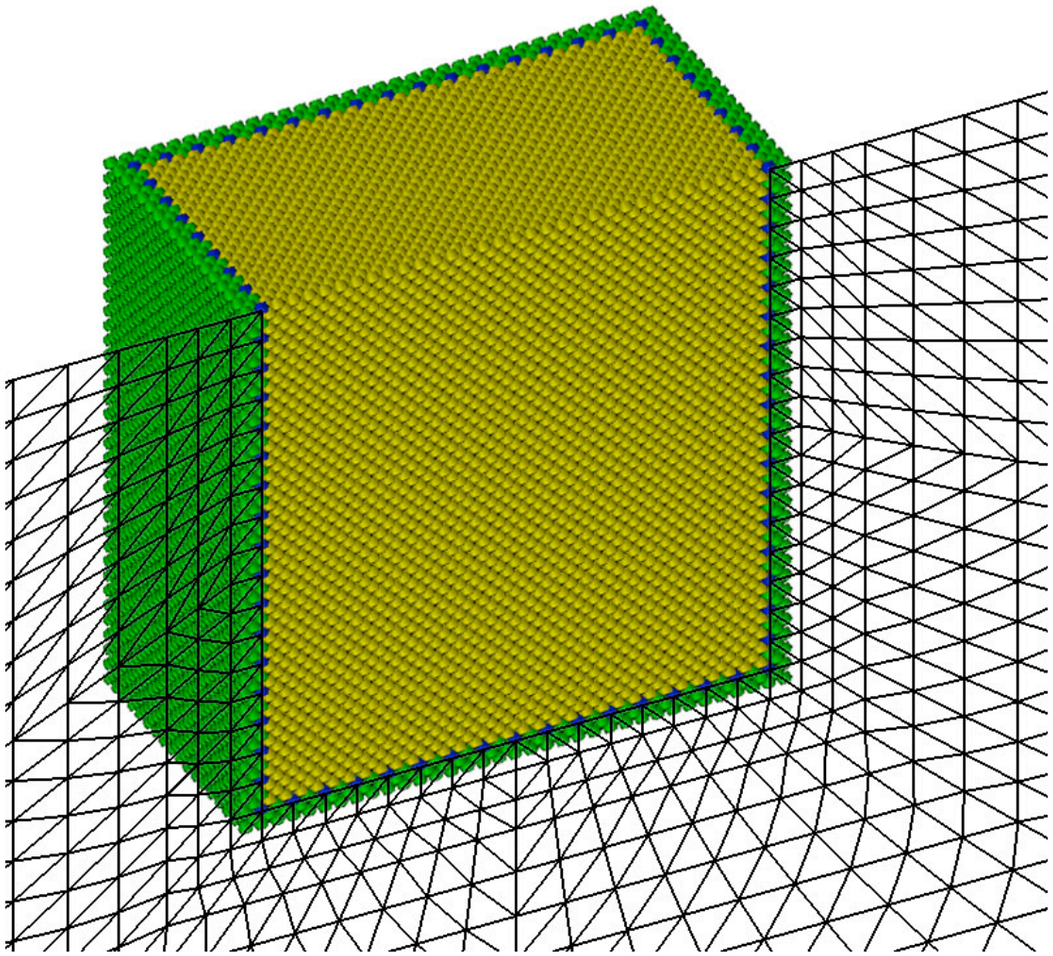
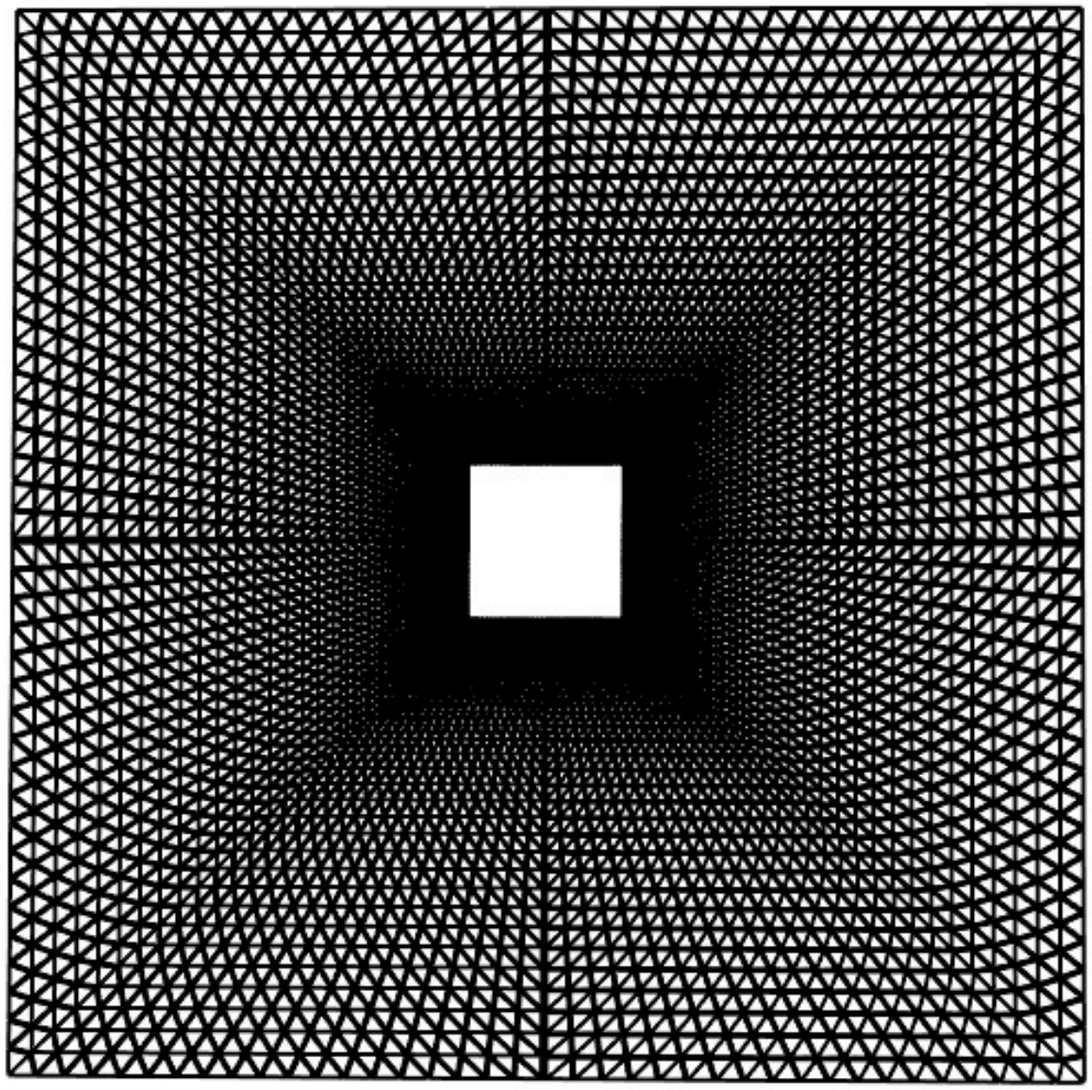
Coupling





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Coupled Model

- Ghost forces are added to the nodes near the boundary.
- These give a zero initial force on these nodes.
- Imaginary atoms are moved according to the distortion of the element that contains them.
- Linear finite element model is used - assumes distortions are small at the boundary.

E. McGee, R. Smith, S.D. Kenny Int J Mater Res 98 430-437 (2007)

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Results for Ag

- Ackland potential used to describe the Ag interactions.
- Tip was indented to a depth of 14 Å.
- Coupled model results are compared to a atomistic only system containing the same number of atoms.

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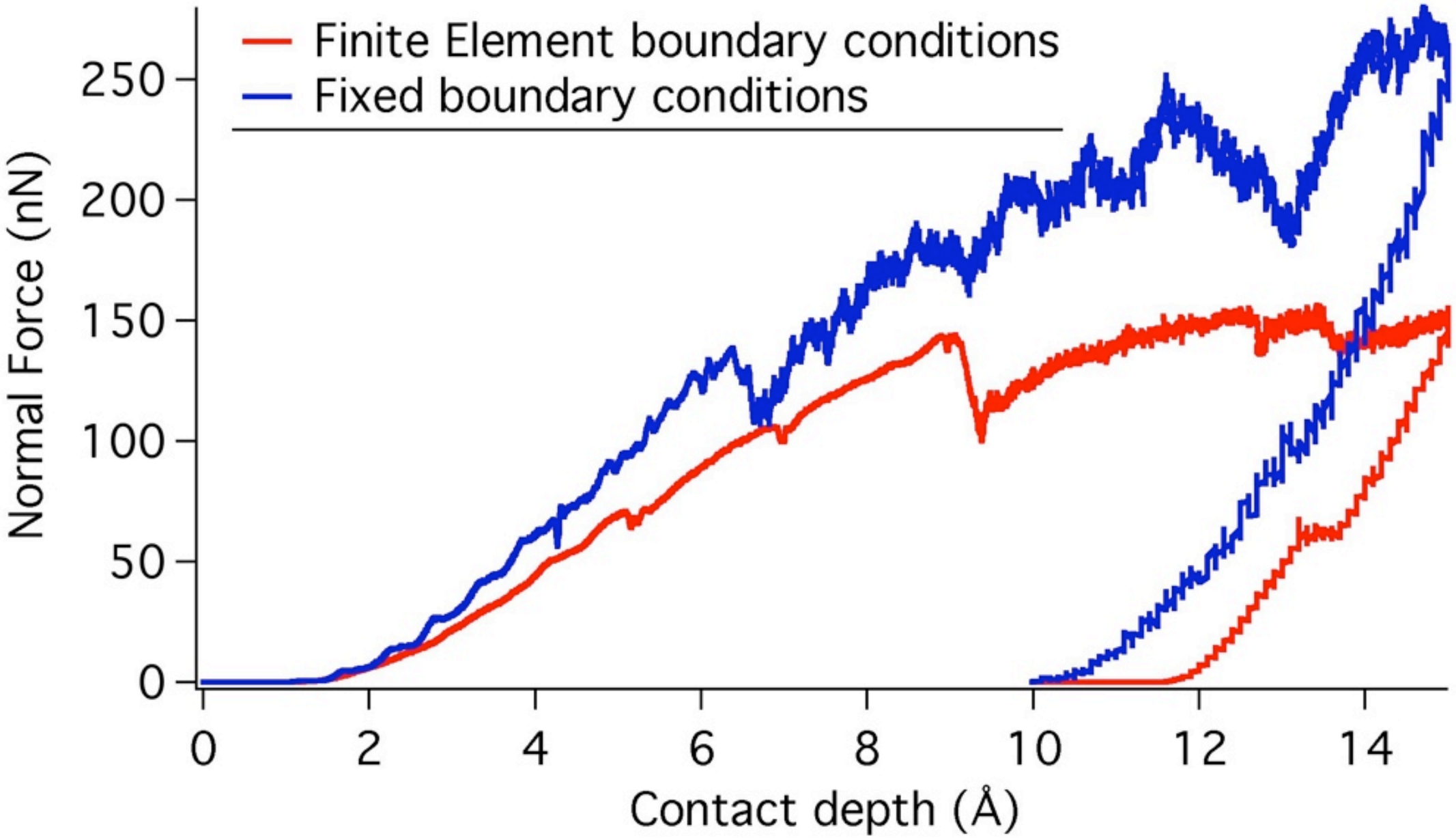
Force-Depth Curve



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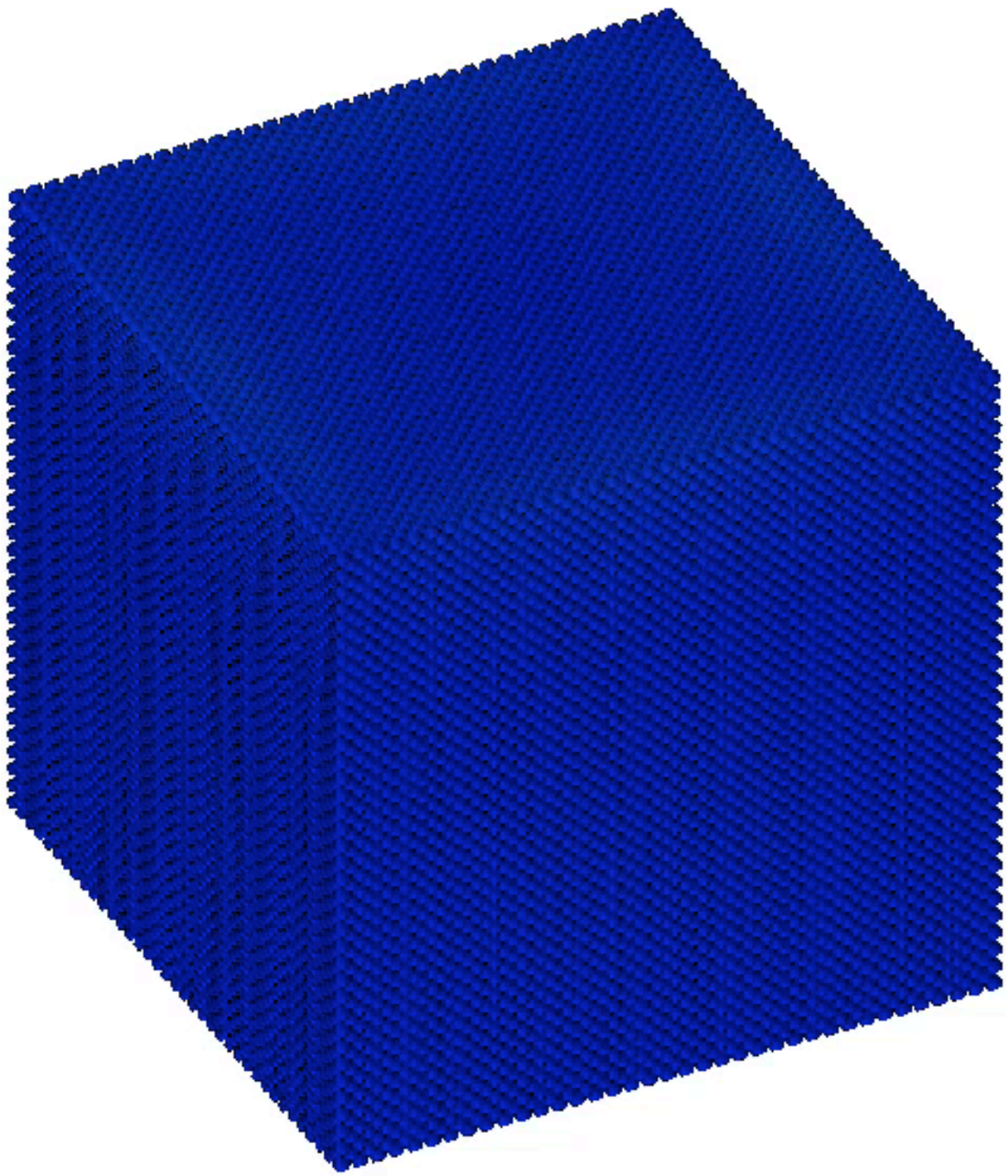

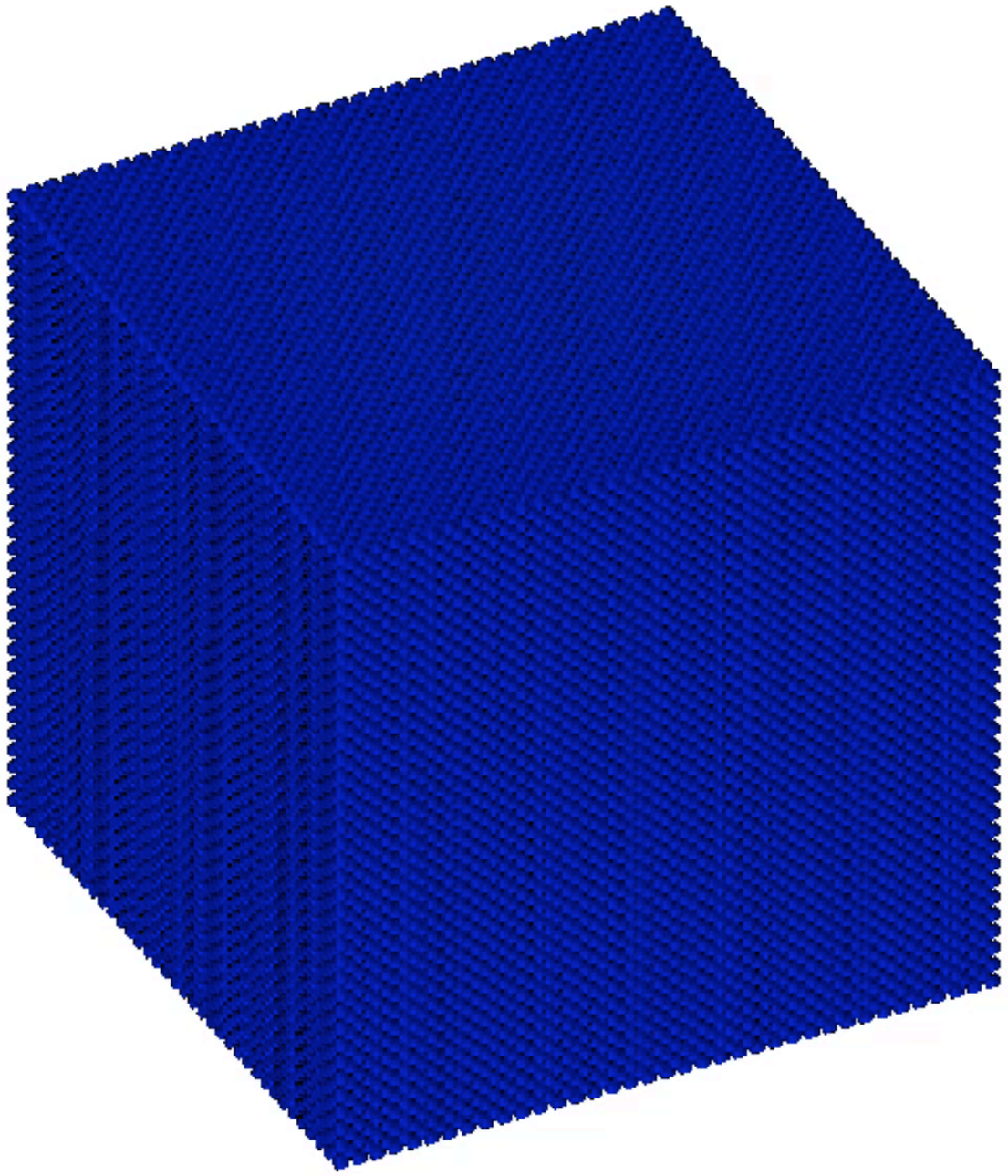

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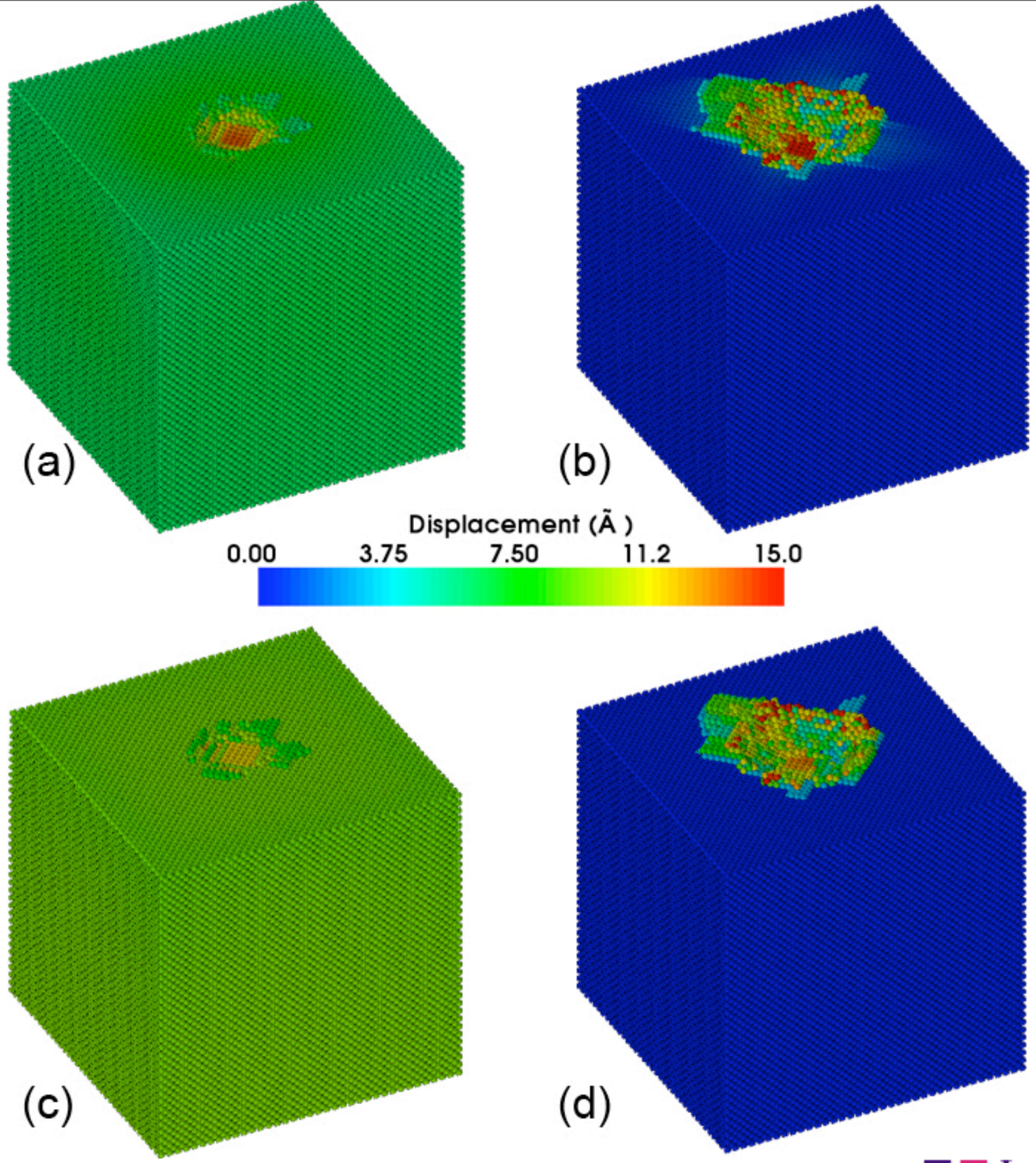

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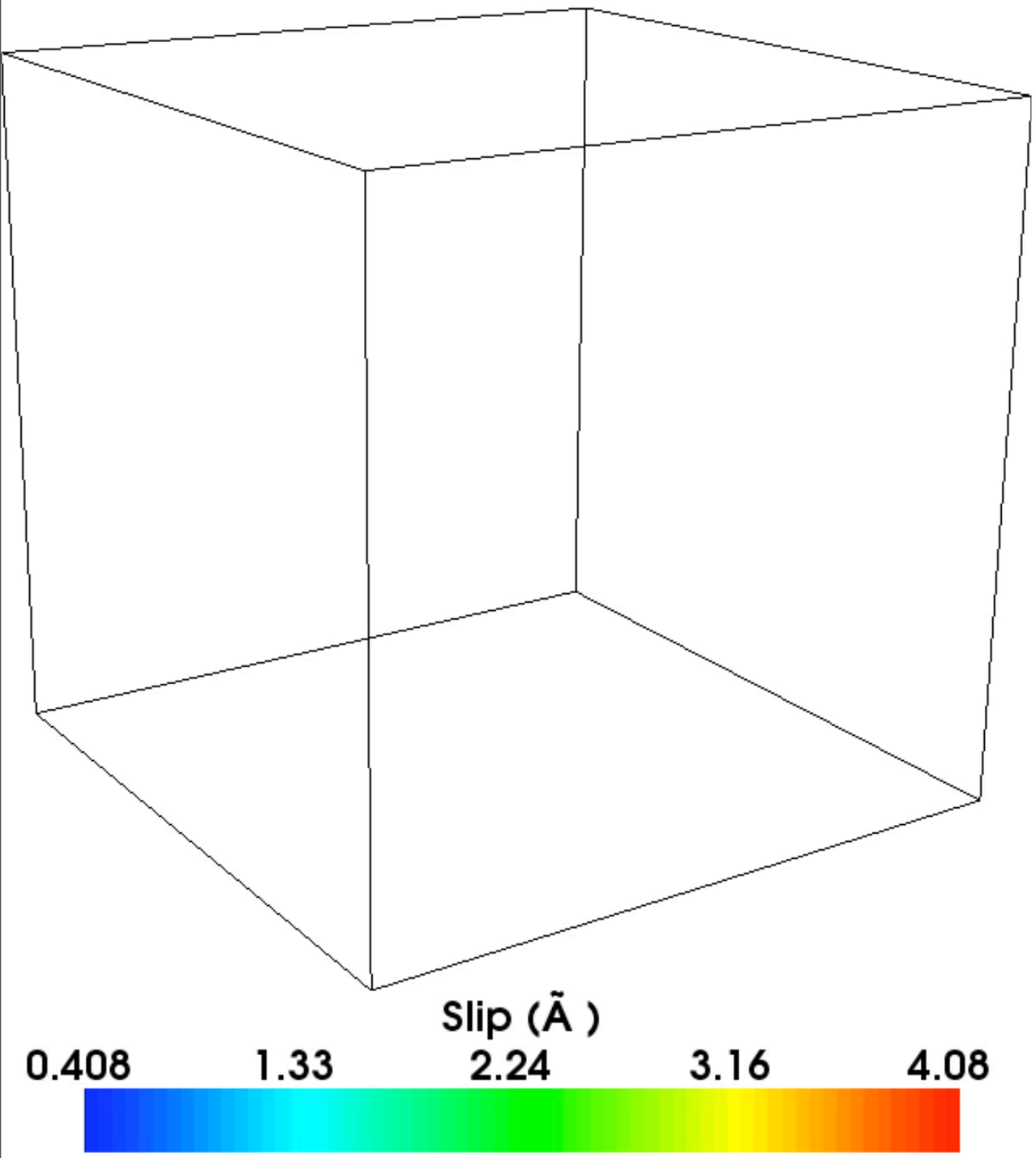
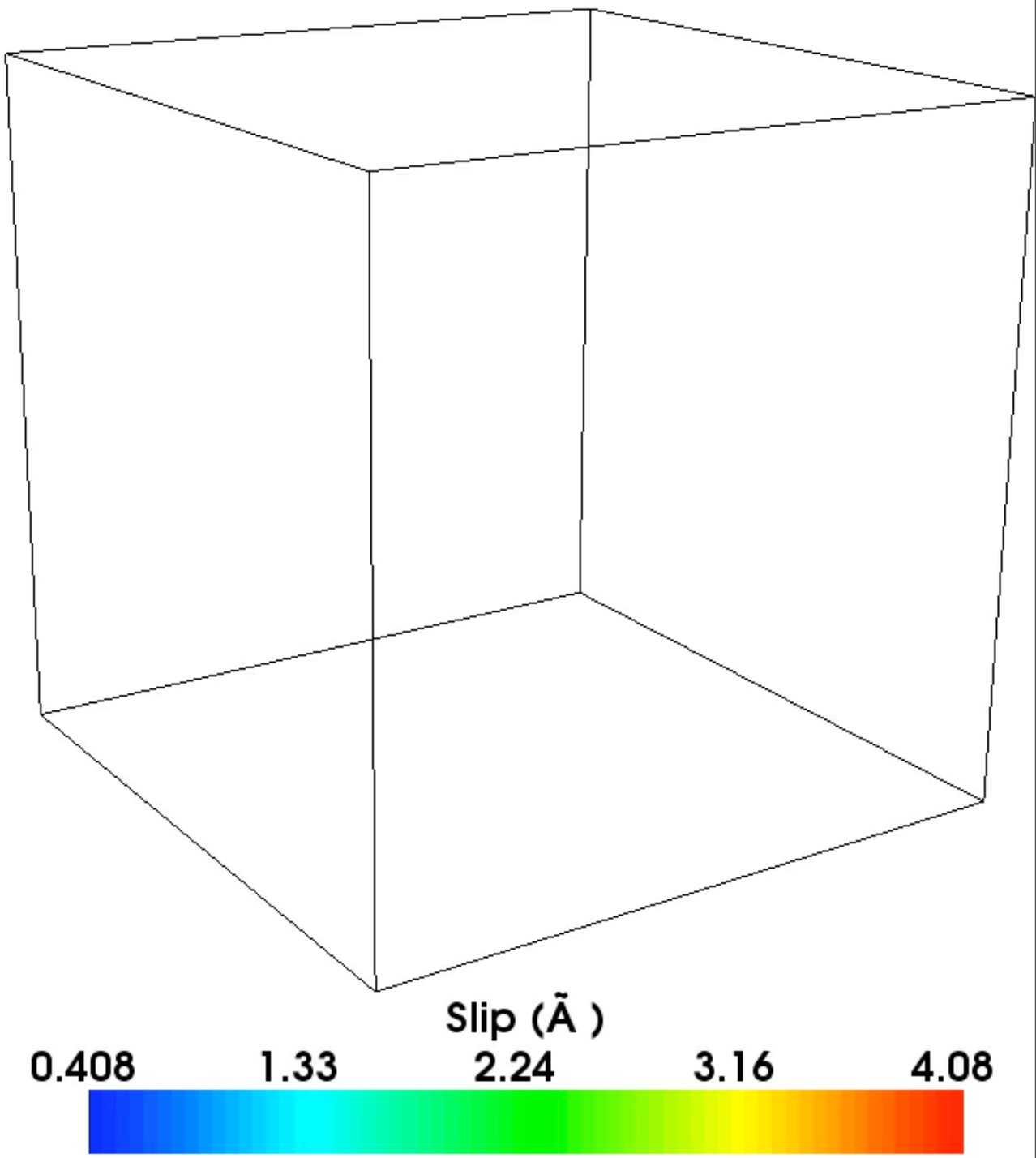
Au Slip Systems





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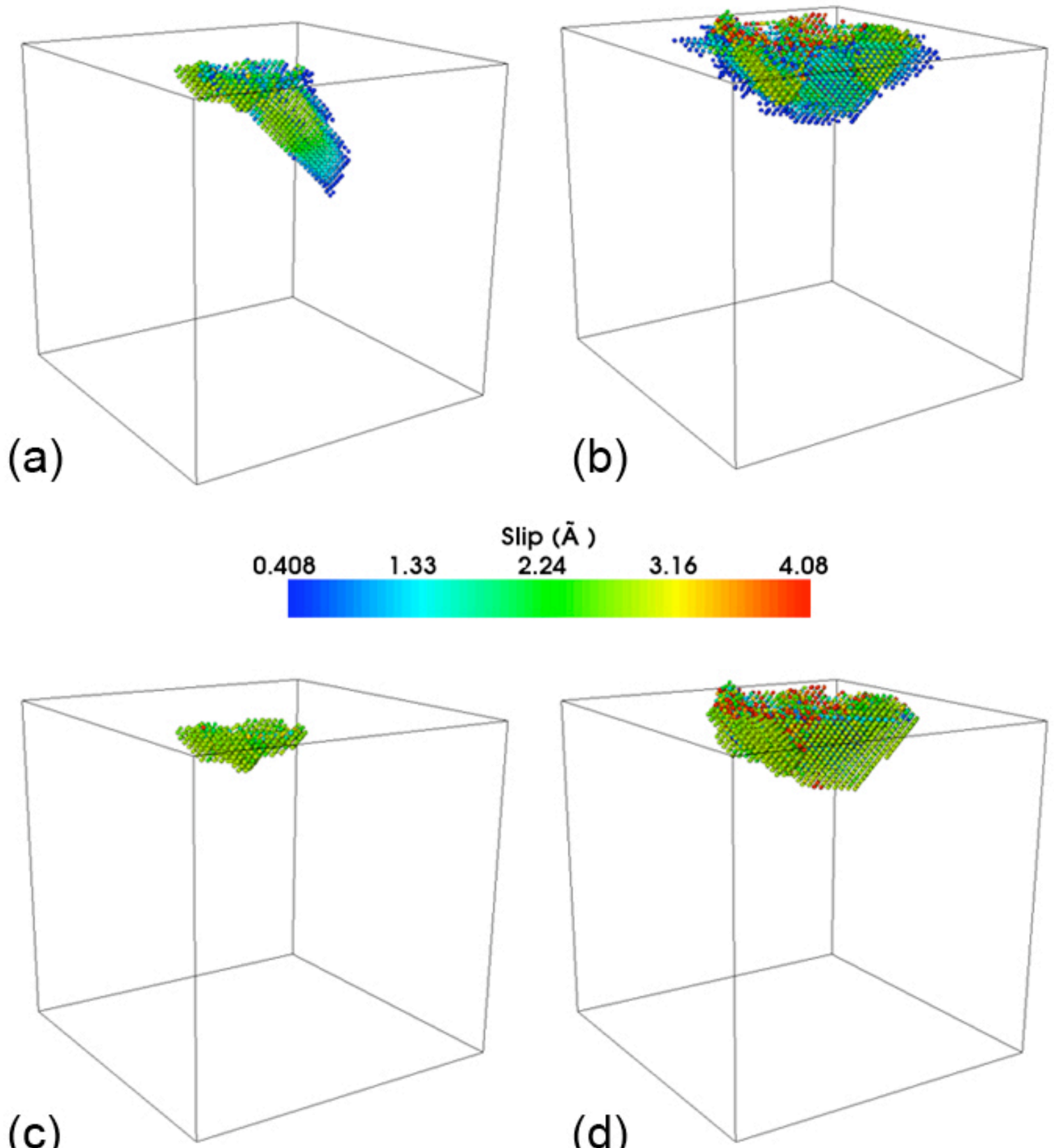

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Multiscale Model Results

- MD region contains 194,509 atoms, FE region contains 32,860 nodes - volume is equivalent to 13.1 x 10^6 atoms.
- Contact pressure from an atomistics only simulation is 19.6 GPa.
- Contact pressure from a coupled model simulation is 17.6 GPa.
- Contact pressure from a coupled model simulation to an equivalent depth is 10.4 GPa.

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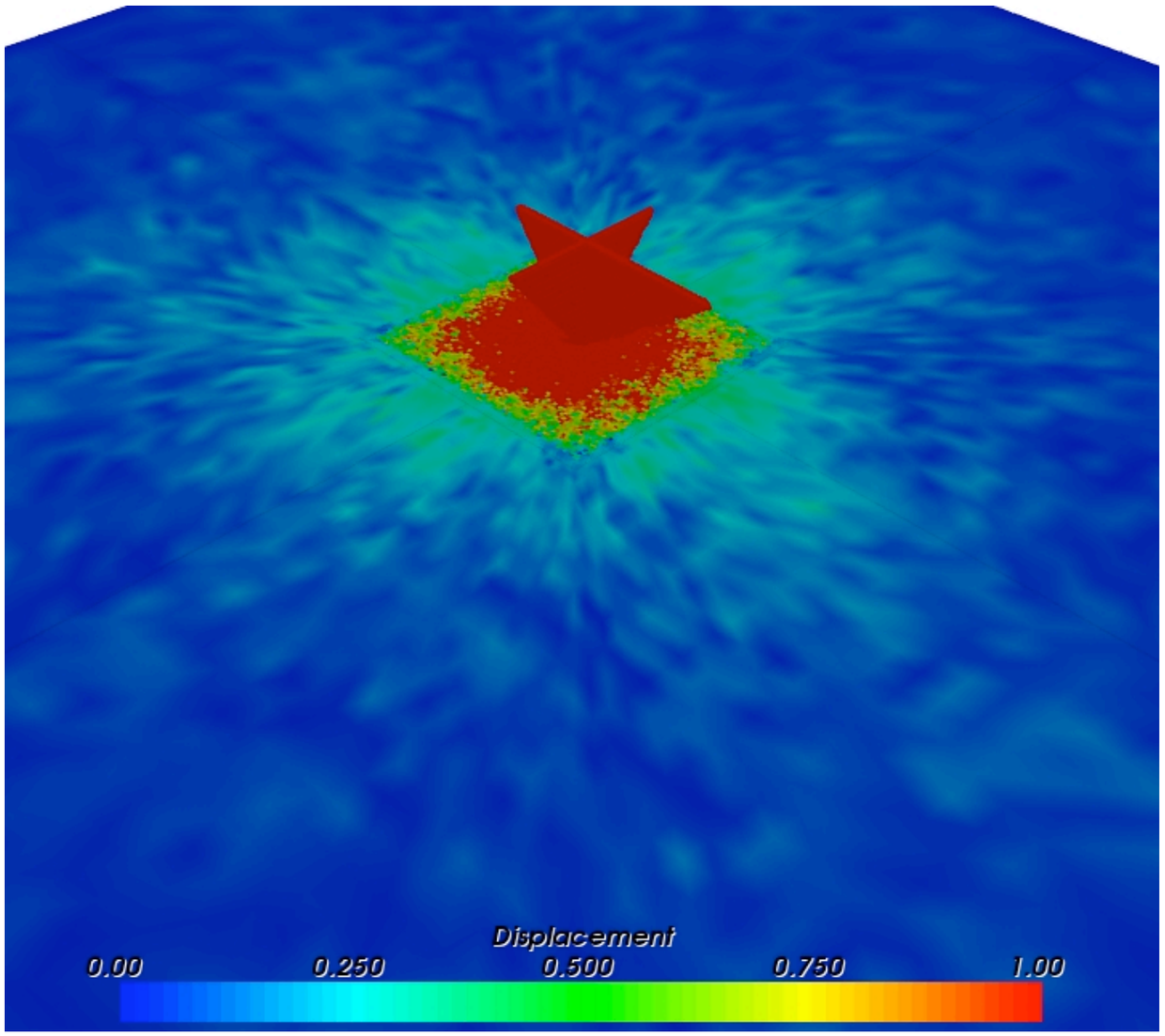
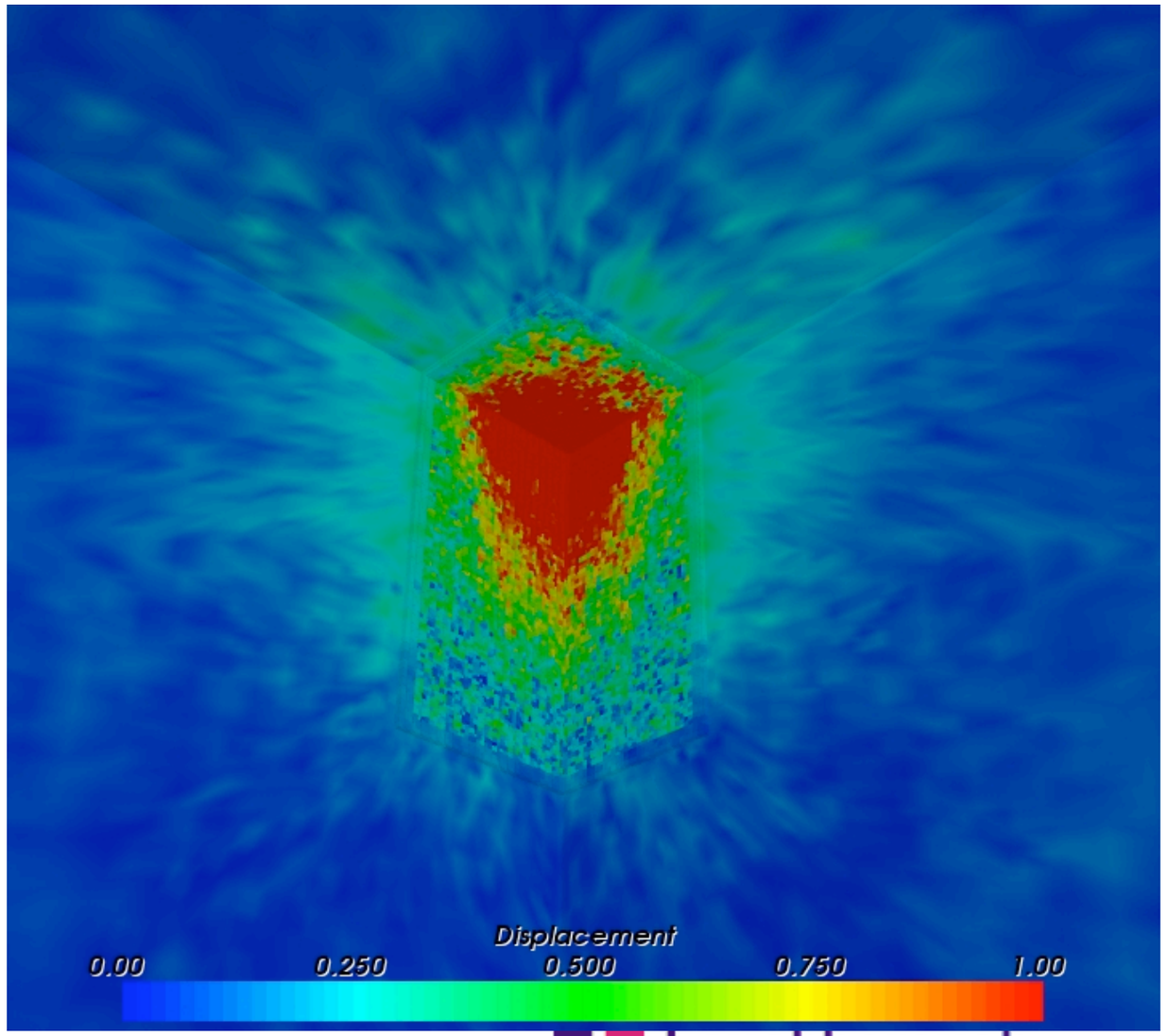
Displacement Field





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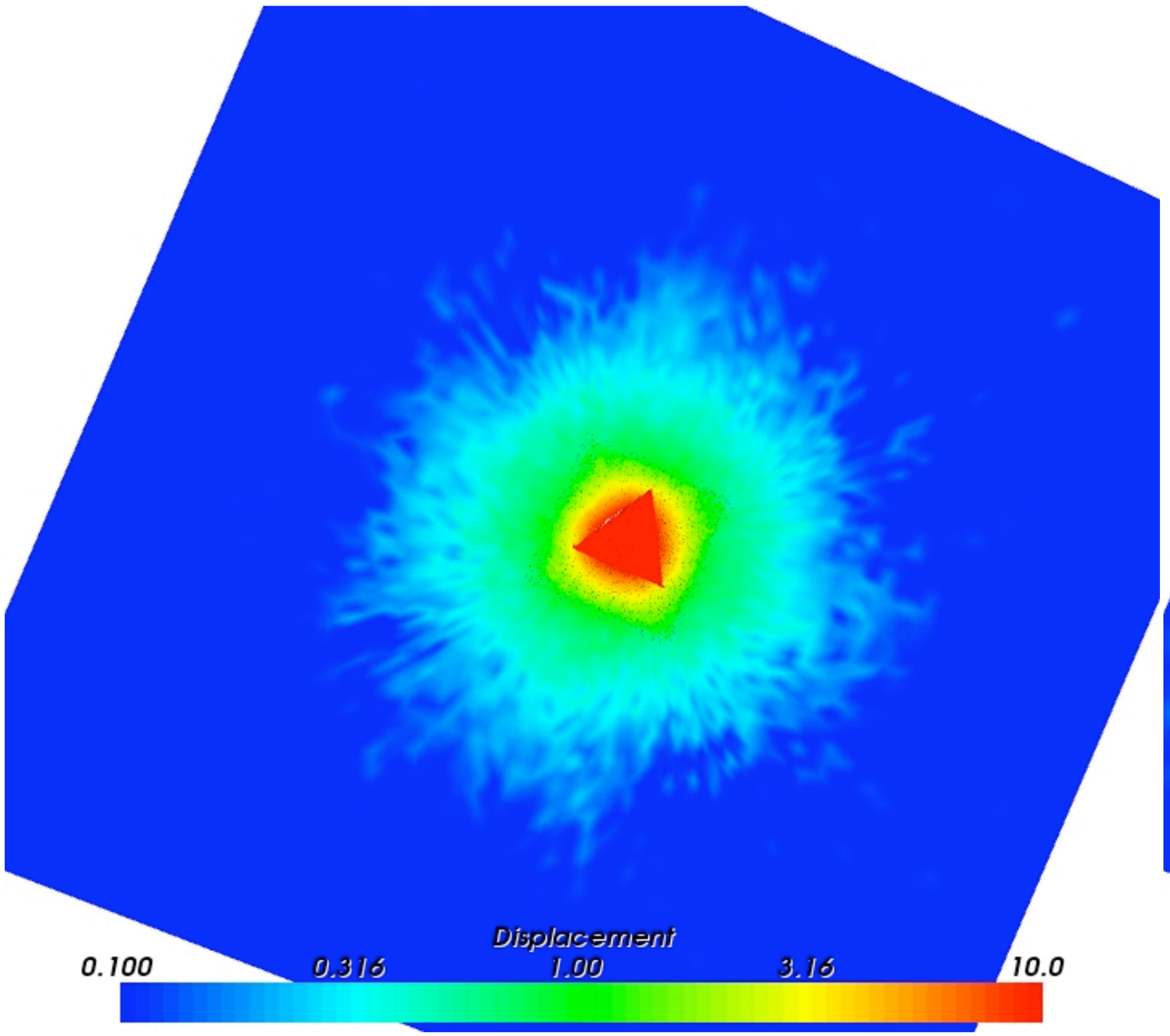
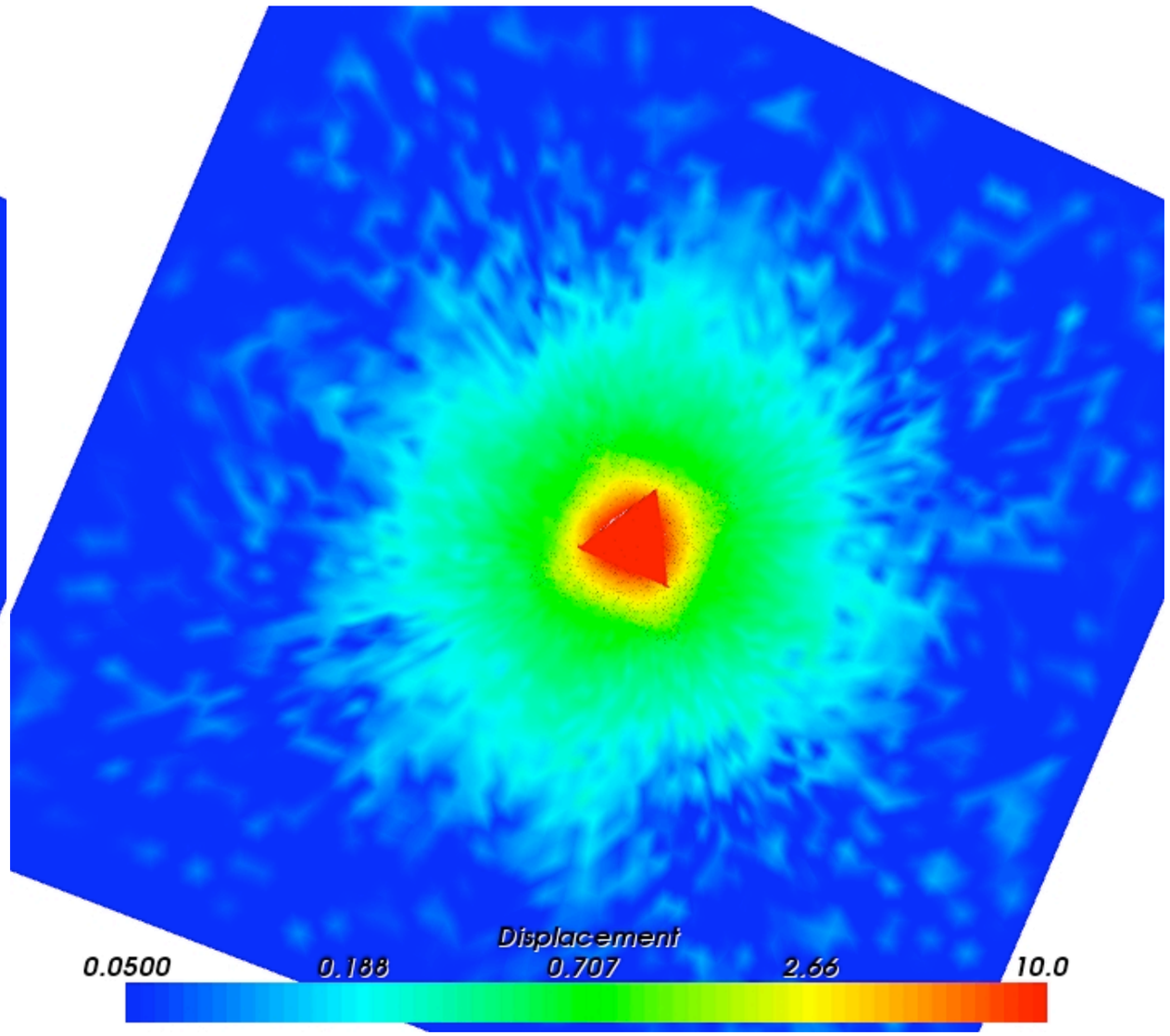
Displacement Field





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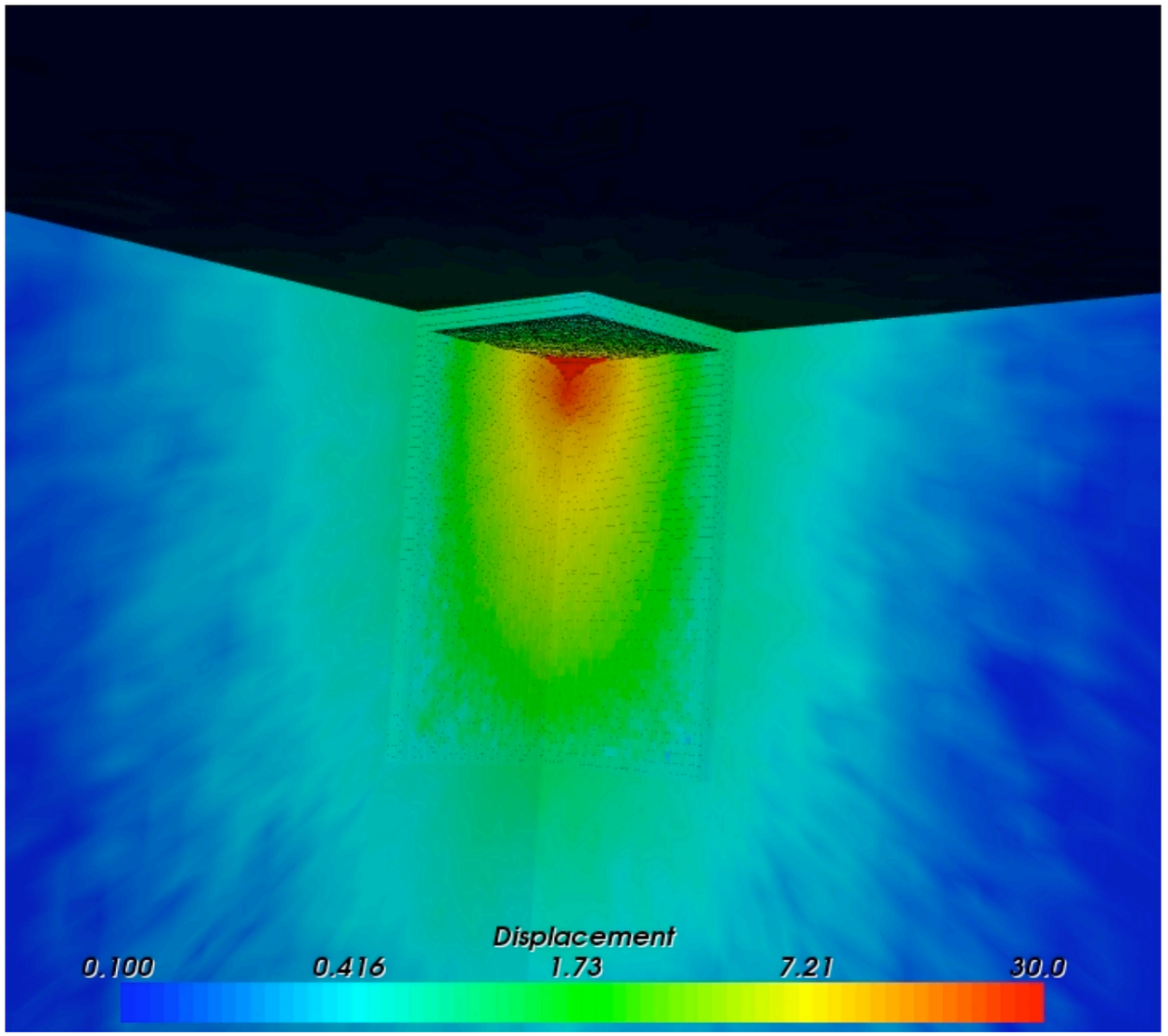
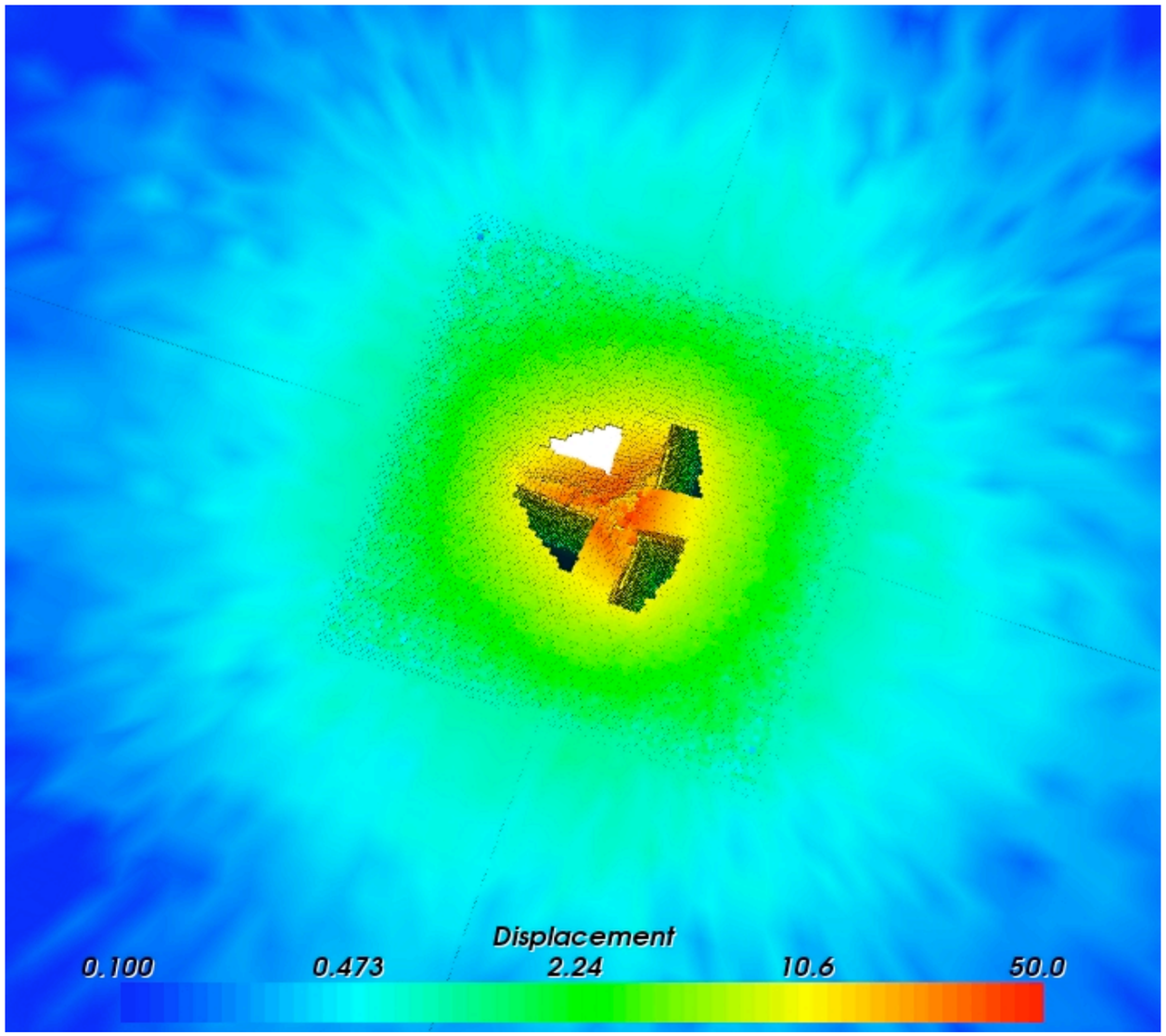
Displacement Field





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System Details

- ZnO
- Bond order potential
- 1.05m atoms
- 226,000 nodes, 1.3m elements
- 150 nm x 73 nm x 150 nm region
- Equivalent to over 140m atoms

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Multiscale Model Results

- For Si at 300K and a depth of 1.5 nm
  - MD only model - 24 GPa
  - Coupled model - 14.8 GPa
  - Experiment - 12 GPa
- For Al at 300K and a depth of 1.5 nm
  - MD only model - 13.3 GPa
  - Coupled model - 4.7 GPa

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Conclusions

- The atomistic-FE multiscale model allows length scales to be bridged.
- The correct description of the long range elastic fields gives a better agreement with experiment.
- The contact pressure is significantly reduced due to the inclusion of the long range elastic field.

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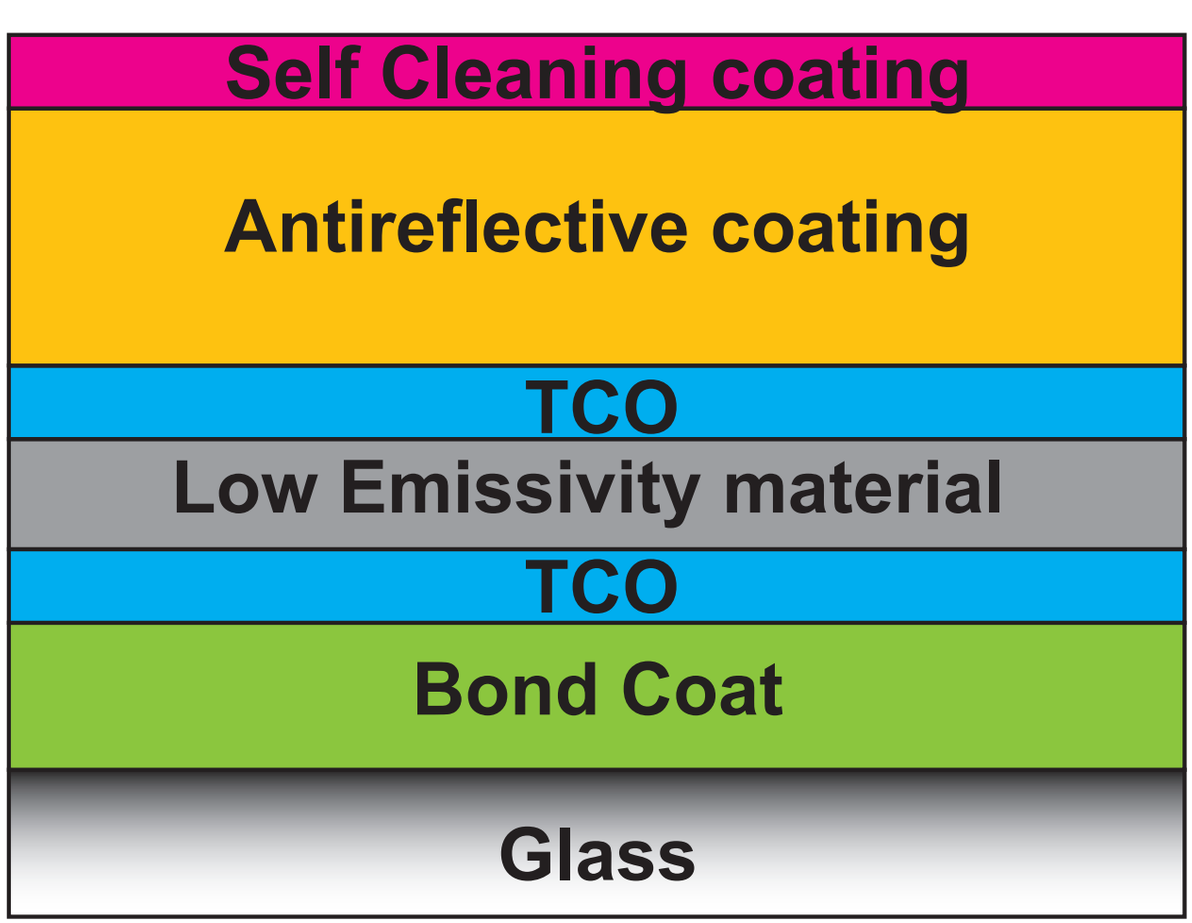
Further Work

- Non-linear elastic model in FE region
- Coulombic Interactions
- Layered systems



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Modelling Long Timescale Dynamics

- Modelling O diffusion in Er_2O_3
- Forms the bixbyite structure
- Radiation tolerant ceramic
- Interested in calculating the prefactor for hTST using Vineyard method

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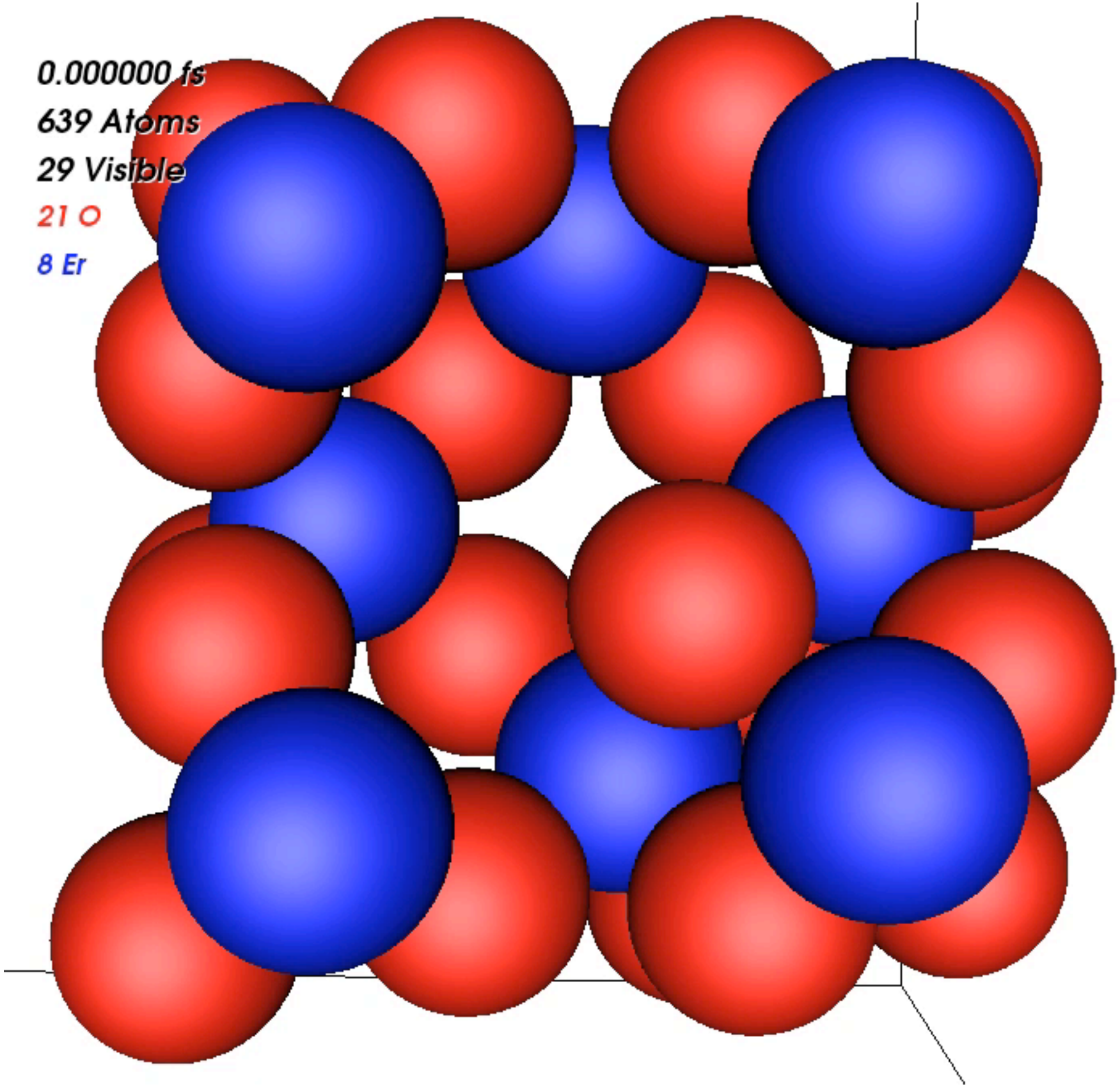

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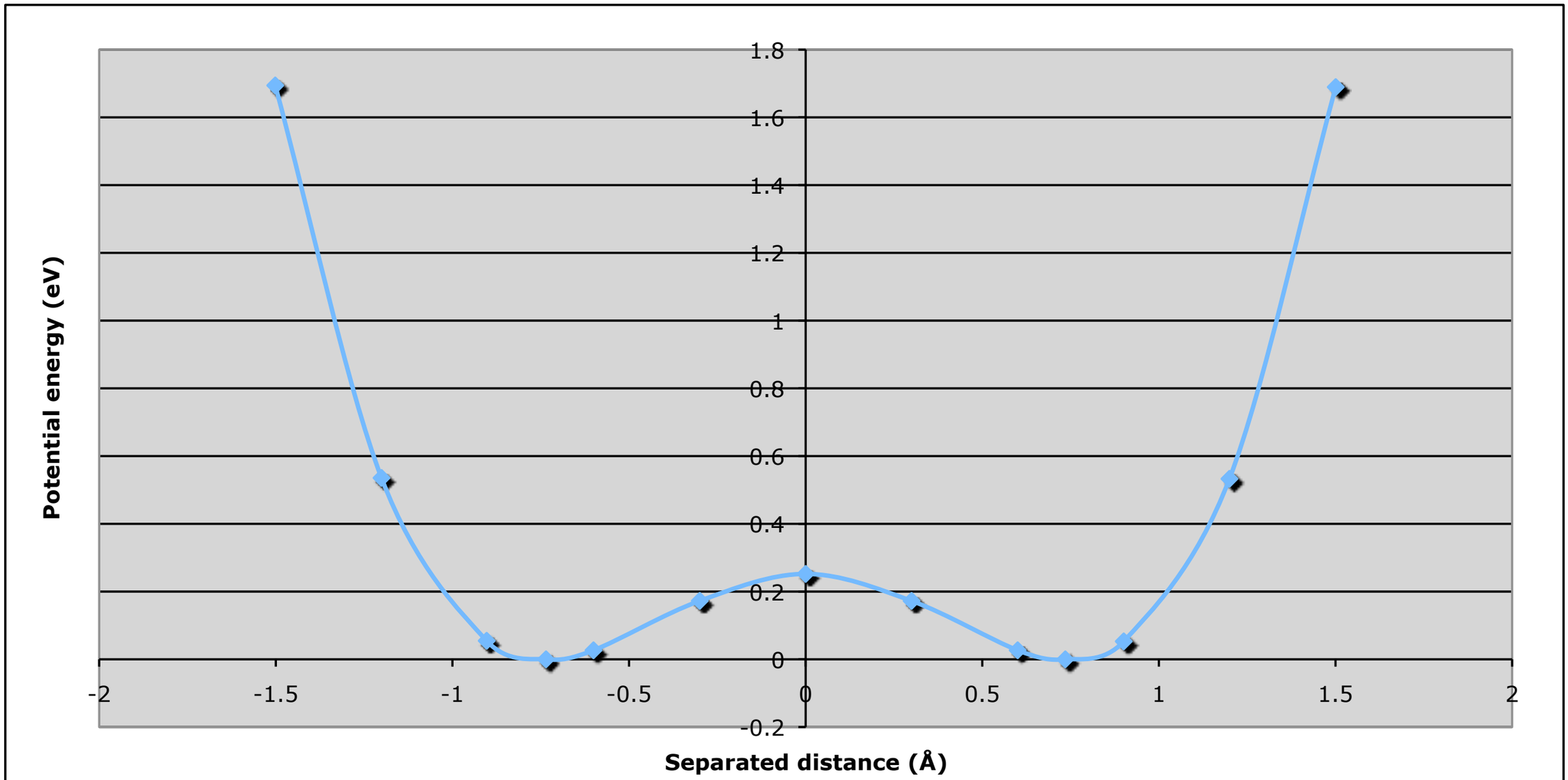
Energy Landscape



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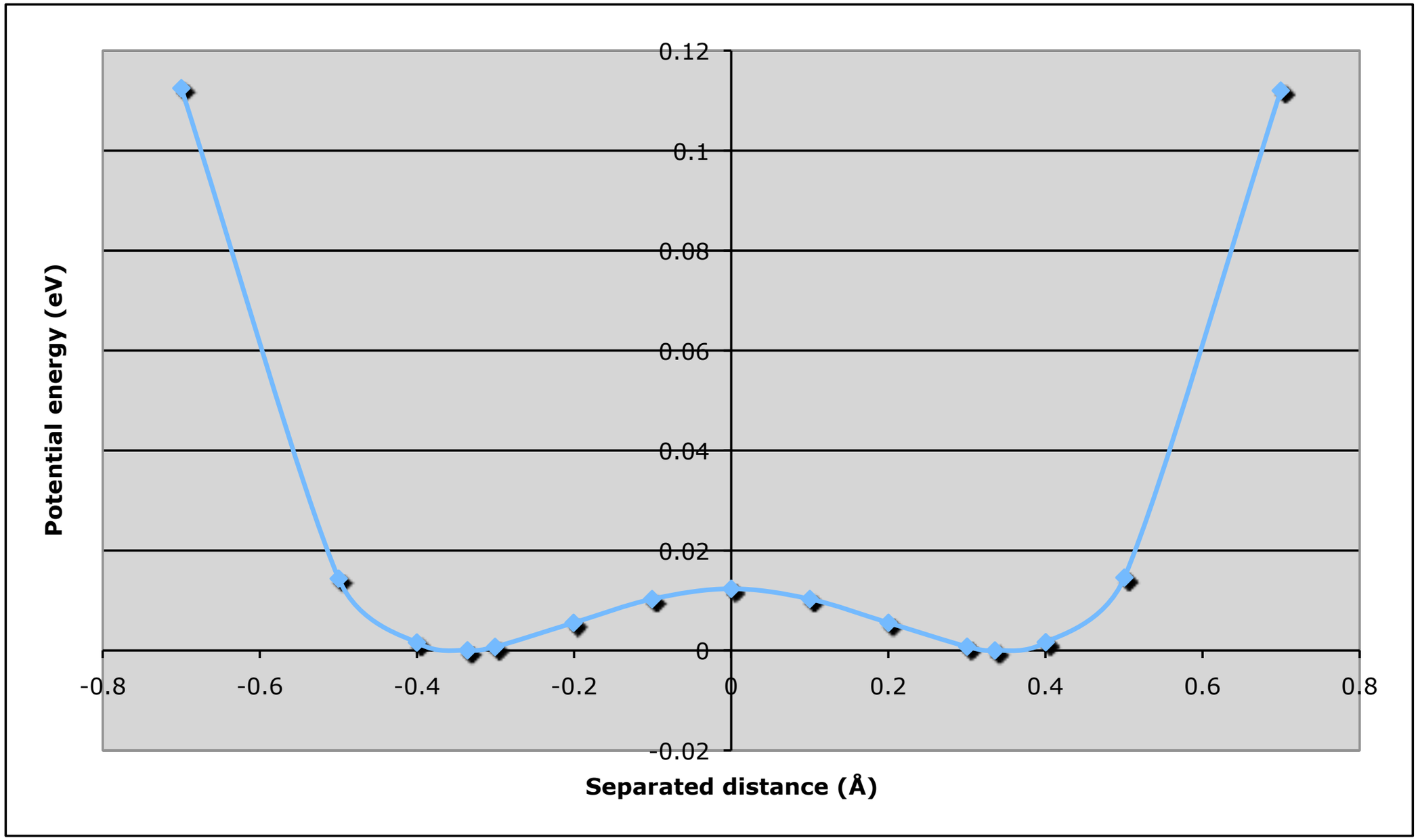
Energy Landscape



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Conclusions

- "Correct" path would not have double negative eigenvalue.
- Do such features exist?
- If so how would we deal with them?

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Acknowledgements

- Ismail Gheewala, Ed McGee, Lanchakorn Kittiratanawasin, Marc Robinson
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