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Dislocation-Interface Interactions in Silicon

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Lucas Hale
Post Doc
Sandia National Laboratories, CA

Jonathan Zimmerman, Xiaowang Zhou, Neville Moody
Sandia National Laboratories, CA

William Gerberich, Roberto Ballarini
University of Minnesota

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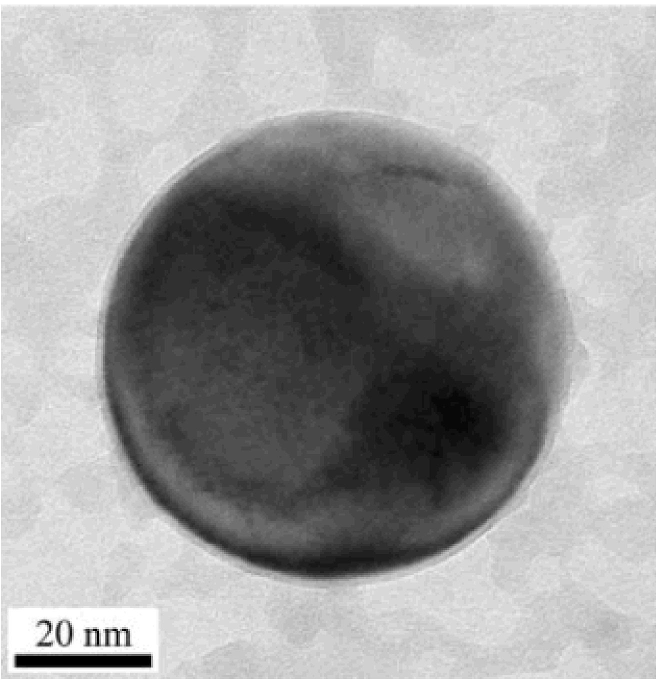
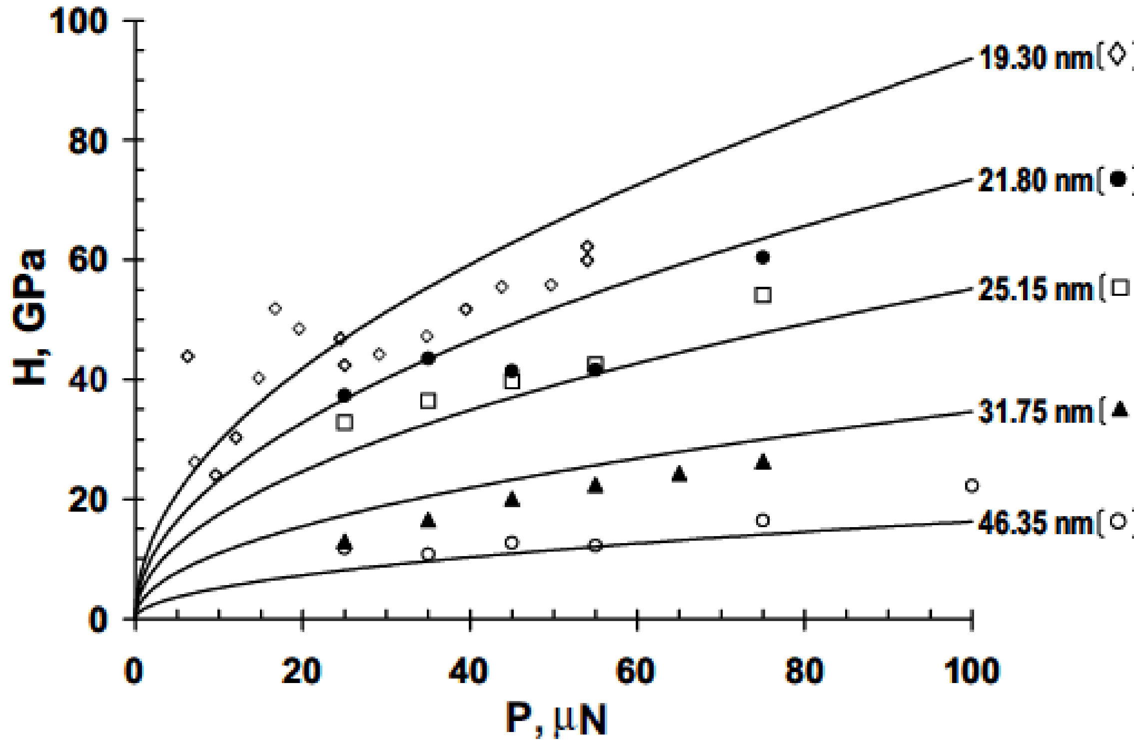
Super Hard Silicon Nanoparticles

- Compressed Si nanoparticles harder than bulk silicon





W.W. Gerberich, et. al, *Int. J. of Plasticity* **21** (2005) 2391

W.W. Gerberich, et al. *Journal of the Mechanics and Physics of Solids* **51** (2003) 979.

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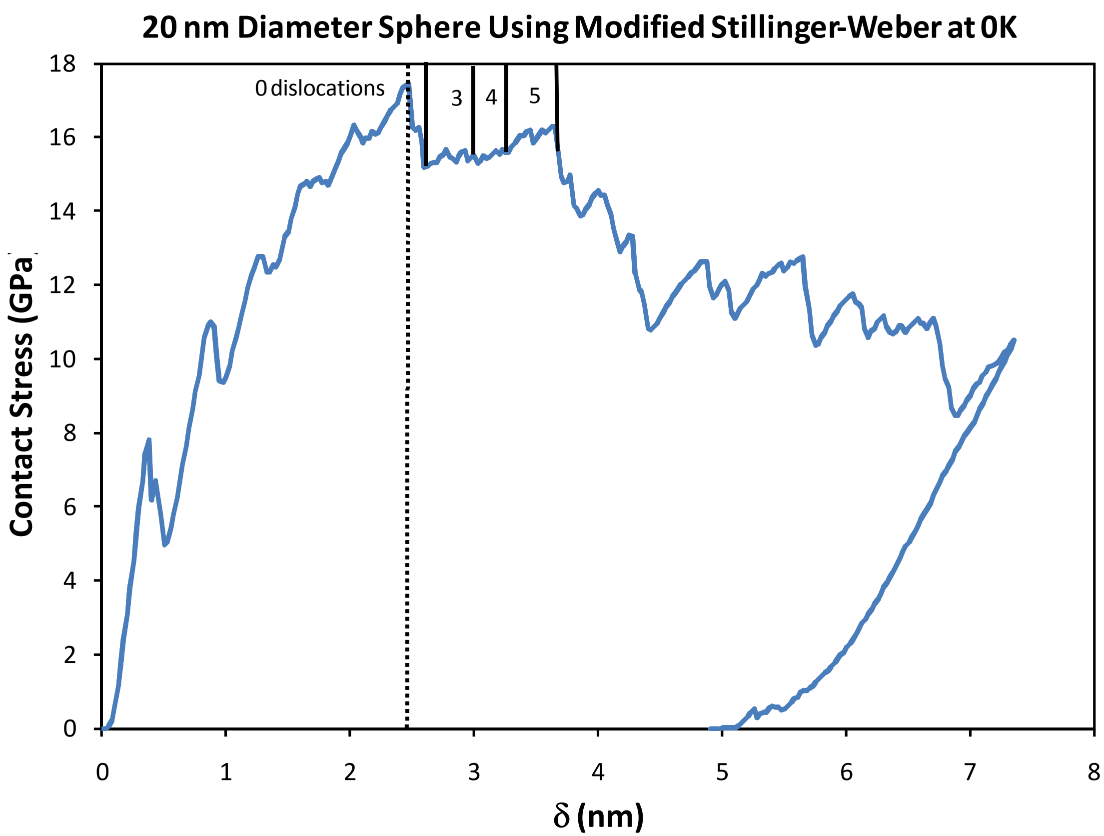
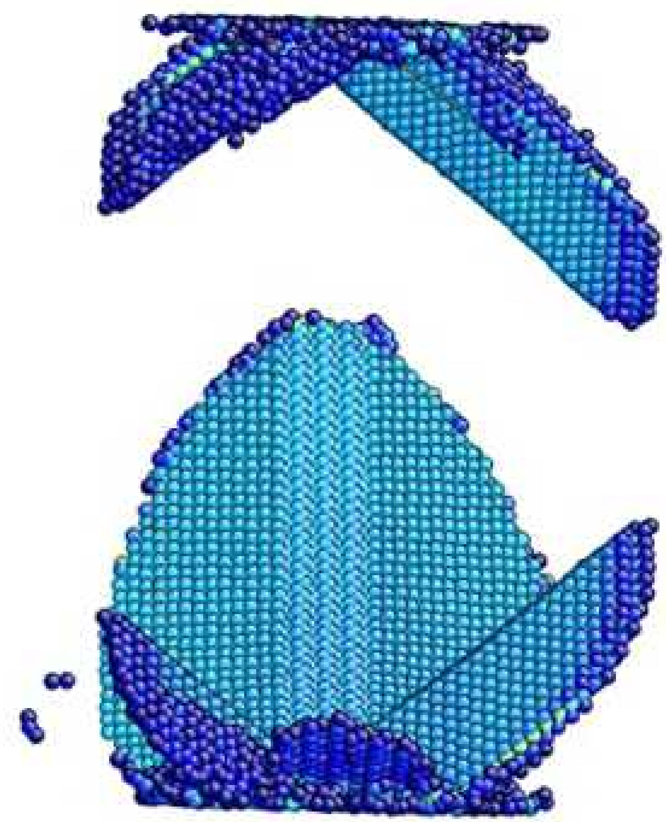
Increasing Number of Dislocations

- **Hardening at low strain with increasing dislocations**
- **Softening at high strains – dislocations reach surfaces**



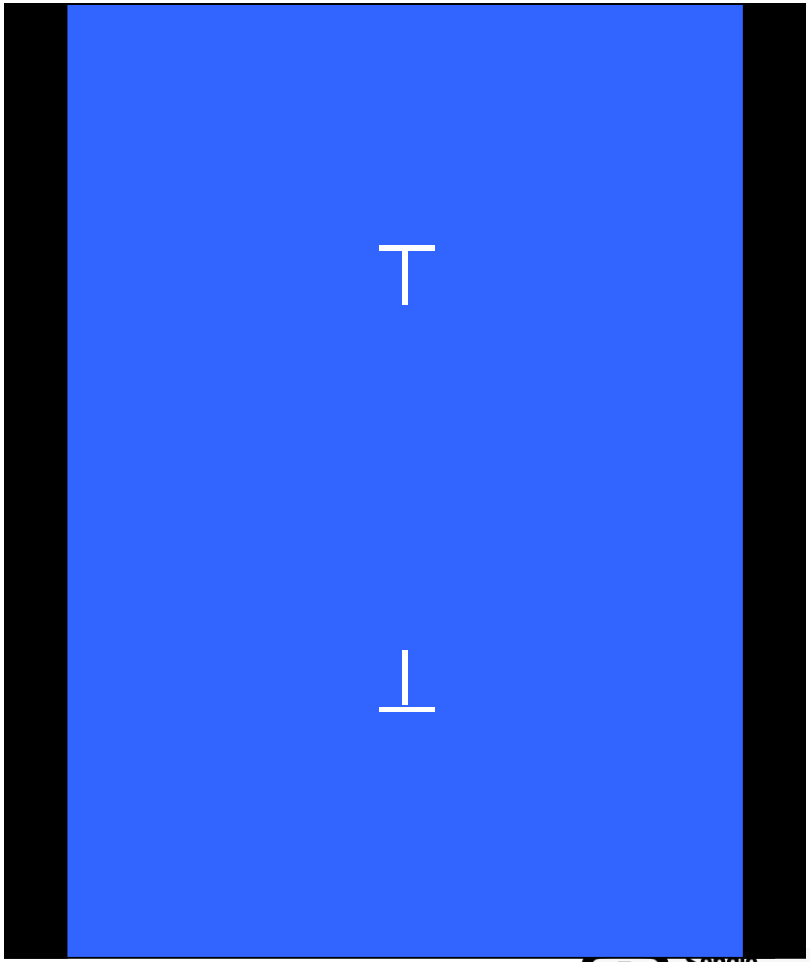


Dislocation Interaction Simulations

- **Will dislocation interactions in MD match elasticity based models?**
- **Can mechanically realistic material-oxide systems be simulated?**
- **Will oxide retain dislocations for hardness increase?**

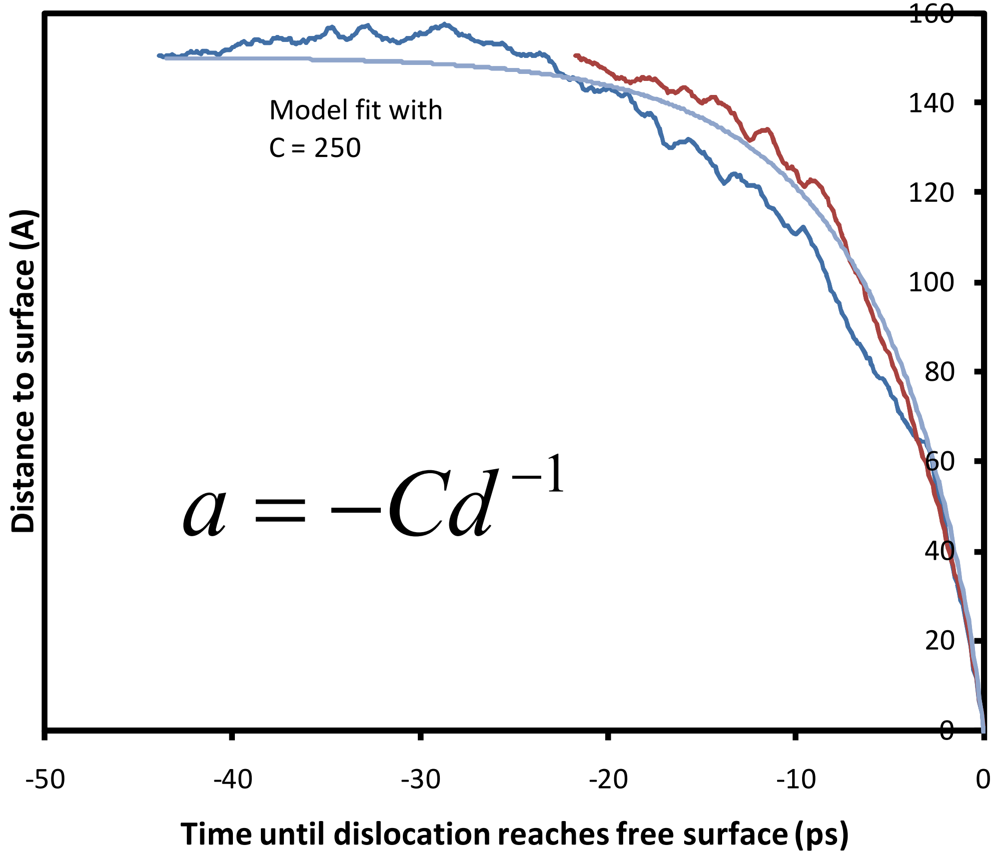
Simulation Design

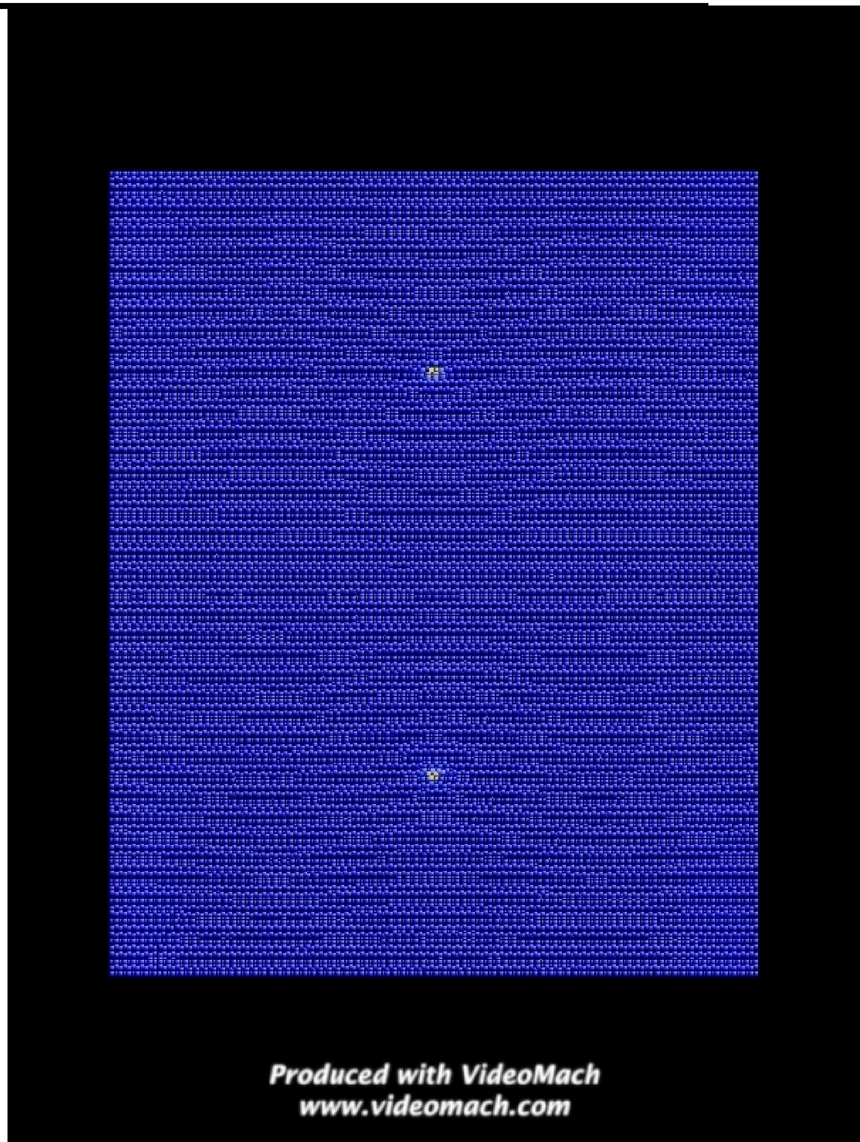
- Perfect edge dislocations
- Systems of 37920, 85648, 152640, and 238784 atoms used
- Stillinger-Weber silicon
- Two testing methods
  - All atoms unconstrained
  - Rigid y boundaries



Free Surface: No Shear Applied

$$F_X^{\text{Im}} = m_{\perp} a = -\frac{\mu b^2}{4\pi(1-\nu)d}$$





Si/SiO_2 Potential

- **Watanabe et al.[1] modification of the Stillinger-Weber is able to model both Si and SiO_2**

- **Introduces bond softening function to 2-body term based on Si-O binding energy with coordination**

- **Cutoffs and preferred bond angles less restricted in three-body term**

- **Stable and correct polymorphs**

[1] T Watanabe, H Fujiwara, H Noguchi, T Hoshino, and I Ohdomari, *Jpn. J. Appl. Phys.* **38** (1999) L366

LAMMPS Implementation

- Stillinger-Weber code modified
- 2 parameter sets in literature, both included
- ~2X slower than Stillinger-Weber (coordination dependent)
- Tested values consistent with report
  - Si behaves exactly like Stillinger-Weber
  - Si-O dimer energy and bond length
  - α-Quartz lattice energy and Si-O length

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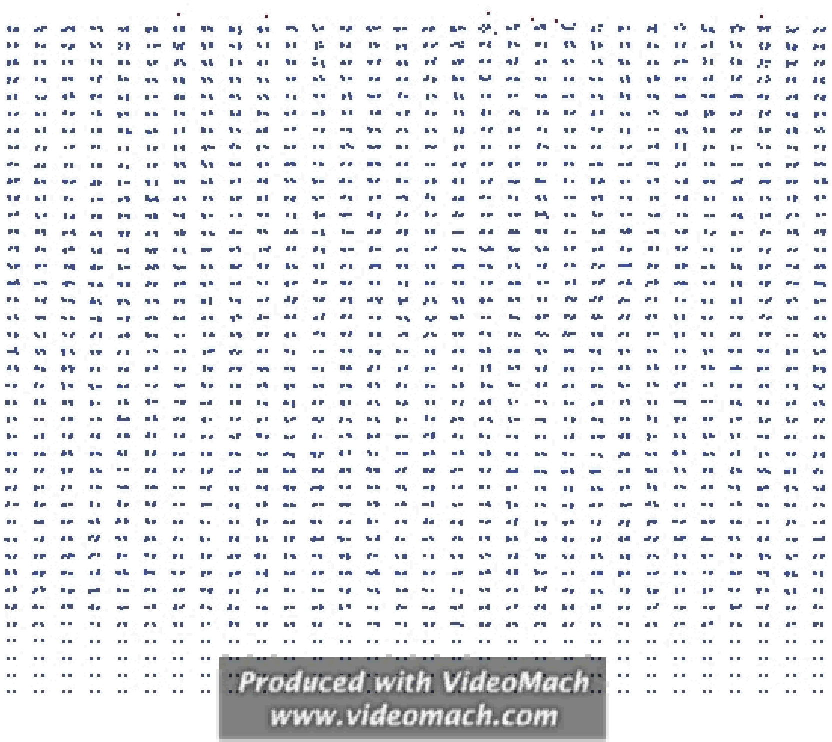
Oxide Growth

- **Use growth routine by Dalla Torre, et al.[1]**

1. **Add O atoms at surface**
2. **Run LAMMPS**
3. **Add new O atoms in leap-frog method**
4. **Repeat 2 and 3 until desired thickness**



[1] J. Dalla Torre, J.-L. Bocquet, Y. Limoge, J.-P. Crocombette, E. Adam, G. Martin, T. Baron, P. Rivallin, and P. Mur, *J. Appl. Phys.* **92** (2002) 1084

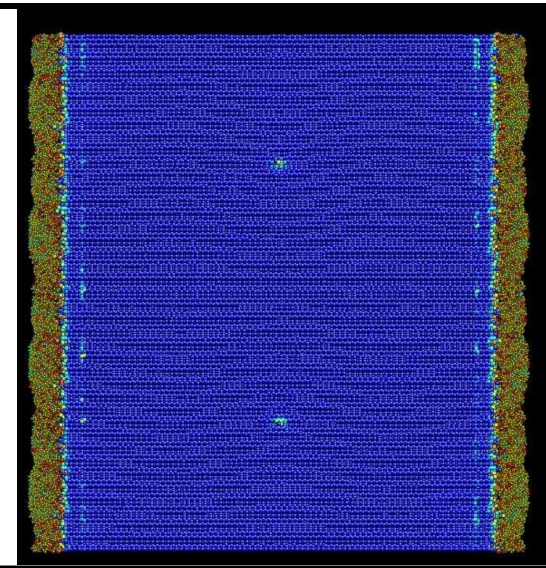
Oxide Interactions

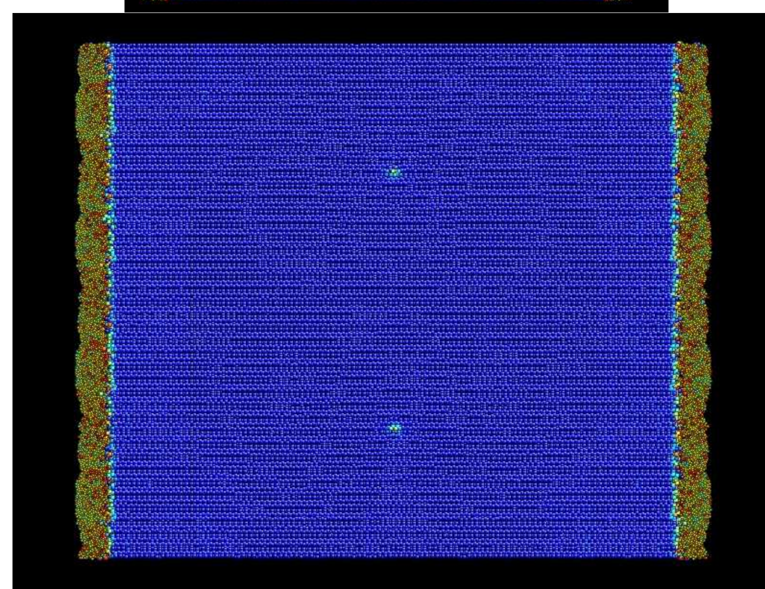
- **Oxide added to free surface system**

- **Dislocation theory:**

$$F_X^{Int} = \frac{\mu b b^*}{4\pi(1-\nu)d} = \frac{\mu - \mu^*}{\mu^* + \mu} F_x^{\mathrm{Im}}$$

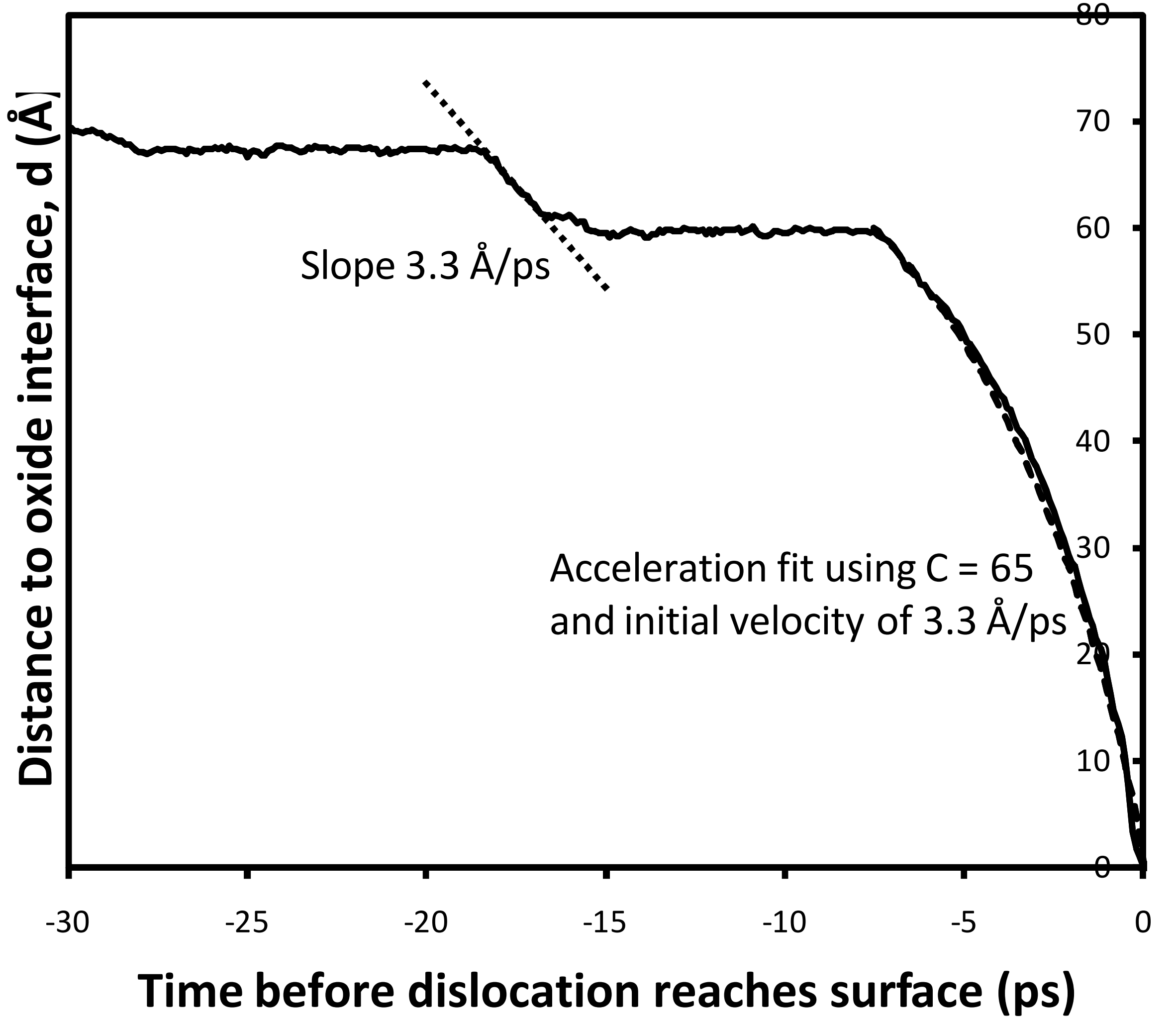
- **Predicted attraction of 1/3-1/4 strength of free surface**





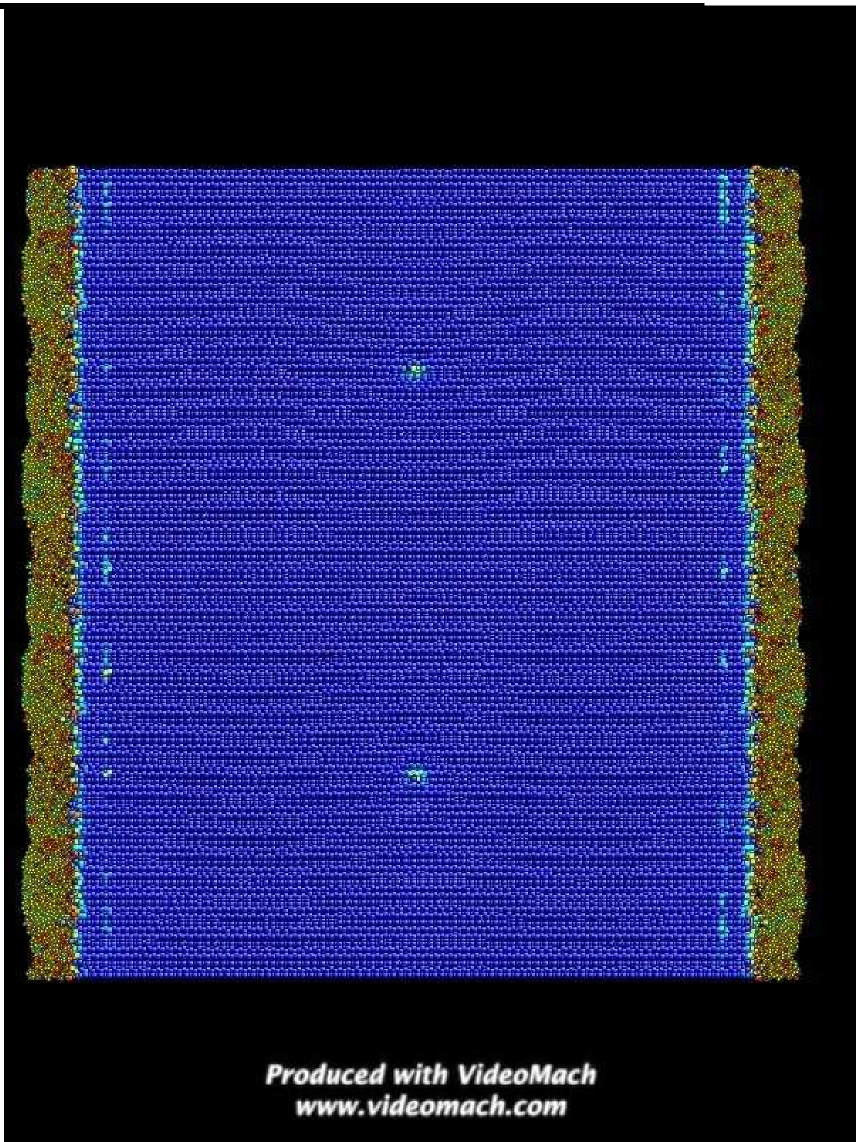
Attraction to Interface

- **Incremental straining with holds**
- **Attraction during last straining**
- **C is 1/4 -1/5 free surface value**



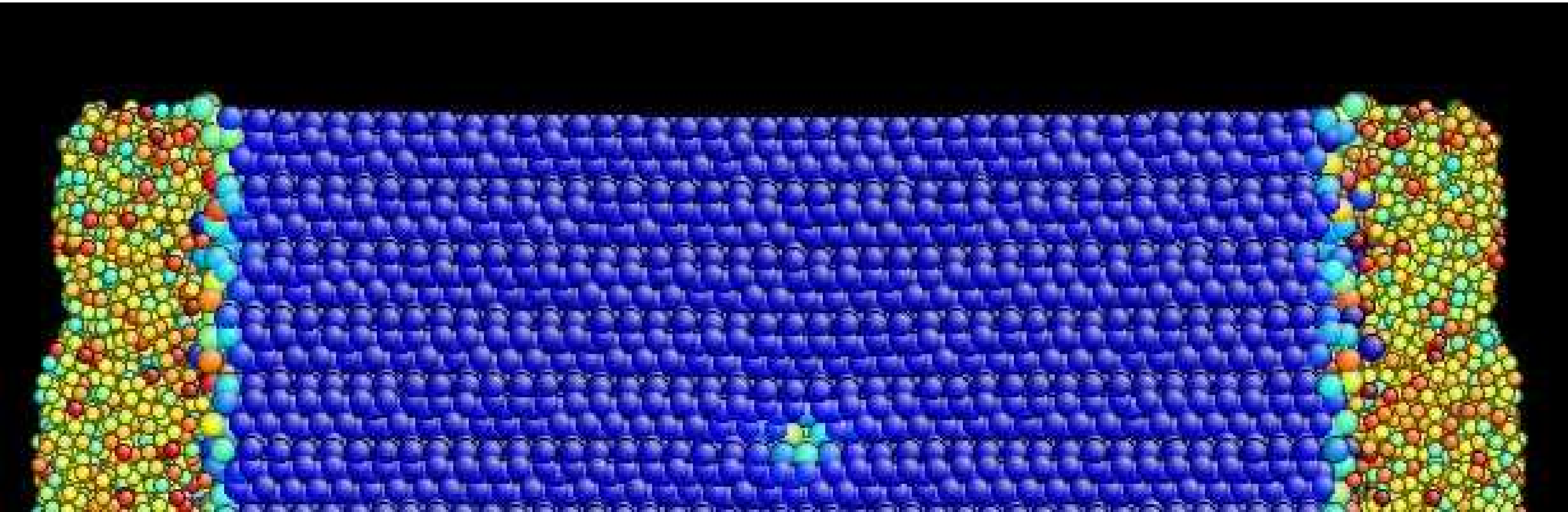
Long Range Repulsion

- **Dislocation positions remain fixed in unconstrained systems**
- **No dislocation-dislocation repulsion seen**
- **Oxide is repulsive**



Stress State

- Oxide places surfaces in tension
- Stress gradient results in shear stresses
- Long range repulsion



Conclusions

- Free surface attraction consistent with image forces
- Short range attraction to oxide interface observed
- Presence of oxide is repulsive at long range due to stress state of system
- Repulsion can lead to dislocation buildup depending on stress state due to oxide