

Dislocation-Interface Interactions in Silicon

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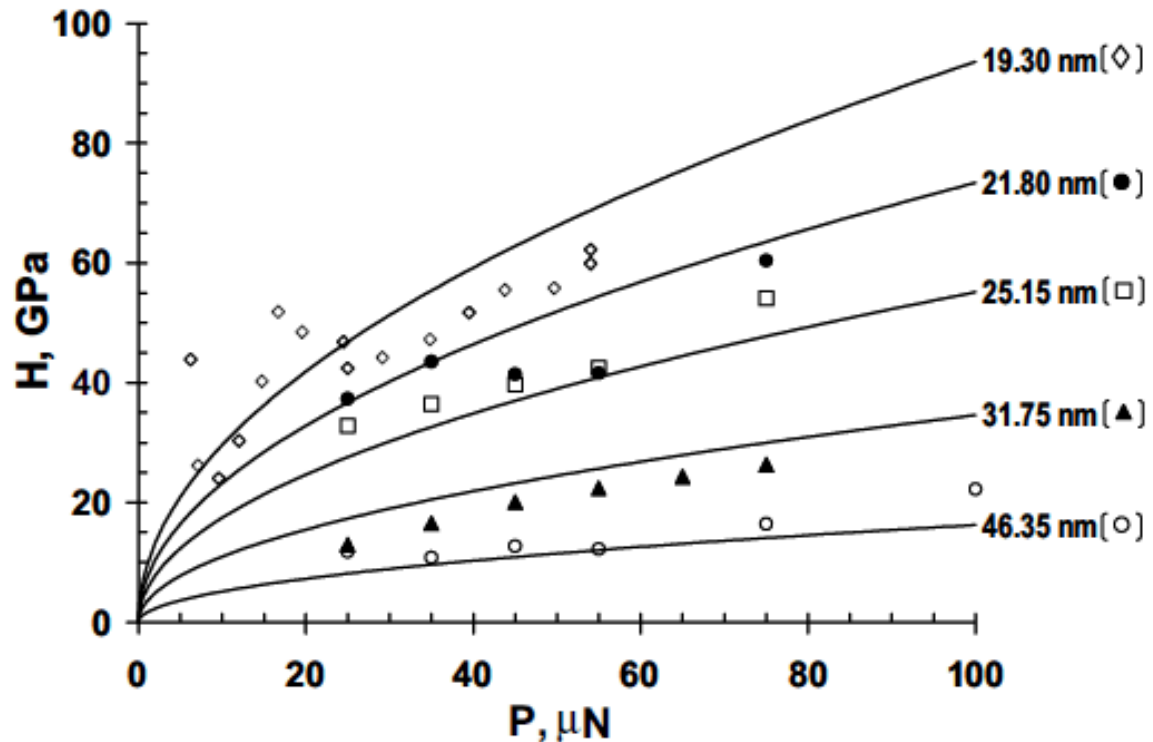
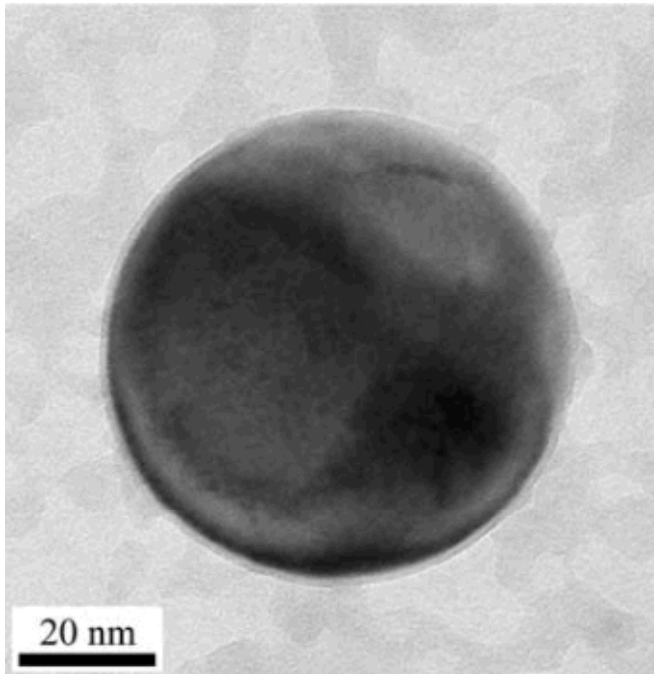
**Jonathan Zimmerman, Xiaowang Zhou, Neville Moody
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Super Hard Silicon Nanoparticles

- Compressed Si nanoparticles harder than bulk silicon



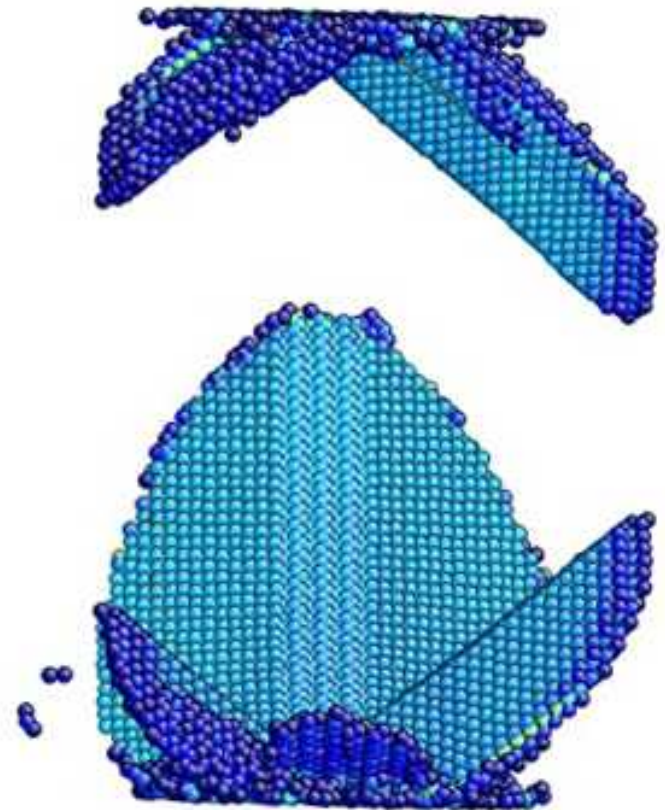
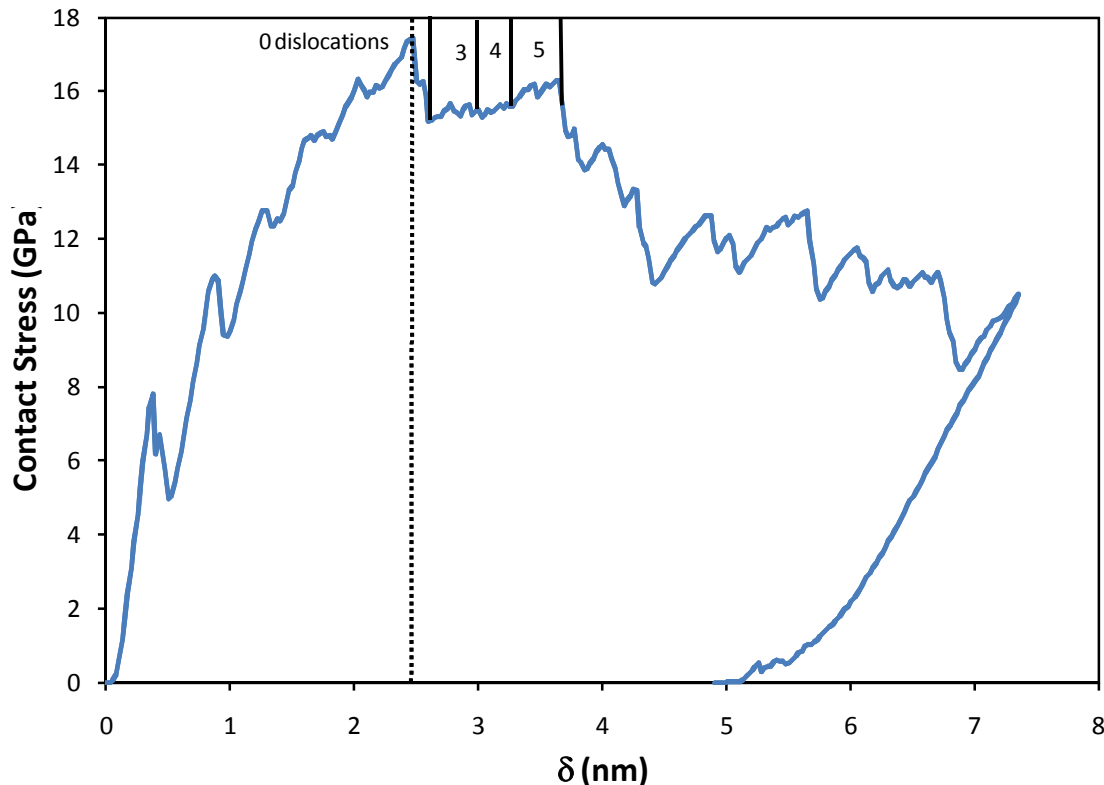
W.W. Gerberich, et. al, *Int. J. of Plasticity* **21** (2005) 2391

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

Increasing Number of Dislocations

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

20 nm Diameter Sphere Using Modified Stillinger-Weber at 0K





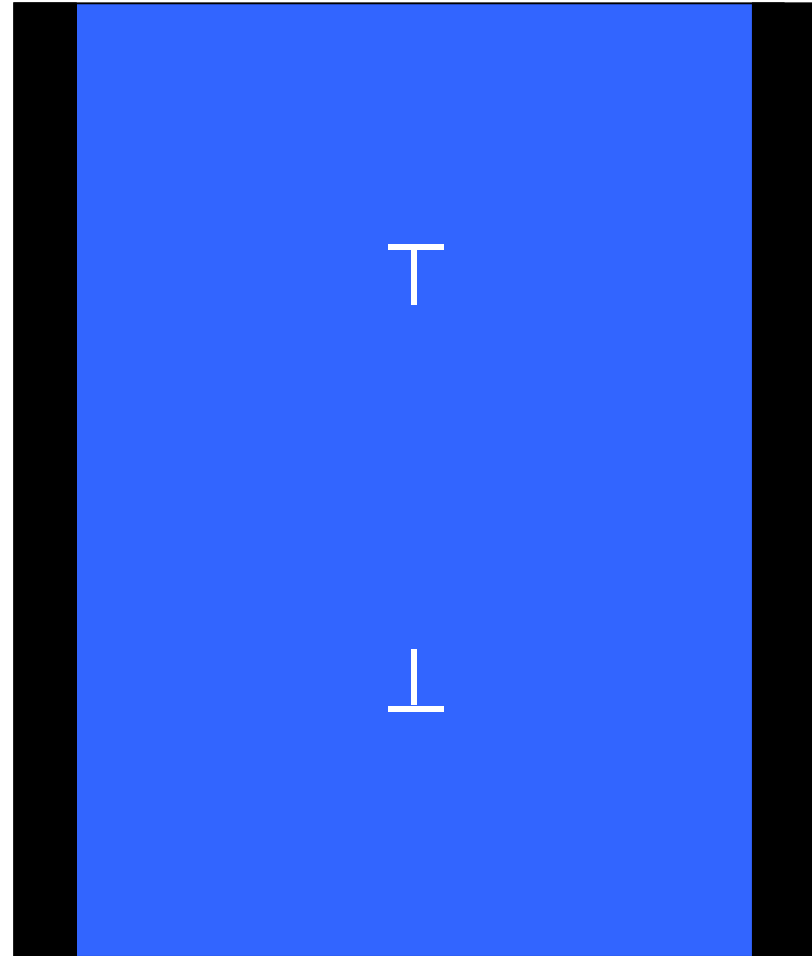
Dislocation Interaction Simulations

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



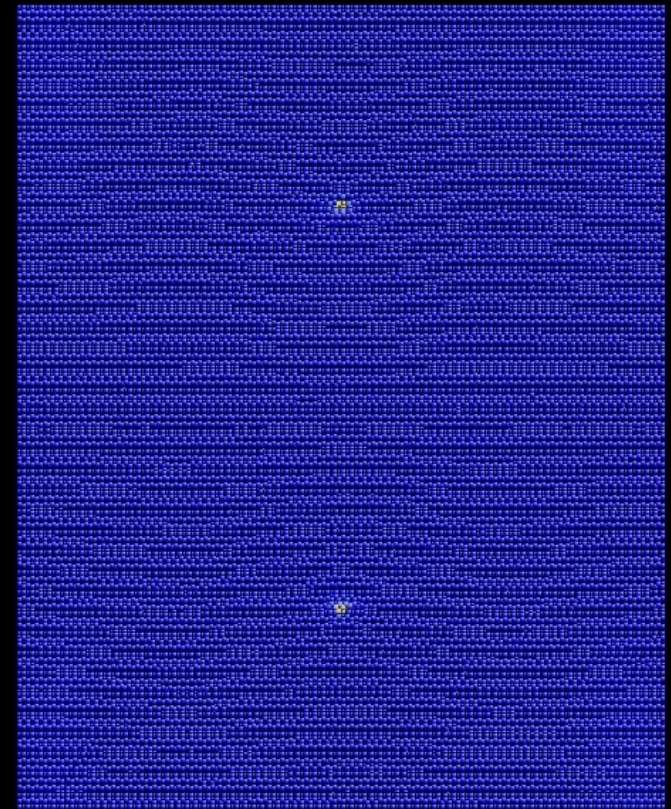
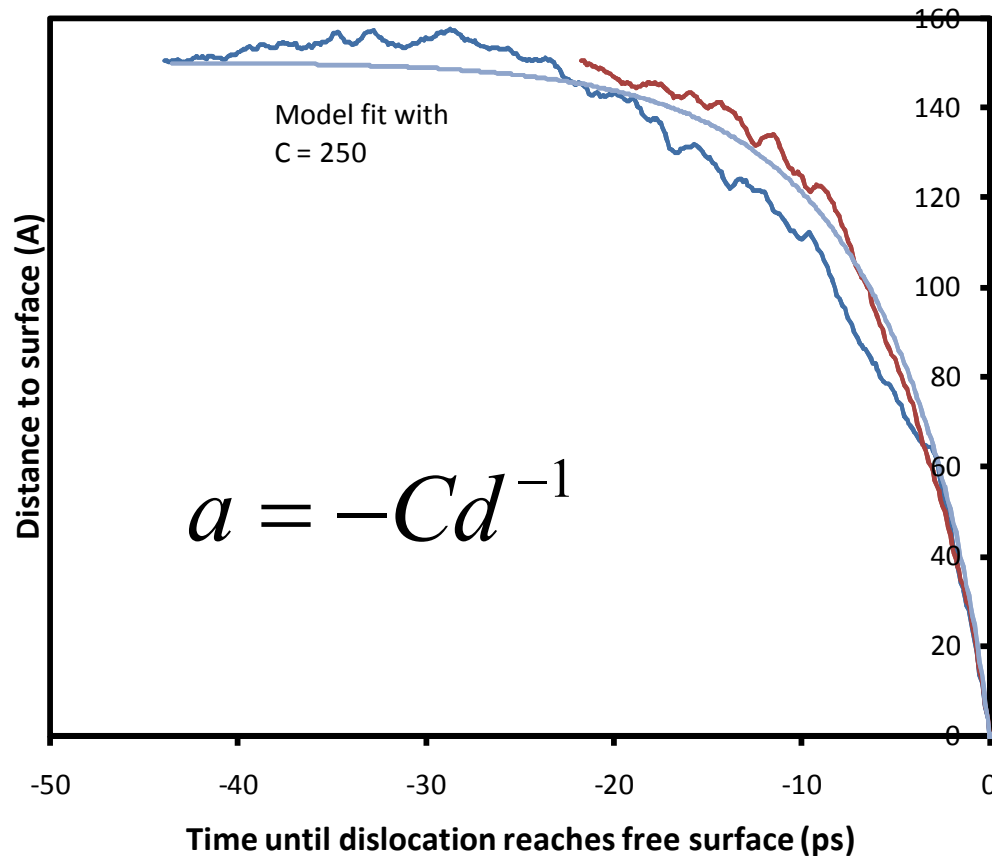
Simulation Design

- **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/SiO₂ Potential

- **Watanabe et al.^[1] modification of the Stillinger-Weber is able to model both Si and SiO₂**
- **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**

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**

00	01	02	03	04	05	06	07	08	09	0A	0B	0C	0D	0E	0F	00	01	02	03	04	05	06	07	08	09	0A	0B	0C	0D	0E	0F
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B0	B1	B2	B3	B4	B5	B6	B7	B8	B9	BA	BB	BC	BD	BE	BF	B0	B1	B2	B3	B4	B5	B6	B7	B8	B9	BA	BB	BC	BD	BE	BF
C0	C1	C2	C3	C4	C5	C6	C7	C8	C9	CA	CB	CC	CD	CE	CF	C0	C1	C2	C3	C4	C5	C6	C7	C8	C9	CA	CB	CC	CD	CE	CF
D0	D1	D2	D3	D4	D5	D6	D7	D8	D9	DA	DB	DC	DD	DE	DF	D0	D1	D2	D3	D4	D5	D6	D7	D8	D9	DA	DB	DC	DD	DE	DF
E0	E1	E2	E3	E4	E5	E6	E7	E8	E9	EA	EB	EC	ED	EE	EF	E0	E1	E2	E3	E4	E5	E6	E7	E8	E9	EA	EB	EC	ED	EE	EF
F0	F1	F2	F3	F4	F5	F6	F7	F8	F9	FA	FB	FC	FD	FE	FF	F0	F1	F2	F3	F4	F5	F6	F7	F8	F9	FA	FB	FC	FD	FE	FF
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www.videomach.com

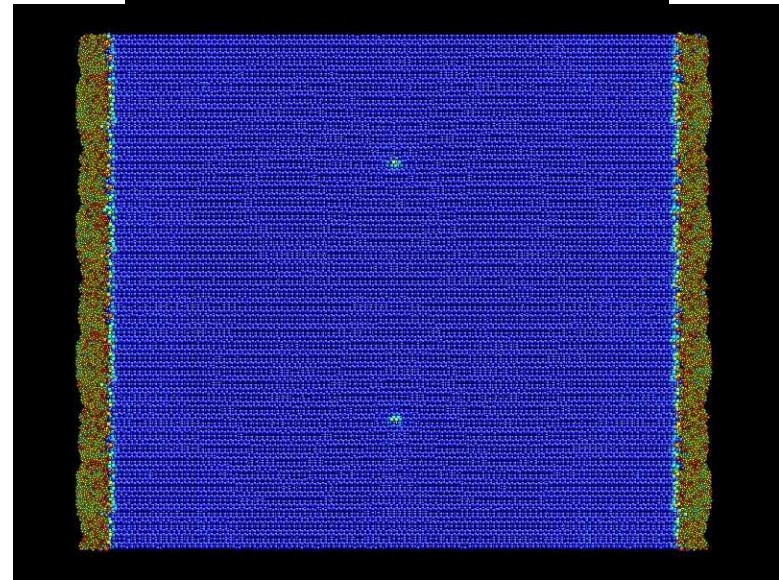
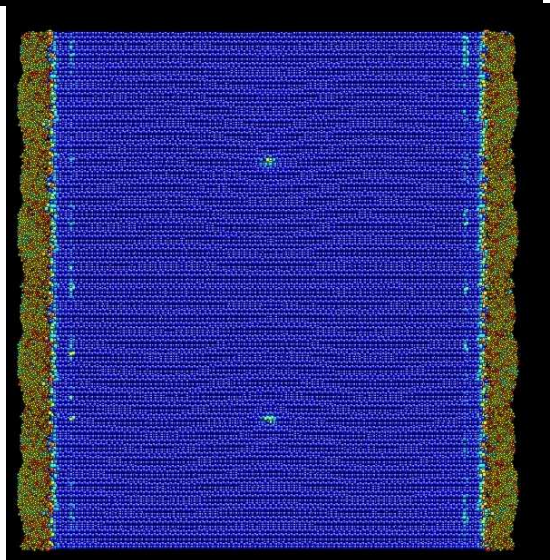
Oxide Interactions

- Oxide added to free surface system

- Dislocation theory:

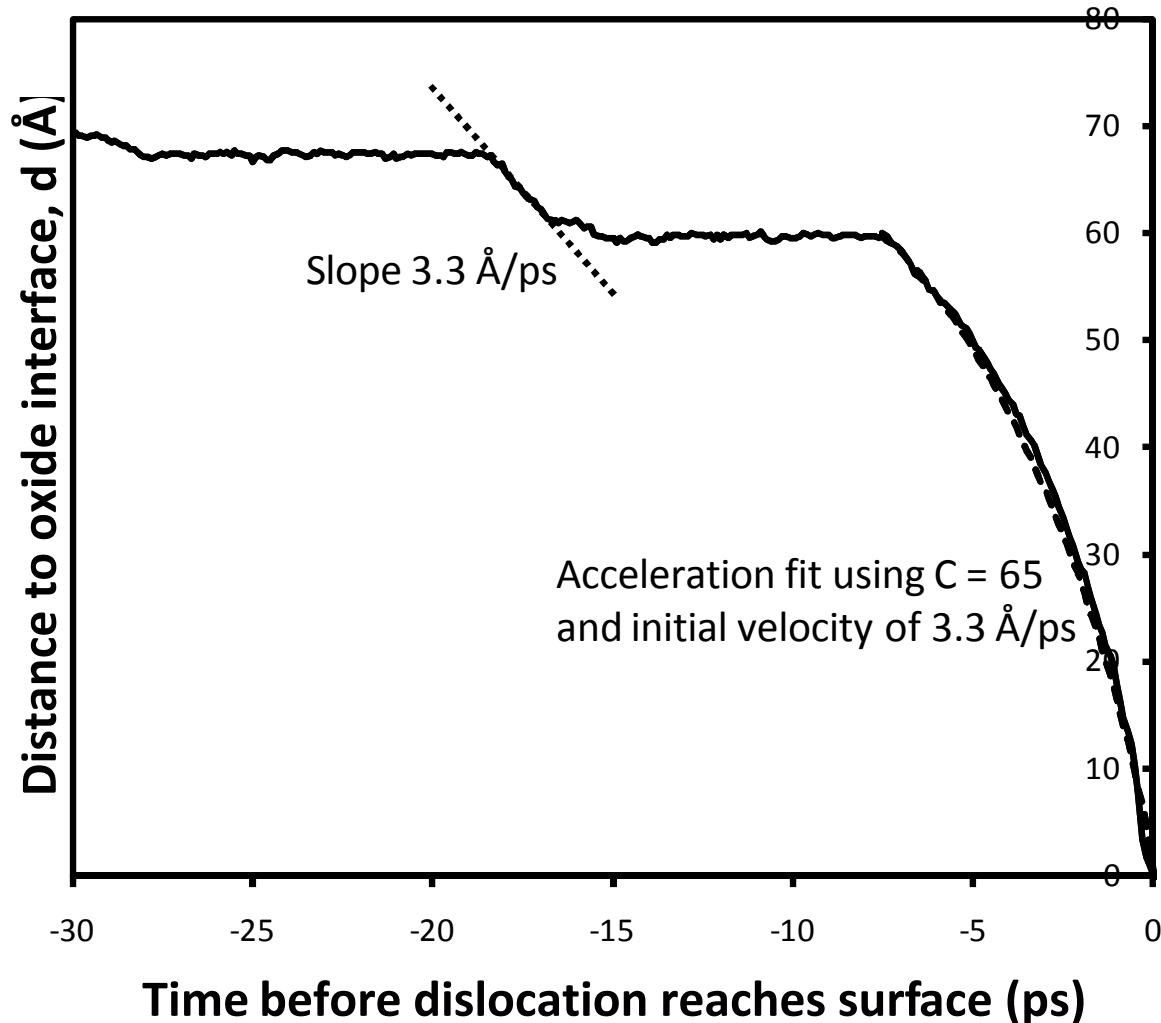
$$F_X^{Int} = \frac{\mu b b^*}{4\pi(1-\nu)d} = \frac{\mu - \mu^*}{\mu^* + \mu} F_x^{Im}$$

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



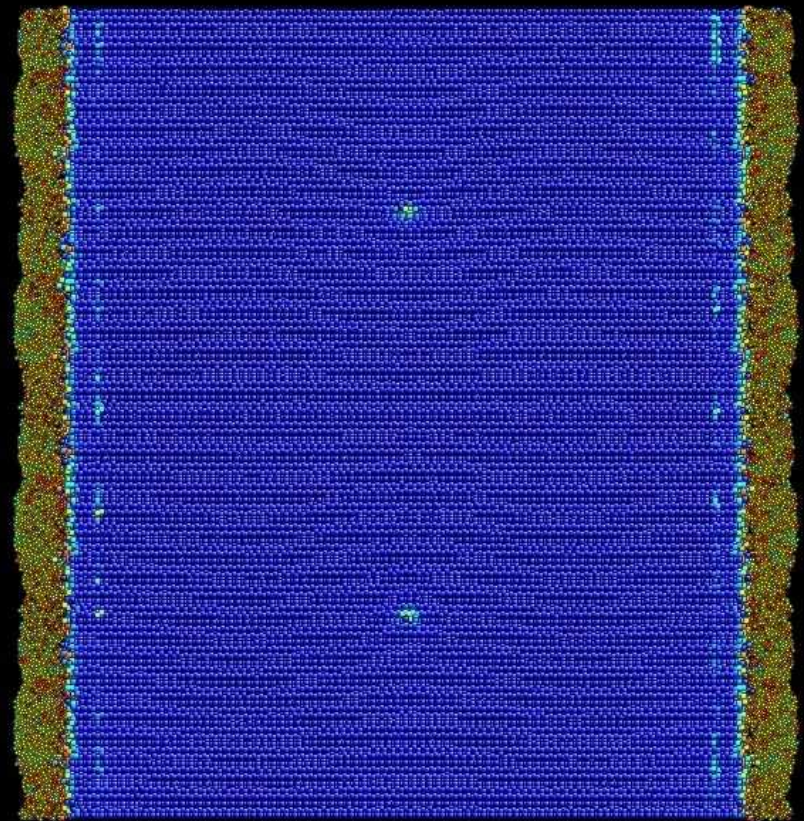
Attraction to Interface

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



Long Range Repulsion

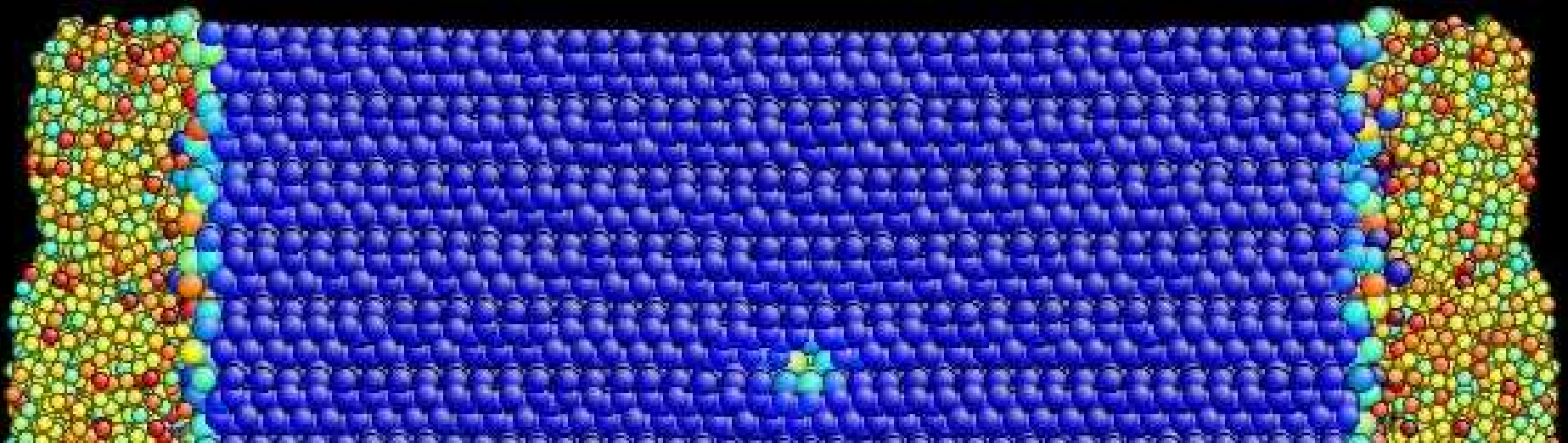
- Dislocation positions remain fixed in unconstrained systems
- No dislocation-dislocation repulsion seen
- Oxide is repulsive





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**

