SciDAC-2: Hierarchical Petascale Simulation Framework for Stress Corrosion Cracking

USC	Priya Vashishta–PI, Rajiv Kalia, Aiichiro Nakano
Harvard	Efthimios Kaxiras
Purdue	Ananth Grama
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Los Alamos	Stephan Eidenbenz, Arthur Voter
Livermore	Randy Hood, John Moriarty, Lin Yang

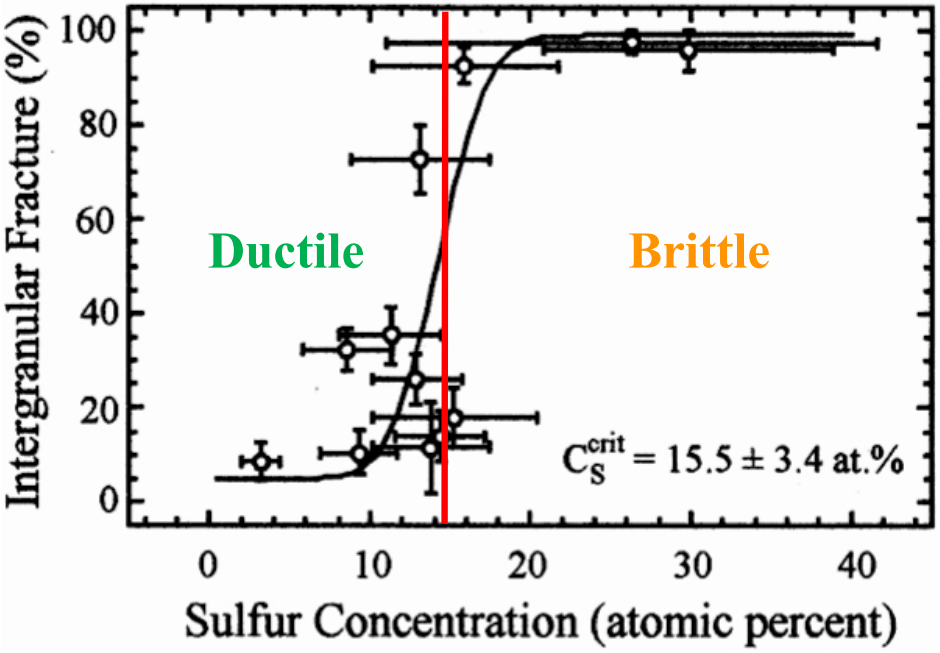
- **DOE-relevant science:** Stress corrosion cracking resistance of nickel-based alloys crucial for next-generation energy systems
- **Advanced computing:** Scalable quantum molecular dynamics (QMD) & reactive molecular dynamics (RMD) simulations

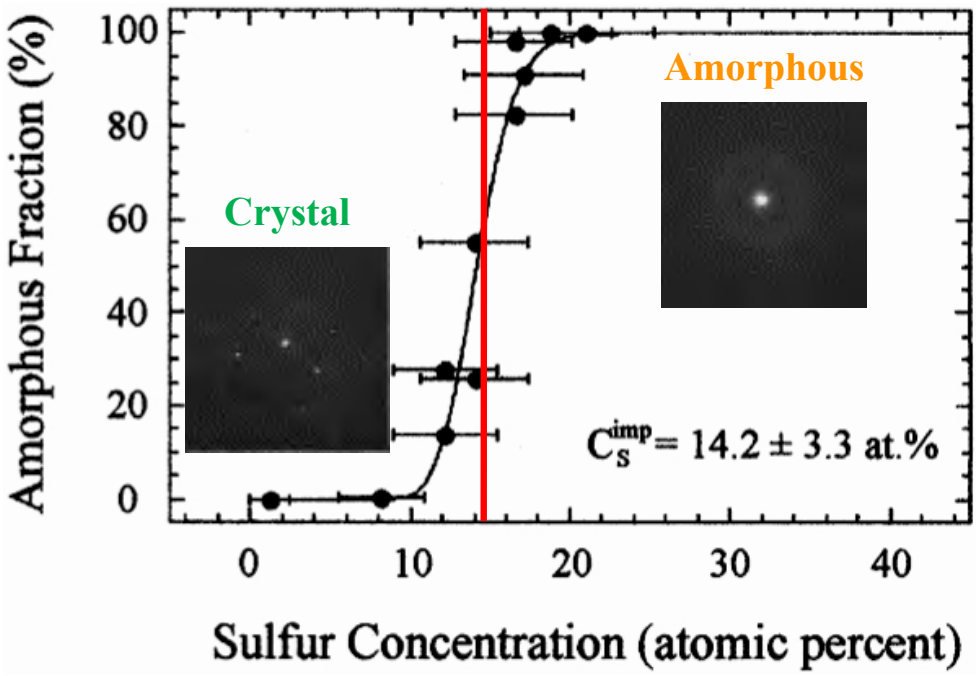
"A Retrospective of SciDAC: Stories That Make Us Unique" Session
SciDAC PI Meeting

Rockville, MD, July16, 2019

Sulfur Segregation-Induced Embrittlement of Nickel

- **Experiments found a crossover from transgranular fracture to intergranular fracture at a critical S concentration of ~15% at grain boundaries**





- **The critical S concentration for embrittlement coincides with that for amorphization during ion implantation**

J. Heuer *et al*., *Appl. Phys. Lett*. **76**, 3403 ('00)
M. Yamaguchi *et al*., *Science* **307**, 393 ('05)

Q: How amorphization causes embrittlement?

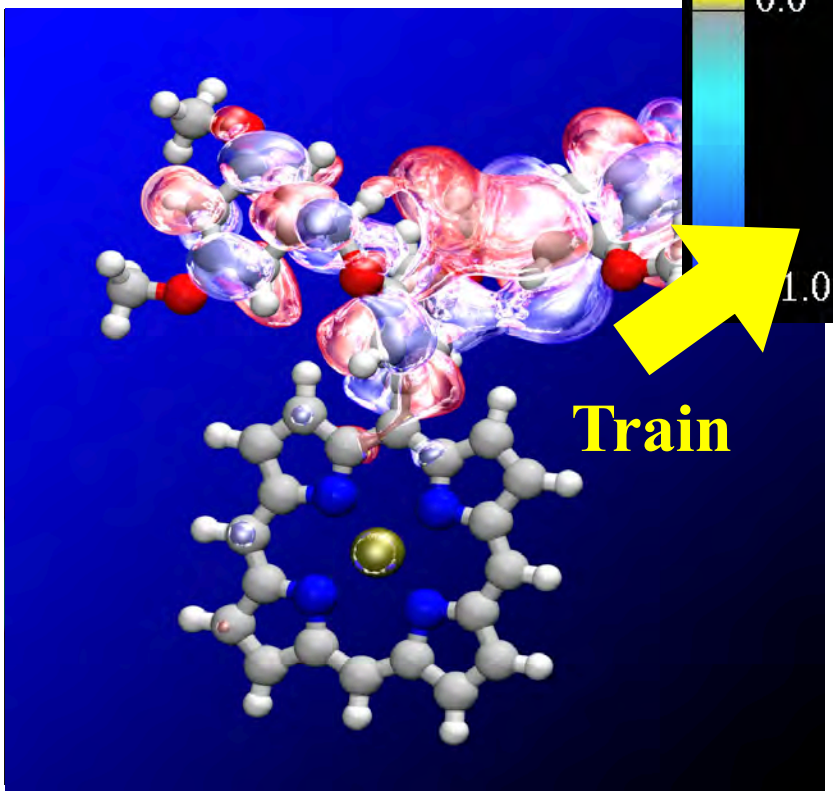
Multiscale Simulation Challenge

Quantum accuracy at scale: RMD!

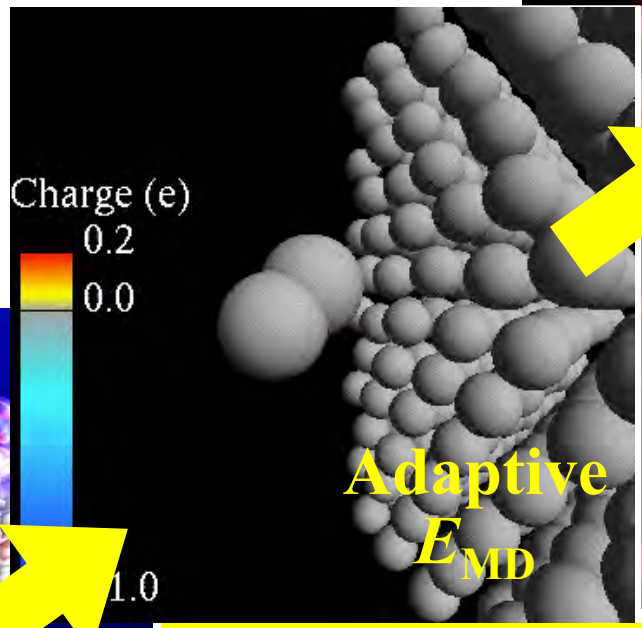
Molecular Dynamics (MD)

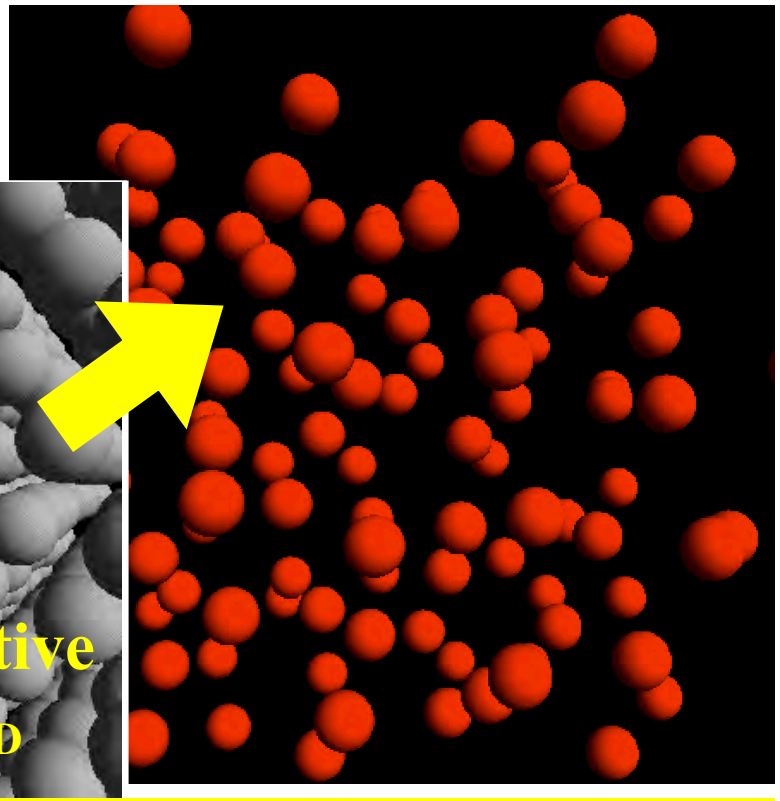
Reactive MD (RMD)

Nonadiabatic quantum MD (NAQMD)



Train





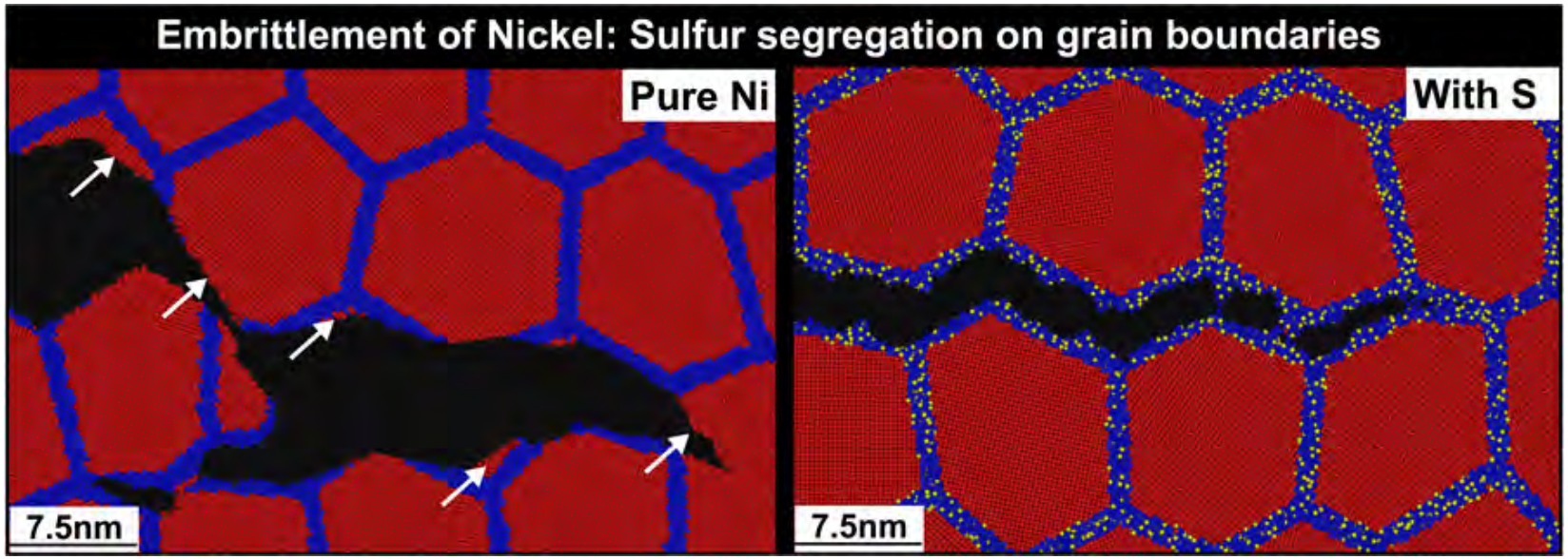
First principles-based reactive force-fields

- **Reactive bond order $\{BO_{ij}\}$**
  → Bond breakage & formation
- **Charge equilibration (QEq) $\{q_i\}$**
  → Charge transfer

Tersoff, Brenner, Sinnott *et al.*; Streitz & Mintmire *et al.*; van Duin & Goddard (ReaxFF)

Highlight: Sulfur-Embrittlement of Ni

- **SciDAC enabled unprecedented 48 million-atom RMD simulation on 163,840-processor IBM Blue Gene/P at Argonne, revealing a direct link between sulfur-induced intergranular amorphization & embrittlement**
- **Highlighted by Dr. William Brinkman, Director of Science, DOE, at the FY 2012 Budget Request to Congress for DOE's Office of Science**

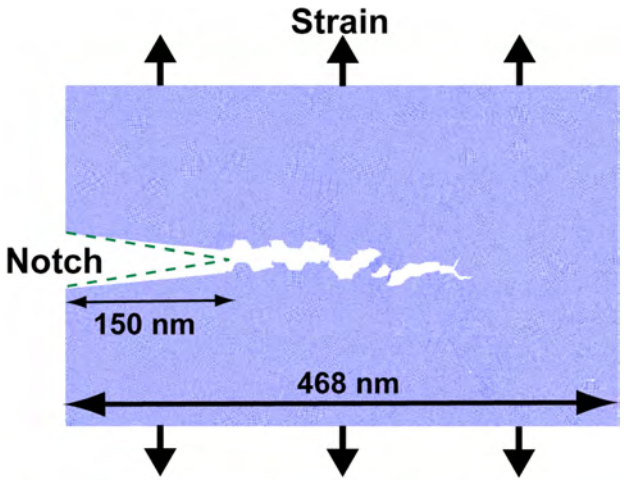


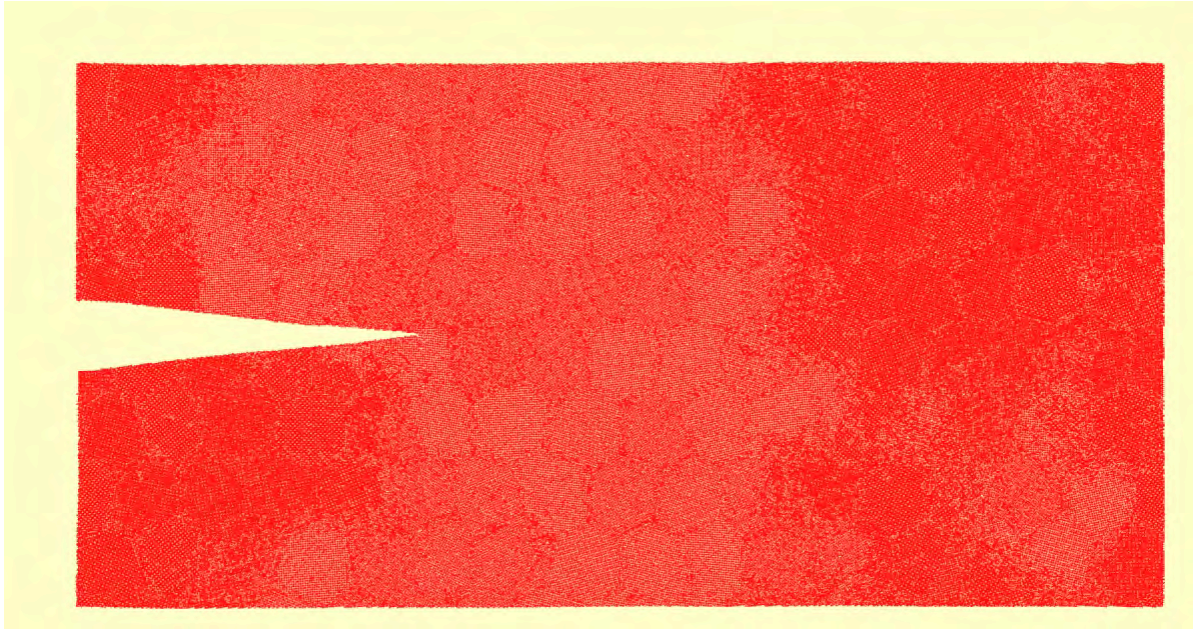
Nickel (bulk)
Ni (grain boundary)
Sulfur

H. Chen *et al.*, *Phys. Rev. Lett.* **104**, 155502 ('10)

48 million-atom RMD Simulations

Pure Ni

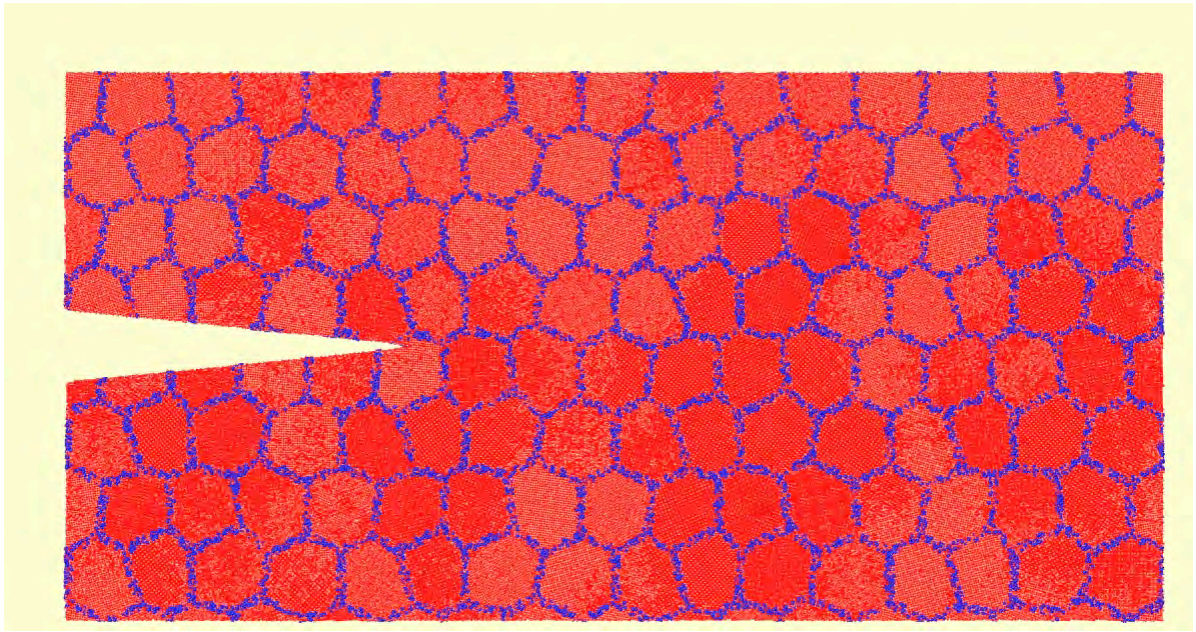




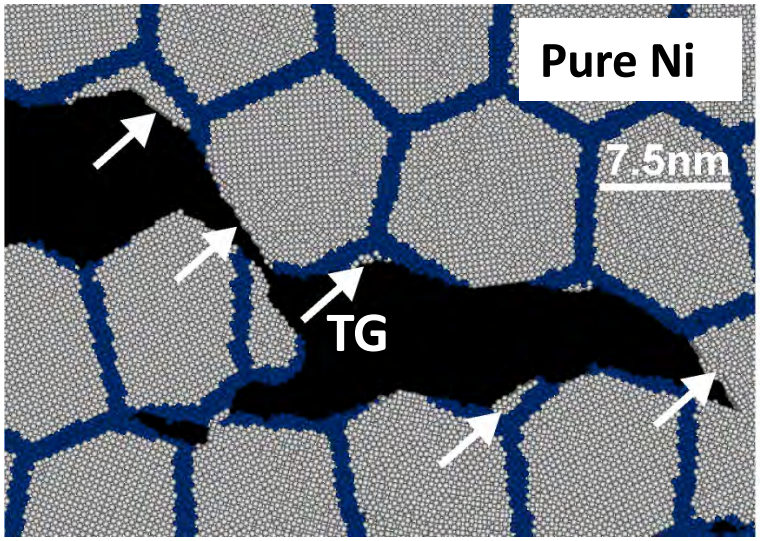
Nickel (bulk)
Sulfur

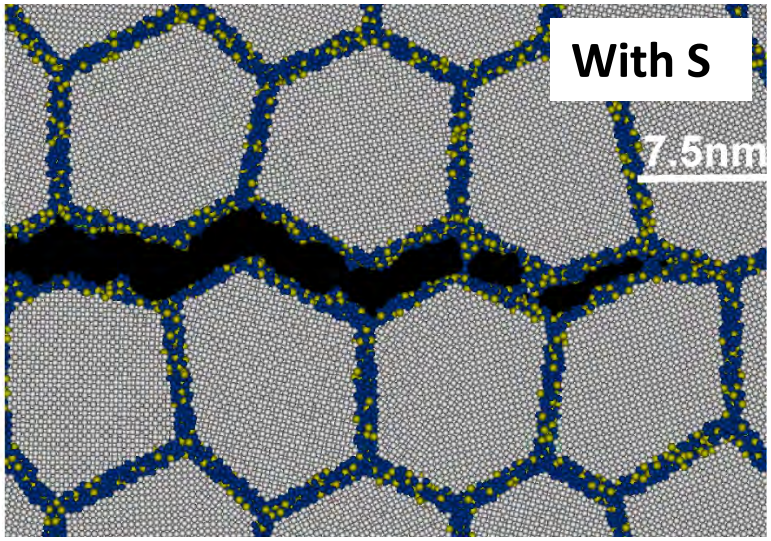
- Ductile tearing (pure Ni) *vs.* brittle cleavage (with S)

With S



Crossover of Fracture Modes





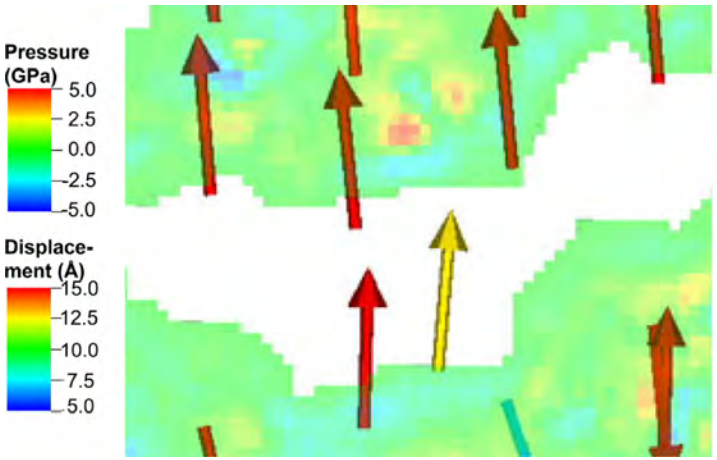
Tensile direction

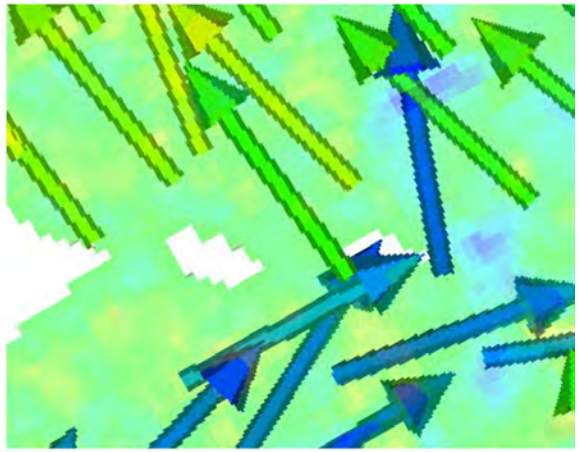
Gray: Ni in grains
Blue: Ni @GB
Yellow: S

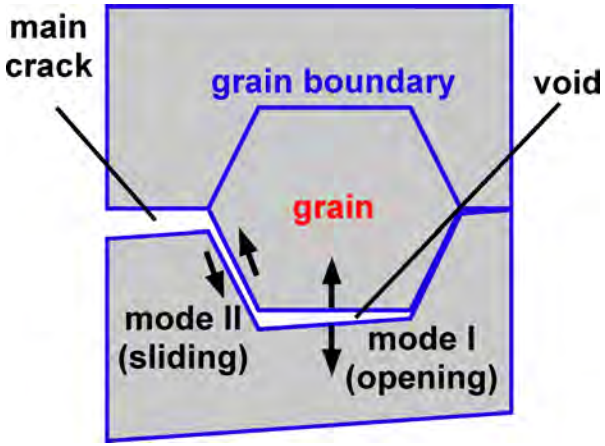
56% intergranular fracture

100% intergranular fracture

- Crossover from mixed intergranular (IG) & transgranular (TG) fracture in pure Ni to purely IG fracture with S, in agreement with experiments



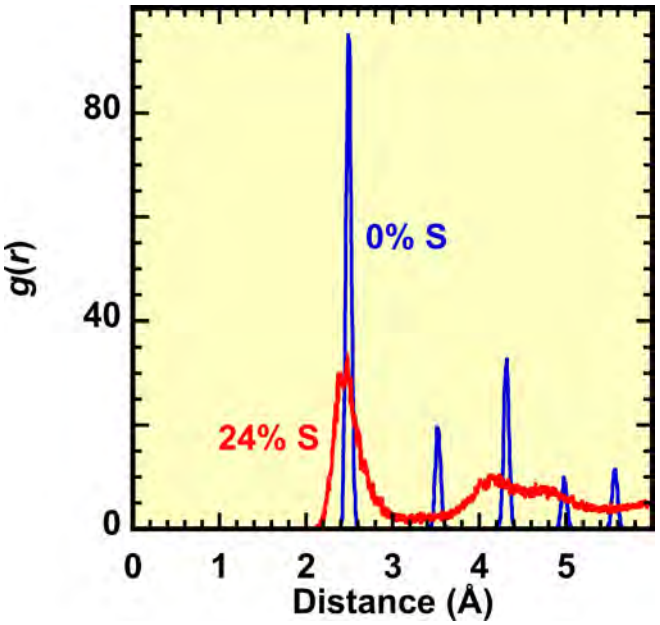


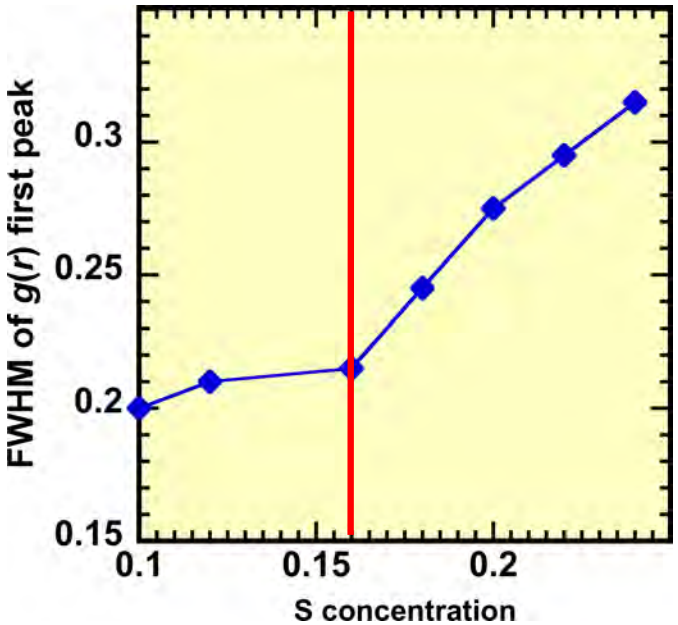


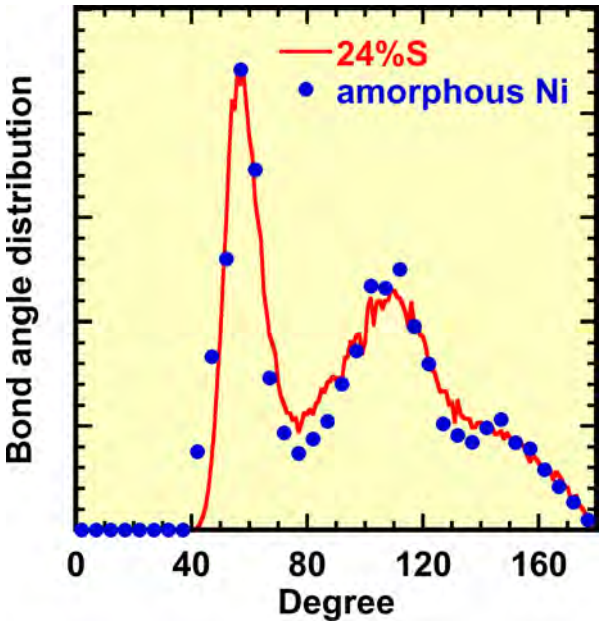
- Crossover from predominantly mode-I (opening) to mixed mode-I & II (opening & sliding) fracture with S

Sulfur-Induced Amorphization of Ni

RMD simulation of S doping in Ni crystal (random substitution)





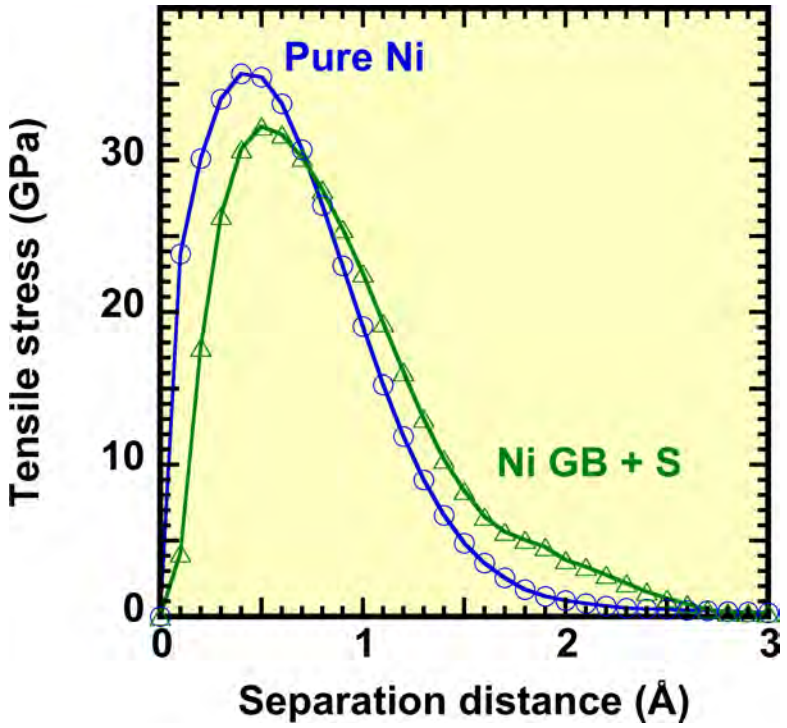


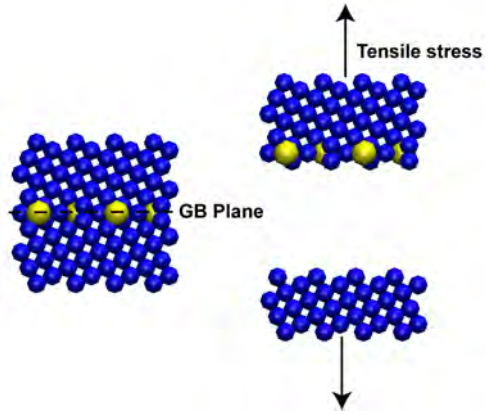
- Increased S concentration broadens peaks in pair distribution function $g(r)$
- The full-width at half-maximum of the first peak of $g(r)$ suddenly increases at 16% S doping, in agreement with the experimental amorphization threshold
- The bond angle distribution above the threshold resembles that of amorphous Ni

- Computed amorphization threshold (16%) is close to the percolation threshold (14%) for S impurities, considering the second nearest-neighbor S-S connectivity (3.5 Å ~ S-S interaction range mediated by lattice distortion)

Mechanism: Tensile-Strength Reduction

- **RMD calculation of the effect of S segregation on Ni-GB tensile test: Ni ∑5(012) grain boundary without/with a monolayer of segregated S atoms**





Tensile stress calculated as the derivative of energy during rigid separation of grains

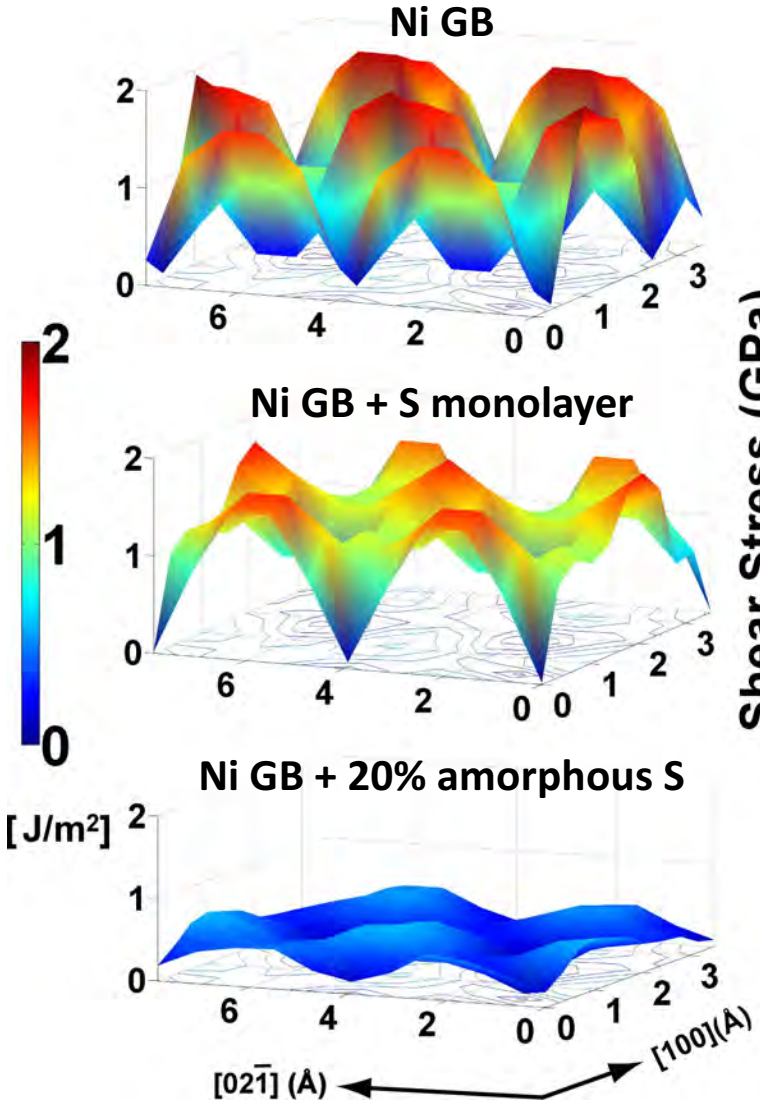
- **S segregation-induced reduction of tensile strength (by 3.5 GPa, confirmed by QMD—4.6 GPa) supports experimentally-observed embrittlement**

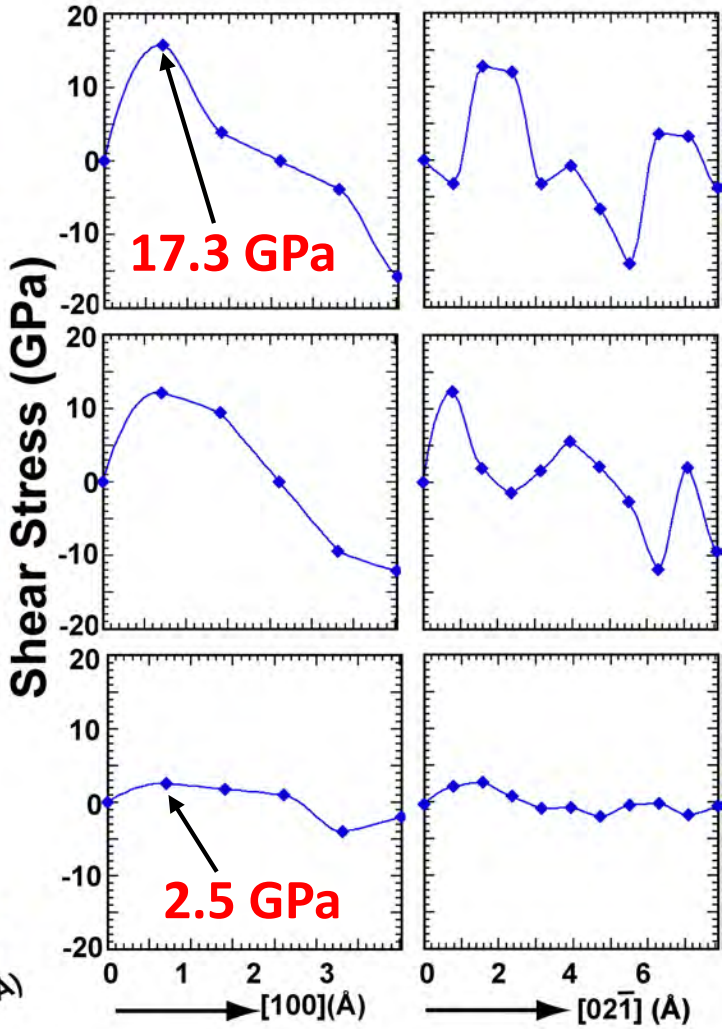
c.f. J.R. Rice & J.-S. Wang, *Mater. Sci. Eng. A* **107**, 23 ('89)
M. Yamaguchi *et al*., *Science* **307**, 393 ('05)

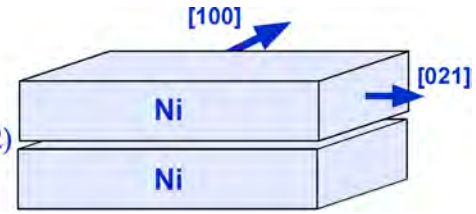
- **However, the tensile-strength-reduction mechanism alone does not explain the relation between embrittlement & amorphization**

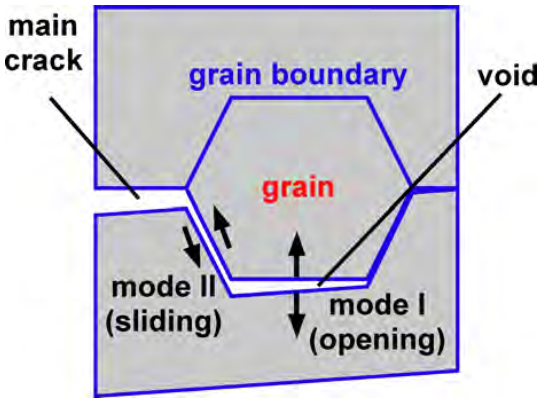
New Mechanism: Shear Strength Reduction

RMD calculation of generalized stacking fault energy of Σ5(012) GB





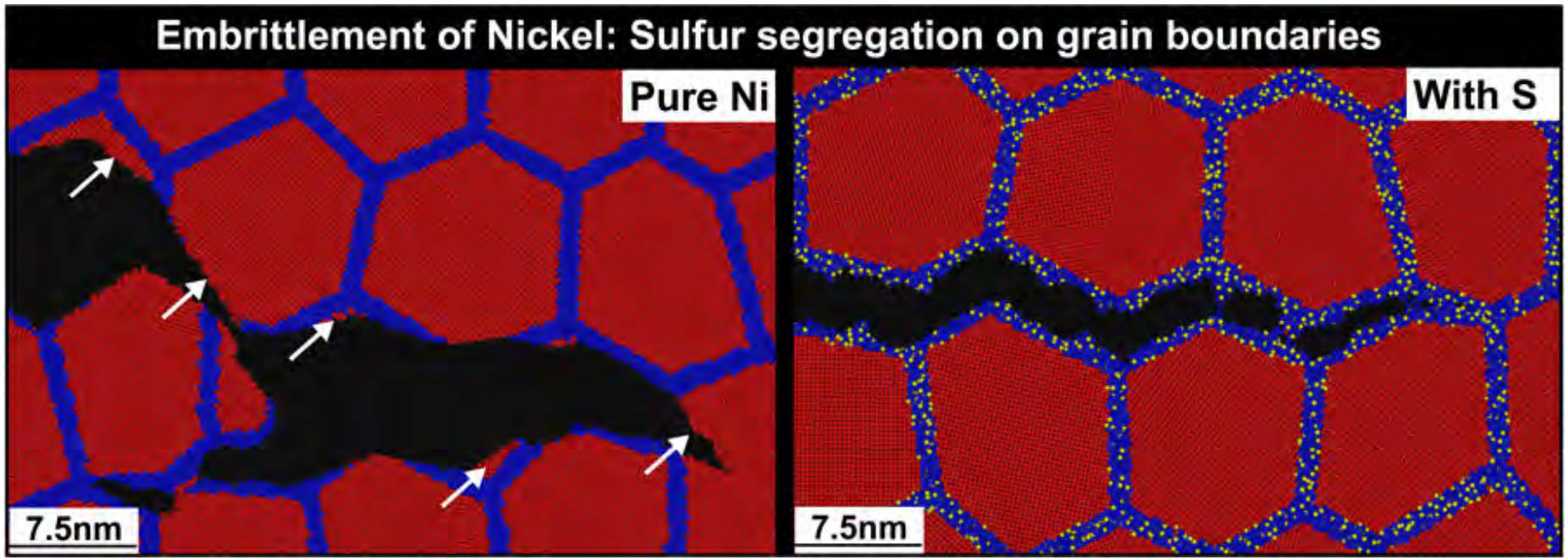




- **First link between S segregation-induced amorphization & embrittlement: Reduction of GB shear strength due to amorphization provides a crack path**

SciDAC Success: Summary

- **Scientific mystery solved: How S-segregation-induced amorphization causes embrittlement of Ni in nuclear reactors?**
- **48 million-atom SciDAC-RMD simulations provided the missing link: An order-of-magnitude reduction of grain-boundary shear strength due to amorphization, combined with tensile-strength reduction, allows the crack tip to always find an easy propagation path along grain boundary**



H. Chen *et al.*, *Phys. Rev. Lett.* **104**, 155502 ('10)

Unique SciDAC Partnership

Full IBM Blue Gene/P simulation with quantum accuracy was only possible by unique SciDAC collaboration

- **Domain science: QMD (Kaxiras, Lu), RMD (Kalia, Vashishta)**
  QMD-accuracy reactive force fields (ReaxFF) for broad use
- **CS/math: scalable parallelization (Nakano), efficient RMD solver & preconditioner (Grama)**
  In-house & LAMMPS (Sandia) implementation for dissemination
- **Collaboration with ASCR SciDAC institute: performance tuning with Bob Lucas–PI, Mary Hall & Jacque Chame at Performance Engineering Research Institute (PERI)**

Cross-SciDAC joint publications

B. Bansal *et al*., *IPDPS* (’07)
Y. Nelson *et al*., *ibid.* (’08)
H. Dursun *et al*., *J. Supercomp.* **62**, 946 (’12)

SciDAC Impact

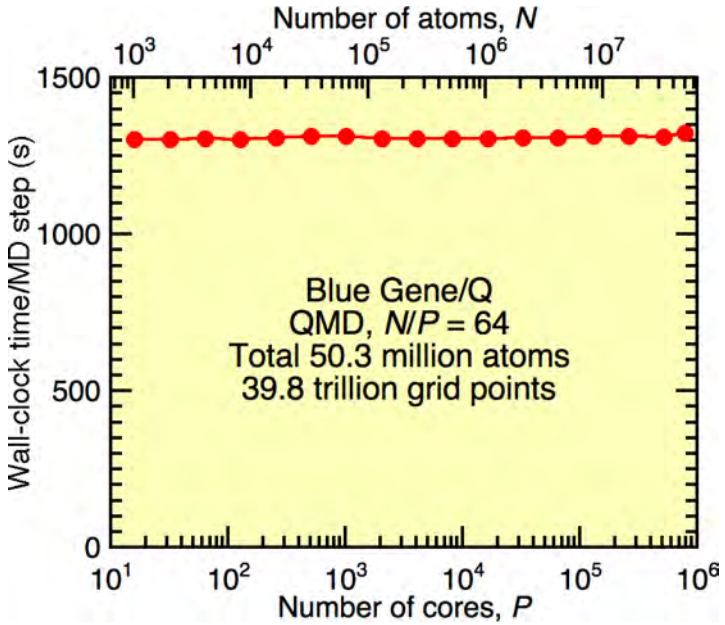
SciDAC partnership established a metascalable (or "design once, scale on future architectures") computing framework for quantum accuracy at scale

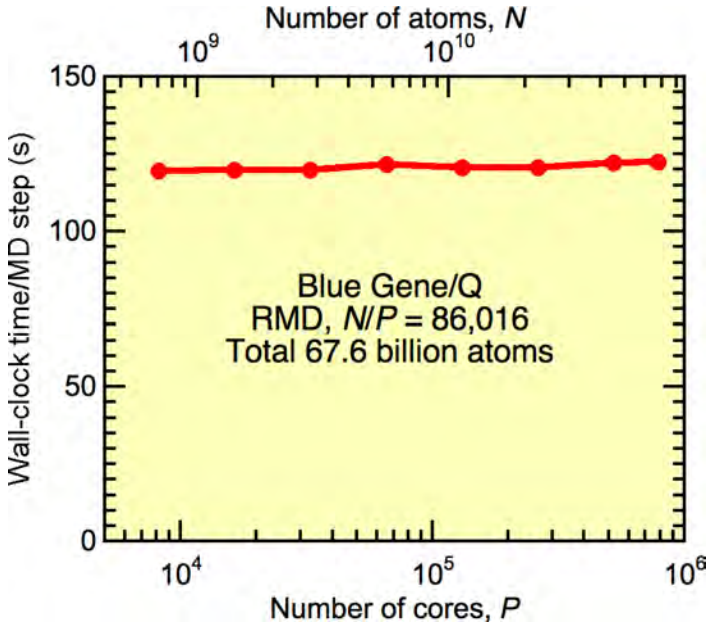
- **Shift-collapse (SC) computation of dynamic *n*-tuples for RMD with provable minimum computation & communication**

  M. Kunaseth *et al.*, *ACM/IEEE Supercomputing, SC13*

- **QMD with parallel efficiency 0.984 & 51% of theoretical floating-point performance on 786,432 IBM Blue Gene/Q processors**

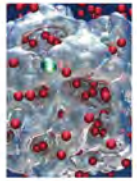
  K. Nomura *et al.*, *IEEE/ACM Supercomputing, SC14*

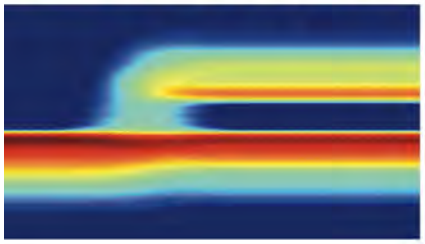




SciDAC impact: quantum accuracy at scale

BES



BASIC ENERGY SCIENCES

EXASCALE REQUIREMENTS REVIEW

An Office of Science review sponsored jointly by
Advanced Scientific Computing Research and Basic Energy Sciences

NOVEMBER 3–5, 2015

ROCKVILLE, MARYLAND

16,661-atom QMD

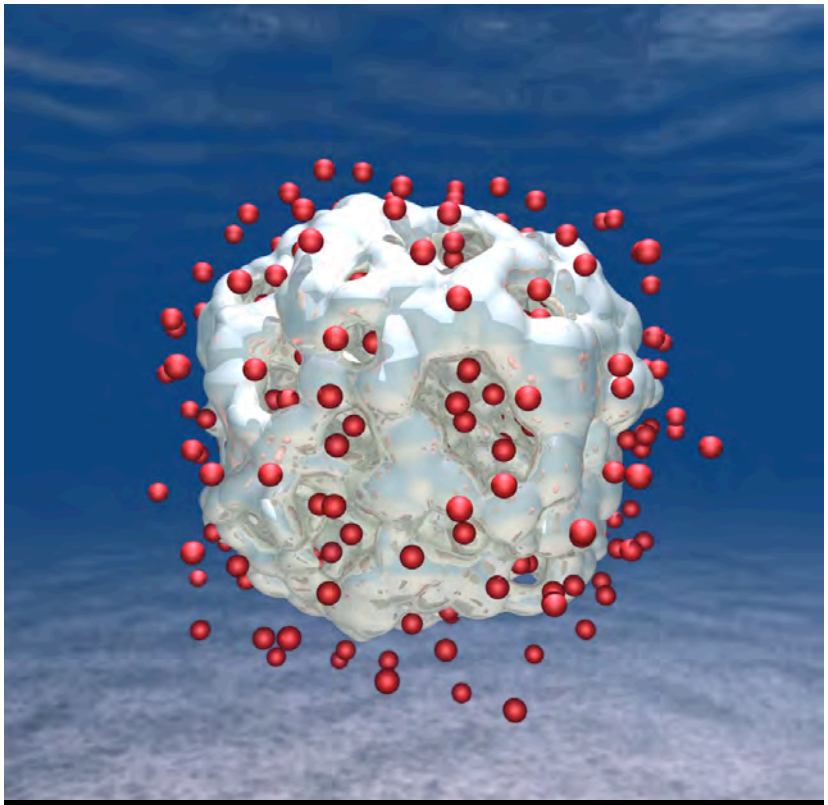
Shimamura *et al.*, *Nano Lett.* **14**, 4090 ('14)

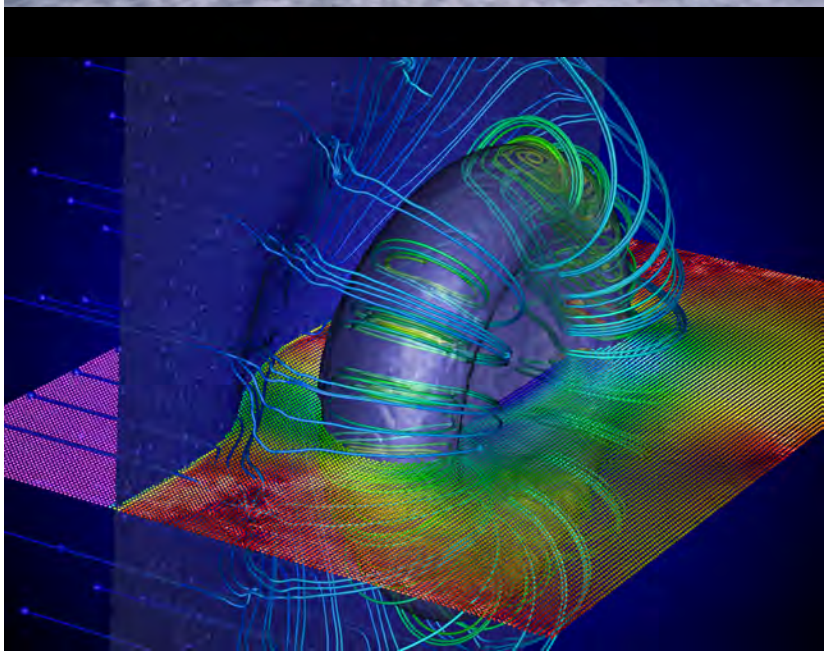
Hydrogen on demand on 786,432-processor IBM Blue Gene/Q

10^9-atom RMD

Shekhar *et al.*, *Phys. Rev. Lett.* **111**, 184503 ('13)

U.S. DEPARTMENT OF ENERGY





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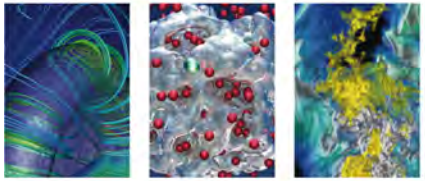

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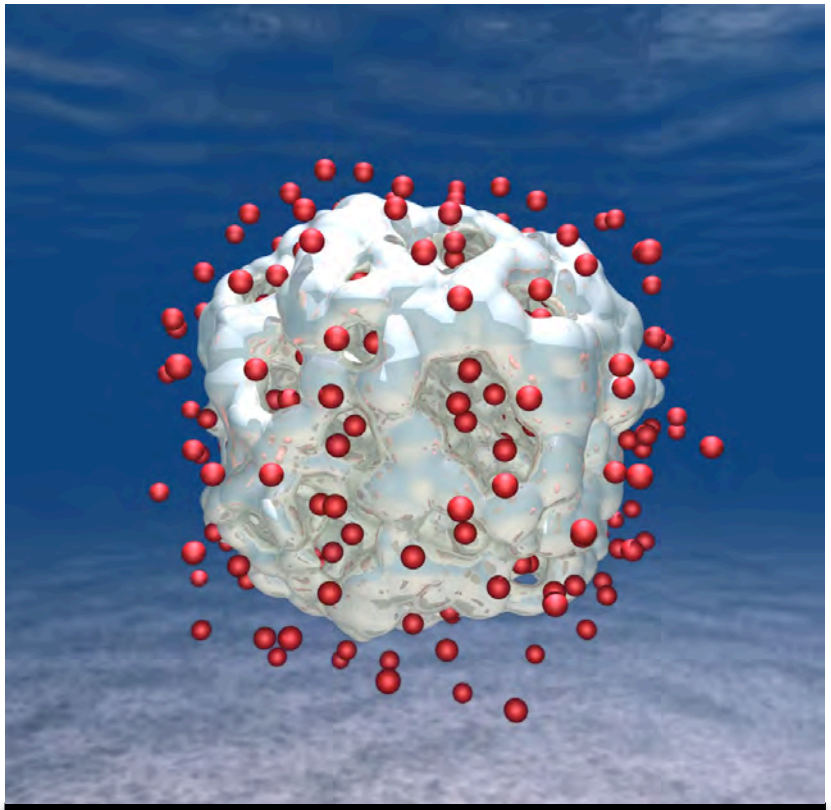
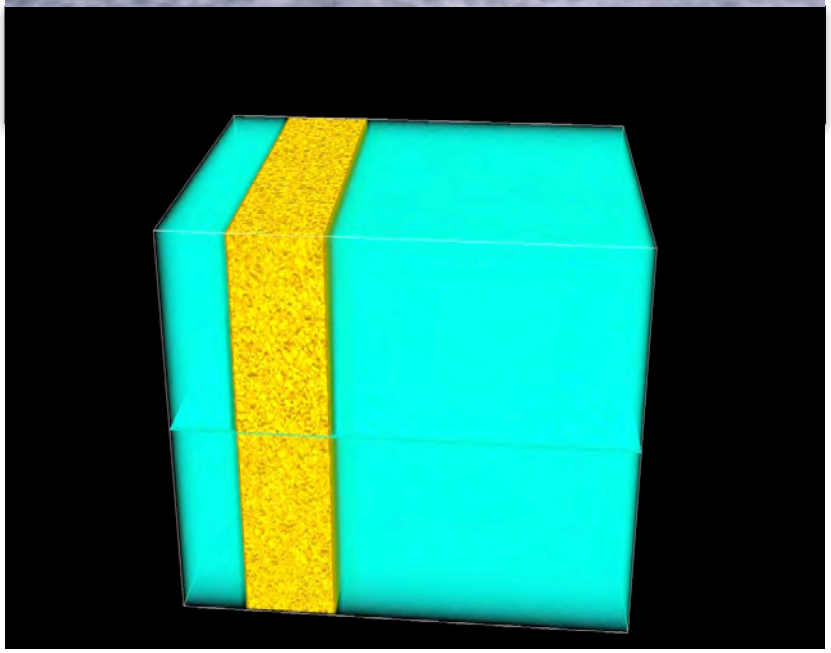


16,661-atom QMD

Shimamura *et al.*, *Nano Lett.* **14**, 4090 ('14)

Cavitation bubble collapse in water (SciDAC2-SCC)



10^9-atom RMD

Shekhar *et al.*, *Phys. Rev. Lett.* **111**, 184503 ('13)

U.S. DEPARTMENT OF ENERGY

SciDAC Impact into Future

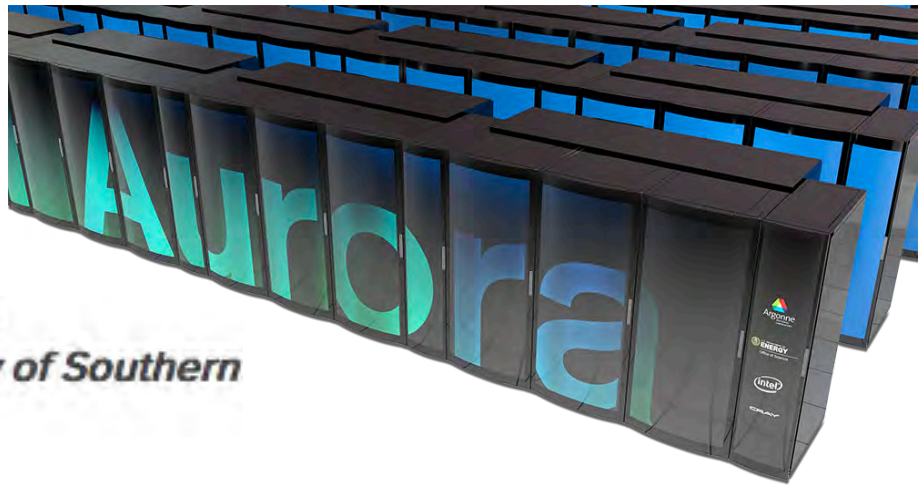
- **One of the 10 initial simulation users of the Nation's first exaflop/s computer, A21**

AURORA | EARLY SCIENCE PROGRAM

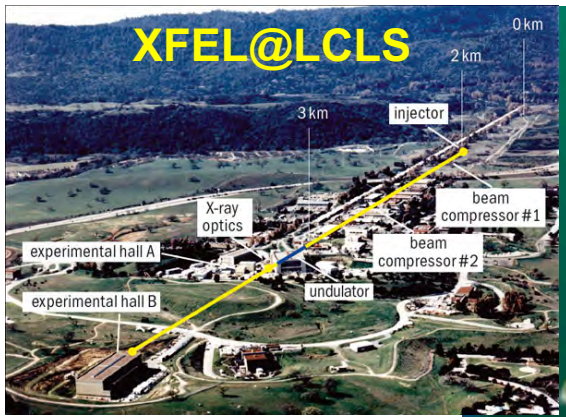
Early Science Projects for Aurora Supercomputer Announced

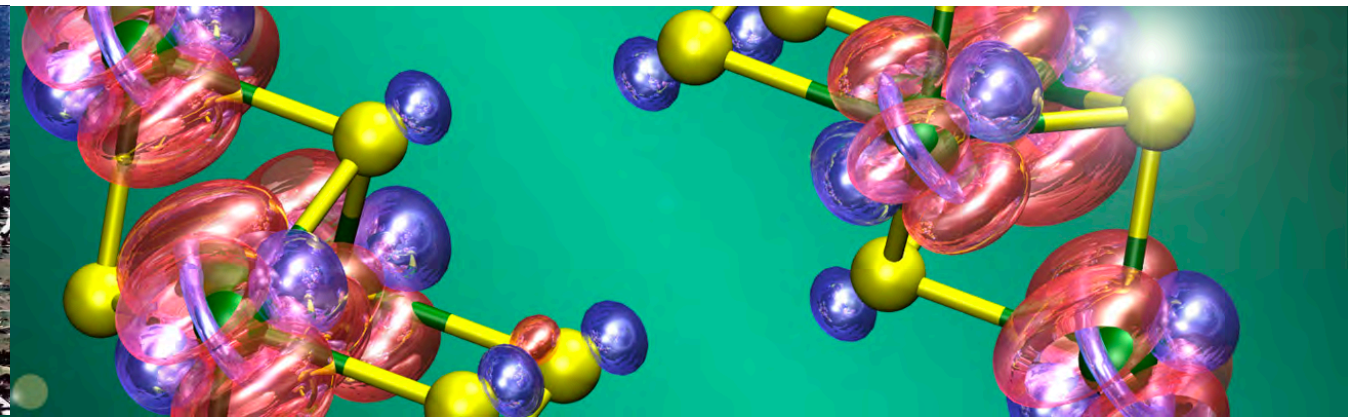
Metascalable layered materials genome

Investigator: Aiichiro Nakano, University of Southern California



- **Metascalable 10^5-atom QMD & 10^{12}-atom RMD simulations on A21 integrated with next-generation X-ray free electron laser (XFEL) experiments at LCLS-II to study ultrafast material processes at exactly the same space & time scales**



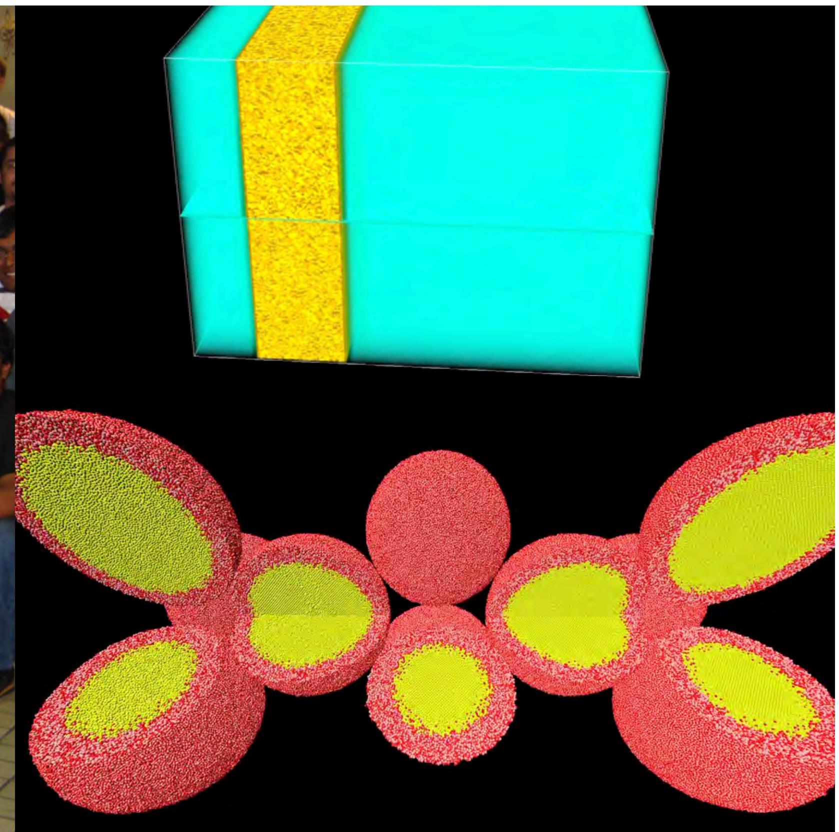


Preliminary advanced-computing + XFEL synergy:

I. Tung *et al*., *Nature Photon.* **13**, 425 ('19)

Summary: SciDAC-2: Hierarchical Petascale Simulation Framework for Stress Corrosion Cracking

SciDAC partnership between domain science + CS + math enabled full-leadership-computer simulation with quantum accuracy, solving a critical scientific problem of DOE relevance—stress corrosion cracking resistance of nickel-based alloys



CACS

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