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

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• 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)

First principles-based reactive force-fields

- Reactive bond order \{BO_{ij}\} → Bond breakage & formation
- Charge equilibration (QEeq) \{q_{ij}\} → 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

48 million-atom RMD Simulations

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

Nickel (bulk)
Sulfur

With S

Pure Ni

Strain

Notch

150 nm

468 nm
Crossover of Fracture Modes

- 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

- 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)

RMD simulation of S doping in Ni crystal (random substitution)
Mechanism: Tensile-Strength Reduction

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

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

  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 $\Sigma 5(012)$ GB

- 17.3 GPa
- 2.5 GPa

- First link between S segregation-induced amorphization & embrittlingment: 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

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 metascaleable (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

BASIC ENERGY SCIENCES

EXASCALE REQUIREMENTS REVIEW

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

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
SciDAC impact: quantum accuracy at scale

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

**Cavitation bubble collapse in water (SciDAC2-SCC)**

10⁹-atom RMD
Shekhar et al., *Phys. Rev. Lett.*
111, 184503 ('13)
SciDAC Impact into Future

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

- 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)
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