Atomistic Simulation of Materials: Introduction to Molecular Dynamics Method

Priya Vashishta

Collaboratory for Advanced Computing & Simulations

Departments of Chemical Engineering & Materials Science, Physics & Astronomy, and Computer Science

University of Southern California

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CACS

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USC

Outline – Part I

Introduction to Molecular Dynamics Method with Reactive Force Fields on Parallel Computers

Collaboratory for Advanced Computing and Simulations:

Faculty: Rajiv Kalia and Aiichiro Nakano (USC), Fuyuki Shimojo and Postdocs and Grad Students

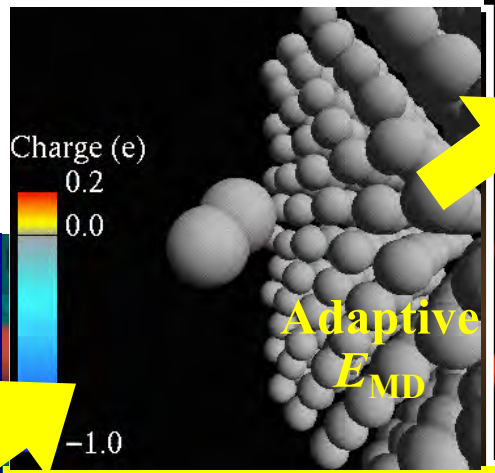
Simulation Methods: NAQMD, RMD and MD

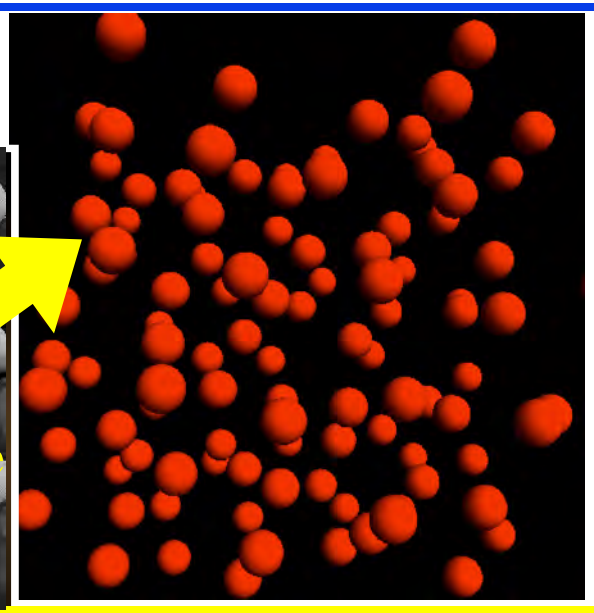
Molecular Dynamics (MD)

Reactive MD (RMD)

Nonadiabatic quantum MD (NAQMD)

Train





First principles-based reactive force-fields

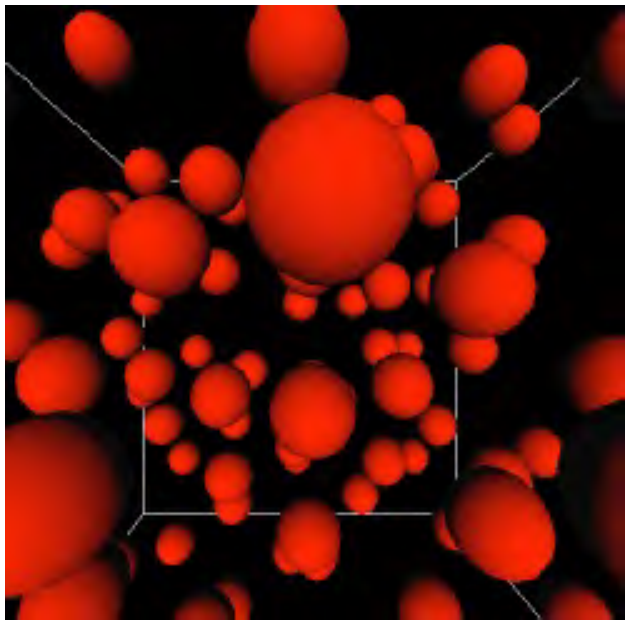
- Reactive bond order $\{BO_{ij}\}$
  → Bond breakage & formation
- Charge equilibration (QEq) $\{q_i\}$
  → Charge transfer

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

Molecular Dynamics Method

Newton's second law of motion:

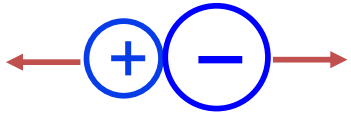
$$\{r_1(t),\ldots,r_N(t)\} \qquad m_i \frac{d^2 r_i(t)}{dt^2} = -\frac{\partial V}{\partial r_i}$$



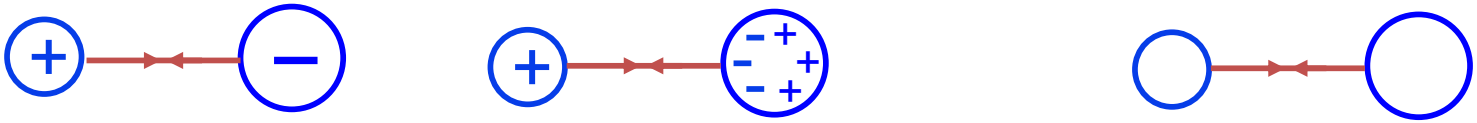
Interatomic potential for SiO_2 & Si_3N_4:

$$V = \sum_{i<j} v_{ij}^{(2)}(r_{ij}) + \sum_{i,j<k} v_{ijk}^{(3)}(r_{ij}, r_{ik})$$

> Two-body: (1) steric repulsion



(2) Coulomb ; (3) charge-dipole ; (4) induced dipole-dipole



> Three-body: covalent bond bending & stretching

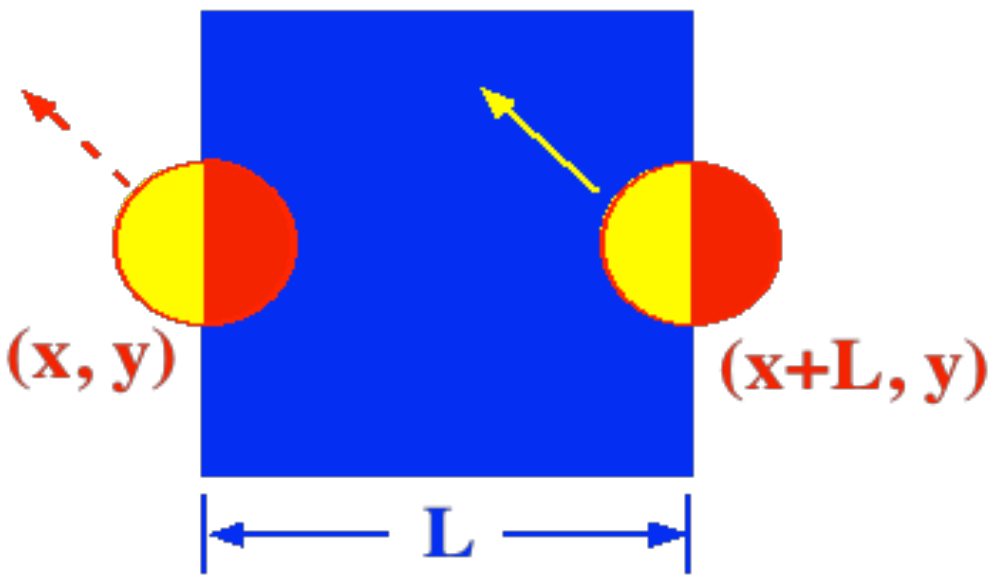
MD Simulation: Numerical Algorithm

- Equations of motion: 2nd order, non-linear, coupled ODE → Finite-difference equations:

$$[\vec{r}_i(t), \vec{p}_i(t)] \longrightarrow [\vec{r}_i(t+\Delta t), \vec{p}_i(t+\Delta t)]$$

- Initial conditions:
  lattice positions, random velocities
- Boundary conditions:
  periodic boundary conditions (PBC)
- Integration algorithms:
  Gear, Beeman, Verlet, Velocity-Verlet, etc,

Periodic Boundary Conditions (PBC)



- simulation box is taken as basic unit
- the whole space is filled by periodically repeating the basic unit

leaving particle is replaced by its image entering from the opposite side
short-range interactions are between minimum images

Velocity-Verlet Algorithm

Stage 1 $\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \Delta t\vec{v}_i(t) + \frac{1}{2}\Delta t^2\vec{a}_i(t)$

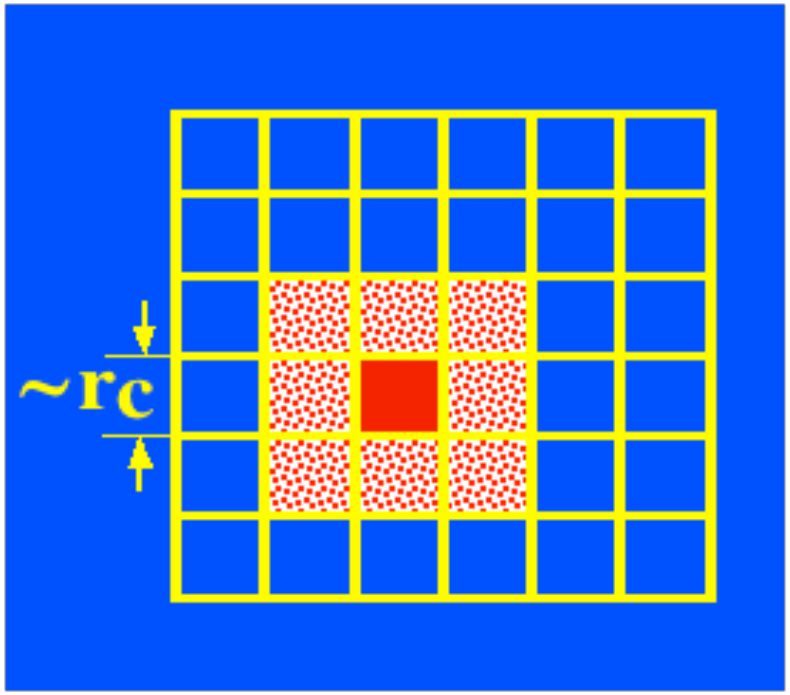
$$\vec{v}_i(t+\frac{1}{2}\Delta t) = \vec{v}_i(t) + \frac{1}{2}\Delta t\vec{a}_i(t)$$

Stage 2 <<<< Force evaluation >>>>

Stage 3 $\vec{v}_i(t+\Delta t) = \vec{v}_i(t+\frac{1}{2}\Delta t) + \frac{1}{2}\Delta t\vec{a}_i(t+\Delta t)$

Time reversible - stability in long time simulations

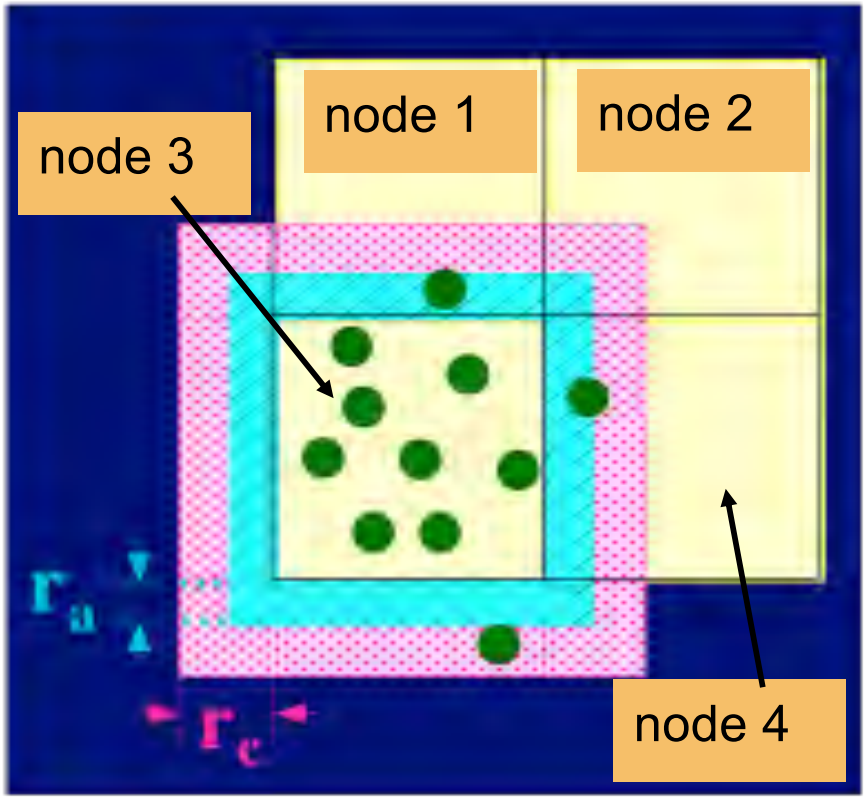
Link-Cell-List Scheme:
$O(N^2) \rightarrow O(N)$



- particles are divided into **cells** of size r_c
- particles are linked in each cell into **link-lists**
- particles in neighbor cells are grouped into **neighbor-lists**

Interactions are evaluated within neighbor lists: $O(NN_b)$

Domain Decomposition Scheme



- system is divided into subsystems
- subsystems are geometrically matched onto nodes
- interaction between neighbor nodes are calculated through message-passing

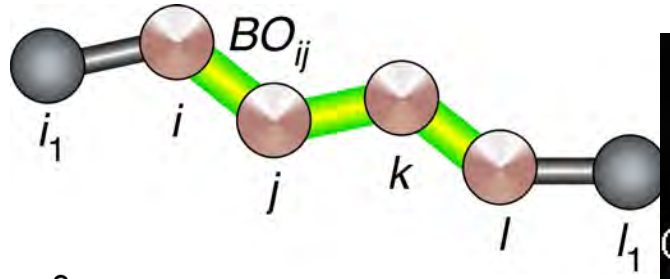
Multiple Time Step: primary surface is copied every Δt
secondary surface is copied every $n\Delta t$

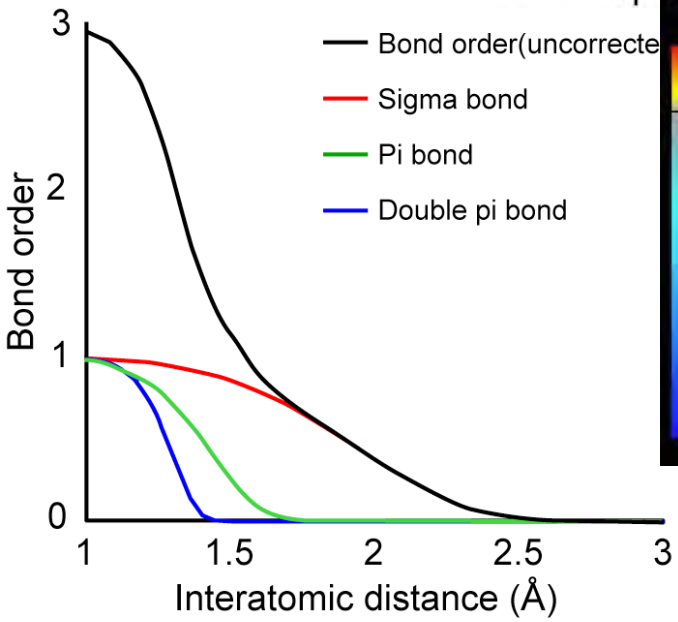
Reactive Force Field (ReaxFF) MD

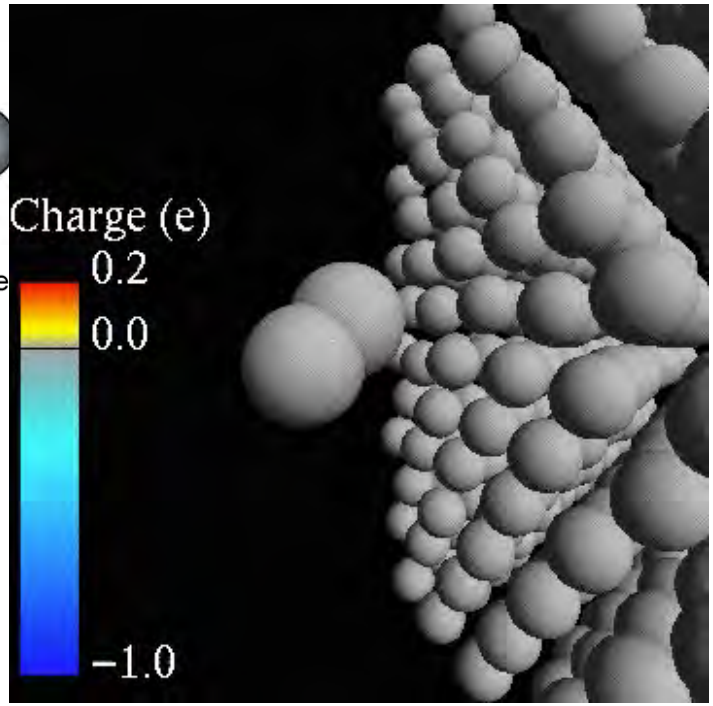
First principles-based reactive force-field [van Duin, Goddard, Caltech]

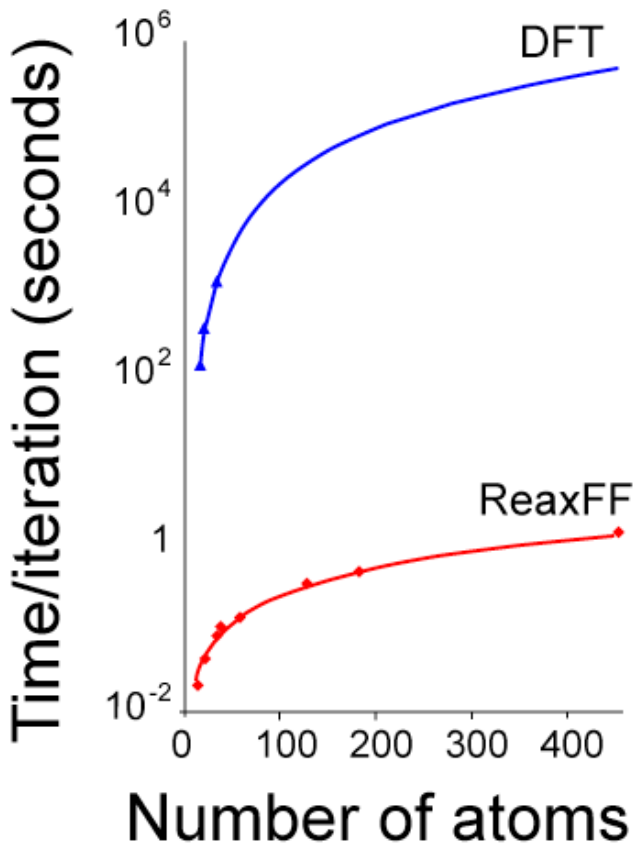
- **Reactive bond order: $E_{BO}(\{r_i,r_j,r_k,r_l\},\{BO_{ij}\})$**
  → **Bond breakage & formation** [Tersoff, '85; Brenner, '90]
- **Charge equilibration (QEq): $\{q_i^*\}$ = argmin $E_{ES}(\{r_i\},\{q_i\})$**
  → **Charge transfer** [Goddard & Rappe, '91; Streitz & Mintmire, '94]

Significantly less computing time than the density functional theory (DFT)

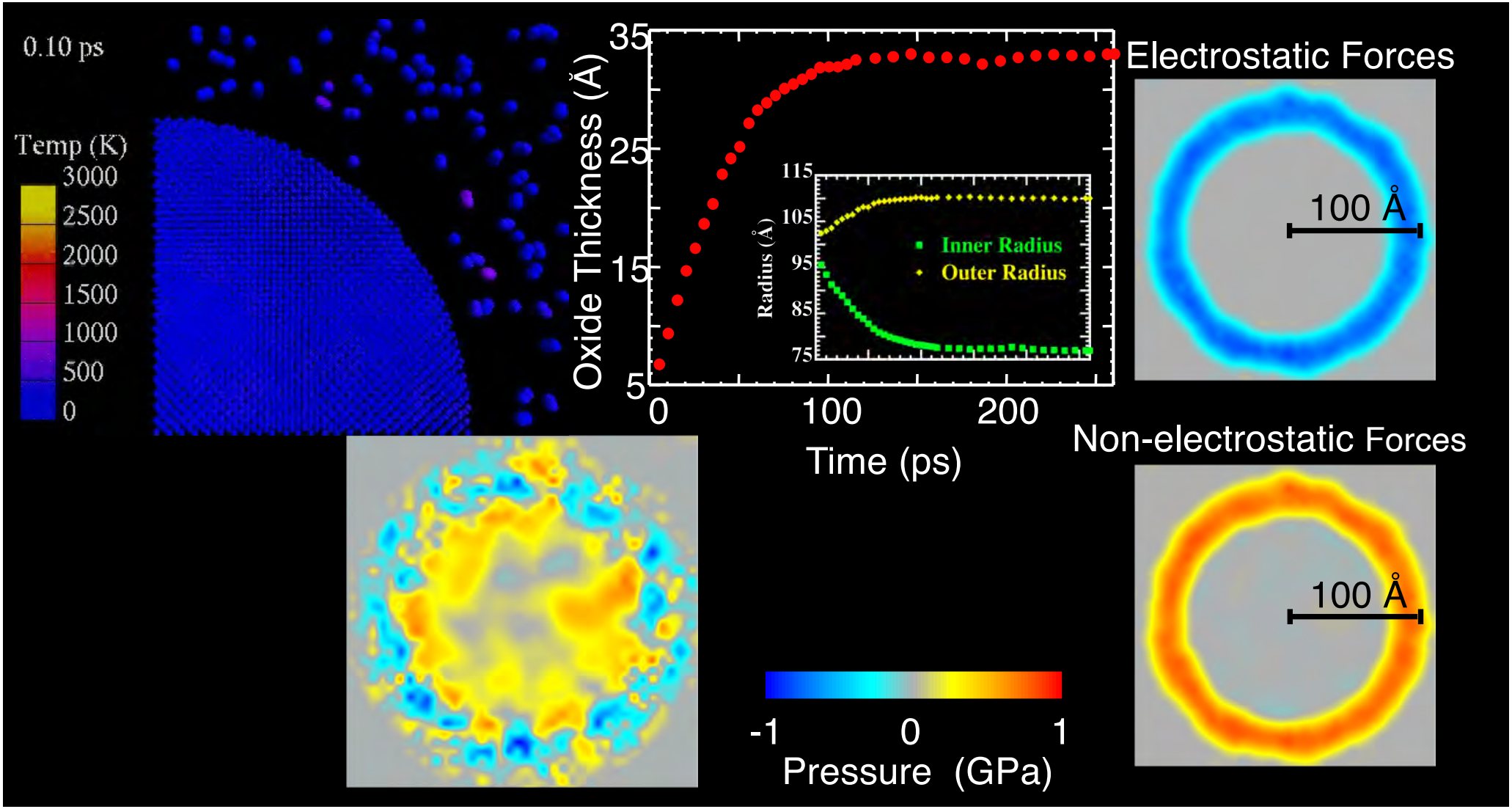






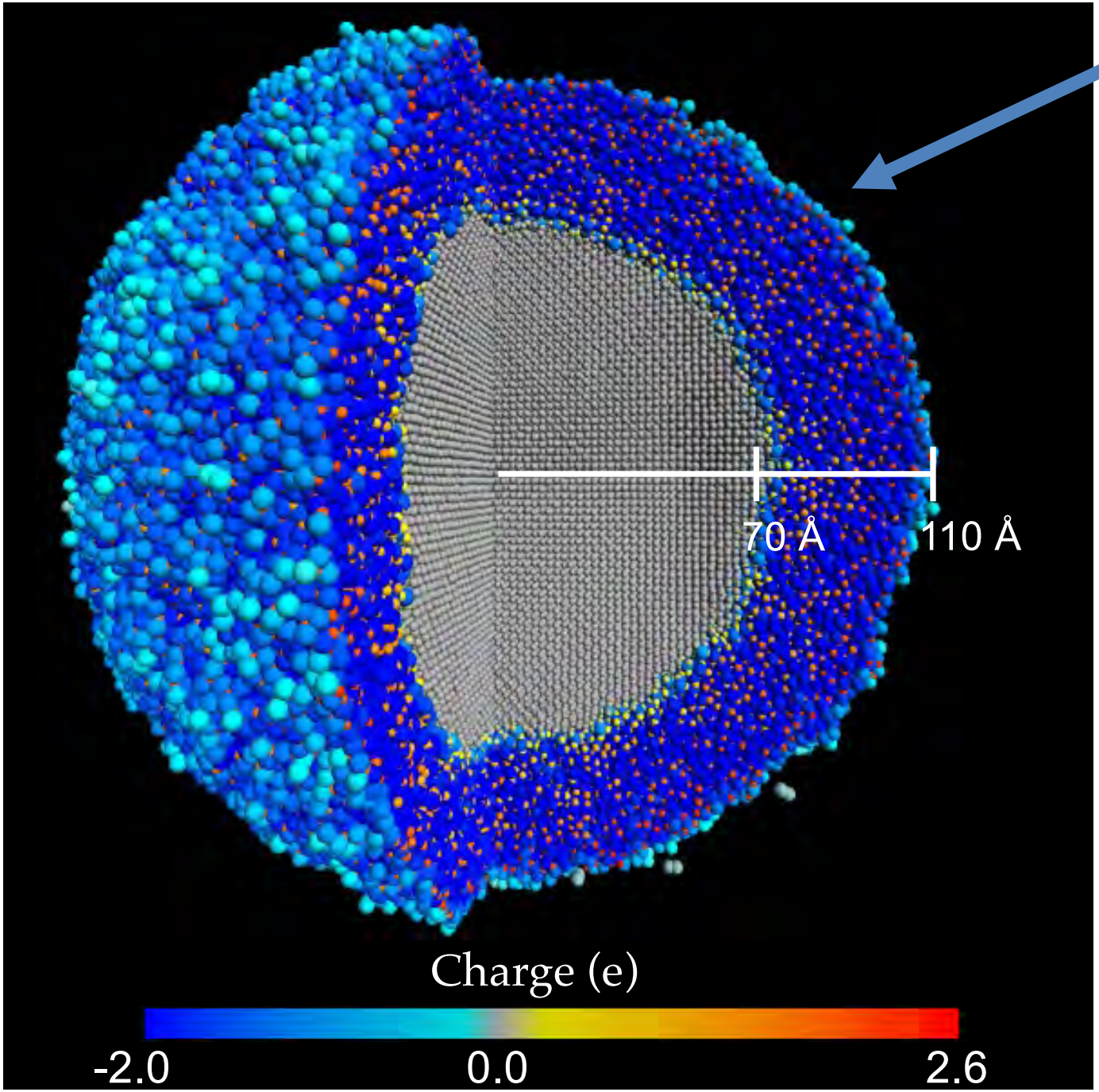


Oxidation of an Al Nanoparticle (n-Al)



- Oxide thickness saturates at 40 Å after 0.5 ns, in agreement with experiments
- Oxide region/metal core is under negative/positive pressure
- Attractive Al-O Coulomb forces contribute large negative pressure in the oxide

Structure of Oxide Scale



Snapshot at 466 ps

Oxide scale is amorphous

Oxide thickness is 40 Å, in agreement with experiment

Average density of oxide is 2.9 g/cm^3; 75% of alumina

EXECUTIVE OFFICE OF THE PRESIDENT
NATIONAL SCIENCE AND TECHNOLOGY COUNCIL
WASHINGTON, D.C. 20502

June 24, 2011

Dear Colleague:

In much the same way that silicon in the 1970s led to the modern information technology industry, the development of advanced materials will fuel many of the emerging industries that will address challenges in energy, national security, healthcare, and other areas. Yet the time it takes to move a newly discovered advanced material from the laboratory to the commercial market place remains far too long. Accelerating this process could significantly improve U.S. global competitiveness and ensure that the Nation remains at the forefront of the advanced materials marketplace. This *Materials Genome Initiative for Global Competitiveness* aims to reduce development time by providing the infrastructure and training that American innovators need to discover, develop, manufacture, and deploy advanced materials in a more expeditious and economical way.

Prepared by an *ad hoc* group of the National Science and Technology Council, this initiative proposes a new national infrastructure for data sharing and analysis that will provide a greatly enhanced knowledgebase to scientists and engineers designing new materials. This effort will foster enhanced computational capabilities, data management, and an integrated engineering approach for materials deployment to better leverage and complement existing Federal investments.

The success of this initiative will require a sustained effort from the private sector, universities, and the Federal Government. I look forward to working with you to make this vision a reality.

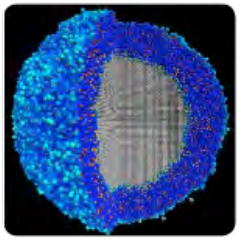
Sincerely,

John P. Holdren
Assistant to the President for Science and Technology
Director, Office of Science and Technology Policy

Computational Tools

Major advances in modeling and predicting materials behavior have led to a remarkable opportunity for the use of simulation software in solving materials challenges. New computational tools have the potential to accelerate materials development at all stages of the continuum. For example, software could guide the experimental discovery of new materials by screening a large set of compounds and isolating those with desired properties. Further downstream, virtual testing via computer-aided analysis could replace some of the expensive and time-consuming physical tests currently required for validation and certification of new materials.

These computational tools are still not widely used due to industry's limited confidence in accepting non-empirically-based conclusions. Materials scientists have developed powerful computational tools to predict materials behavior, but these tools have fundamental deficiencies that limit their usefulness. The primary problem is that current predictive algorithms do not have the ability to model behavior and properties across multiple spatial and temporal scales; for example, researchers can measure the atomic vibrations of a material in picoseconds, but from that information they cannot predict how the material will wear down over the course of years. In addition, software tools that utilize the algorithms are typically written by academics for academic purposes in separate universities, and therefore lack user-friendly interfaces, documentation, robustness, and the capacity to scale to industrial-sized problems. These deficiencies inhibit efficient software maintenance and can result in software failures. Significant improvements in software and the accuracy of materials behavior models are needed.



Open innovation will play a key role in accelerating the development of advanced computational tools. A system that allows researchers to share their algorithms and collaborate on creating new tools will rapidly increase the pace of innovation, which currently occurs in isolated academic settings. An existing system that is a good example of a first step toward open innovation is the nanoHUB, a National Science Foundation program run through the Network for Computational Nanotechnology.[8] By providing modeling and simulation applications that researchers can download and use on their data, nanoHUB.org supports the use of computational tools in nanotechnology research. Researchers can access state-of-the-art modeling algorithms and collaborate with colleagues via the website. To rapidly increase knowledge of first principles and advance modeling algorithms, it is essential for the materials industry to accept open innovation and design these tools on an open platform.

The ultimate goal is to generate computational tools that enable real-world materials development, that optimize or minimize traditional experimental testing, and that predict materials performance under diverse product conditions. An early benchmark will be the ability to incorporate improved predictive modeling algorithms of materials behavior into existing product design tools. For example, the crystal structure and physical properties of the materials in a product may change during the product's processing, due to varying conditions. It could be disastrous to the performance of a product if, for instance, the tensile strength of its bolts changed during manufacture. The ability to model these morphology and property changes will enable faster and better design.

Achieving these objectives will require a focus in three necessary areas: (1) creating accurate models of materials performance and validating model predictions from theories and empirical data; (2) implementing an open-platform framework to ensure that all code is easily used and maintained by all those involved in materials innovation and deployment, from academia to industry; and (3) creating software that is modular and user-friendly in order to extend the benefits to broad user communities.

Experimental Tools

The emphasis of the Initiative is on developing and improving computational capabilities, but it is essential to ensure that these new tools both complement and fully leverage existing experimental research on advanced materials. Effective models of materials behavior can only be developed from accurate and extensive sets of data on materials properties. Experimental data is required to create models as well as to validate their key results. Where computations based on theoretical frameworks fall short, empirical testing will fill in the

Laser Heating

48 nm

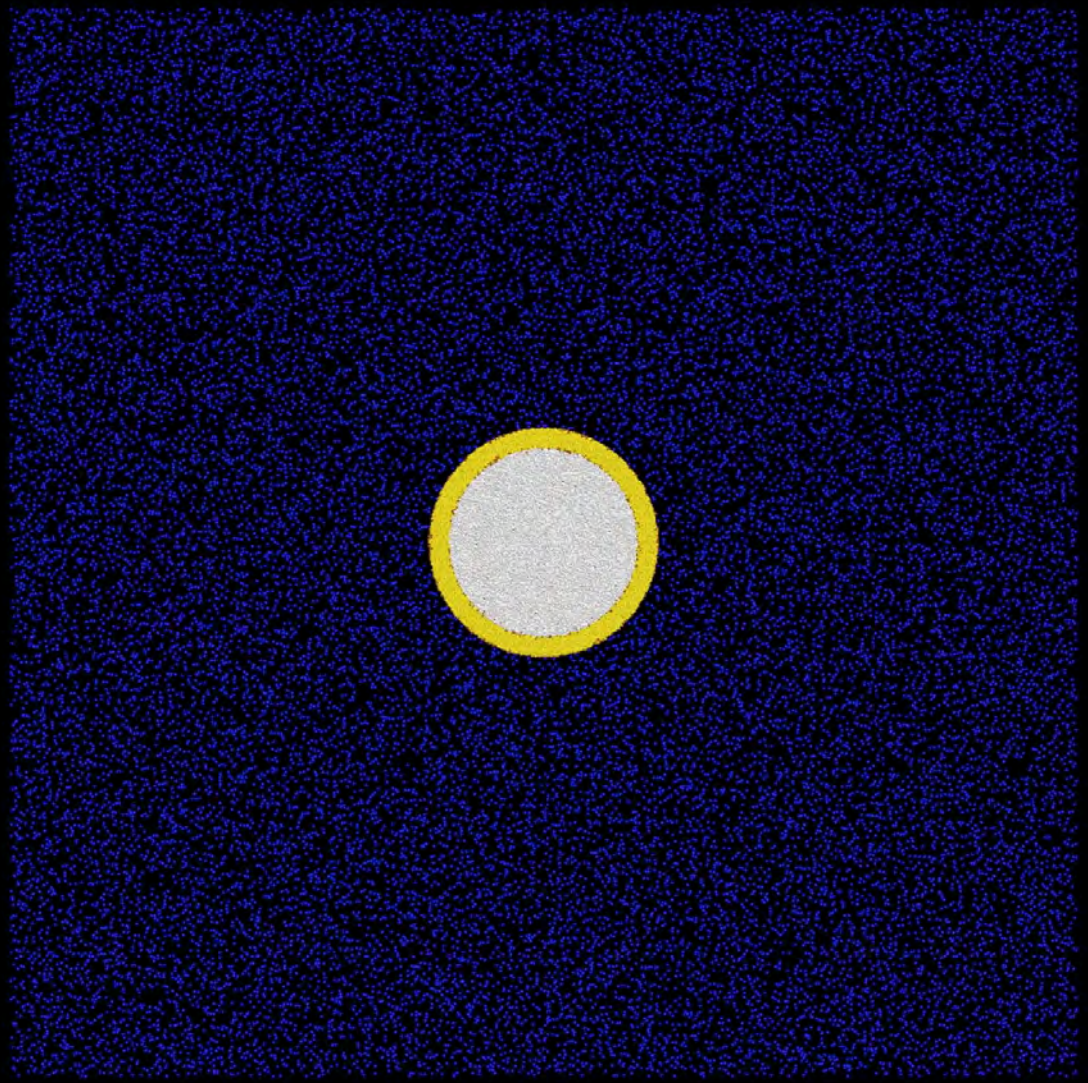
Nanoparticle with

4 nm

Alumina Nanoshell

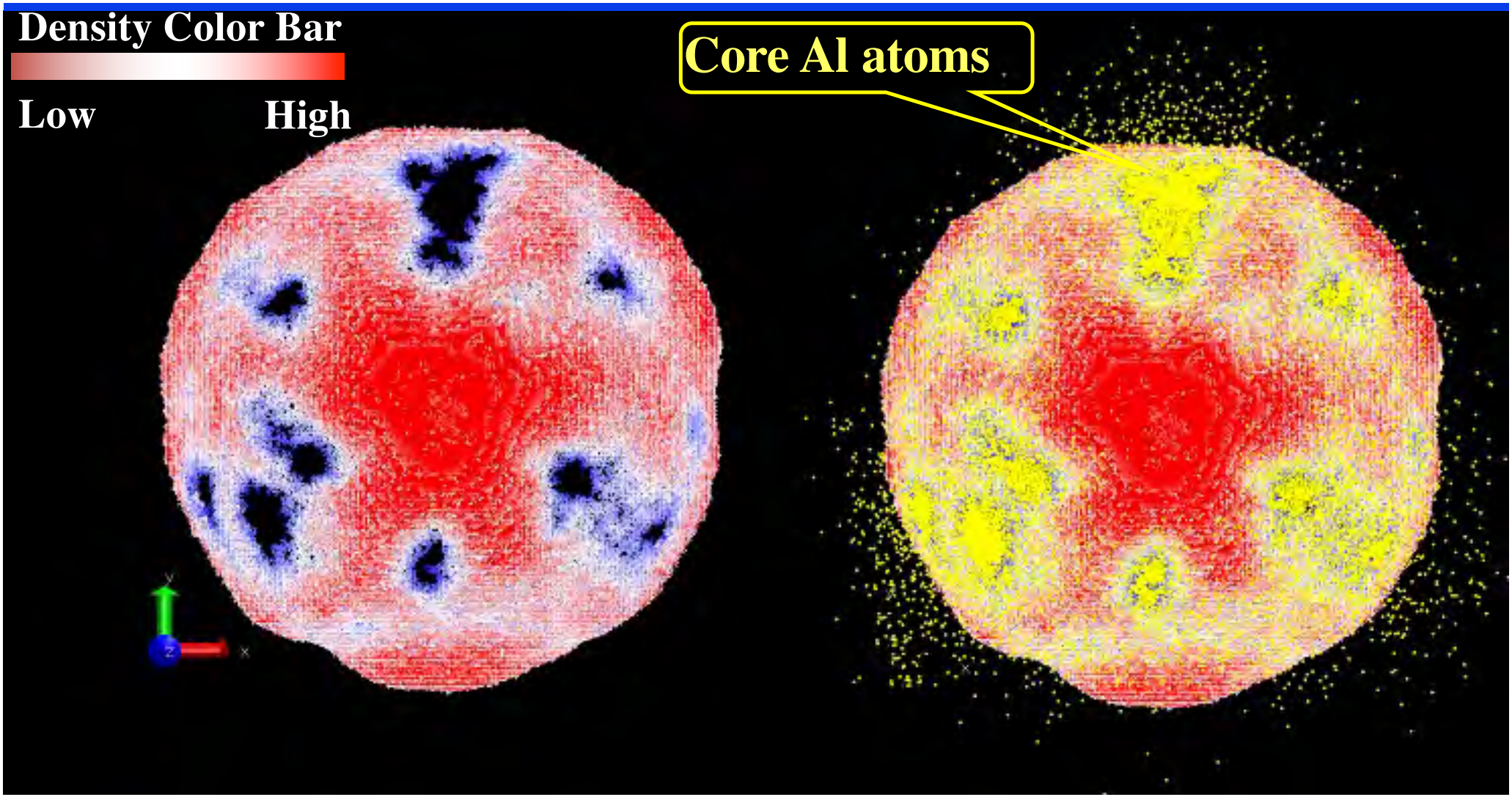
Nanoparticle Explosion

Tcore = 9000K, D= 48nm, S = 4nm



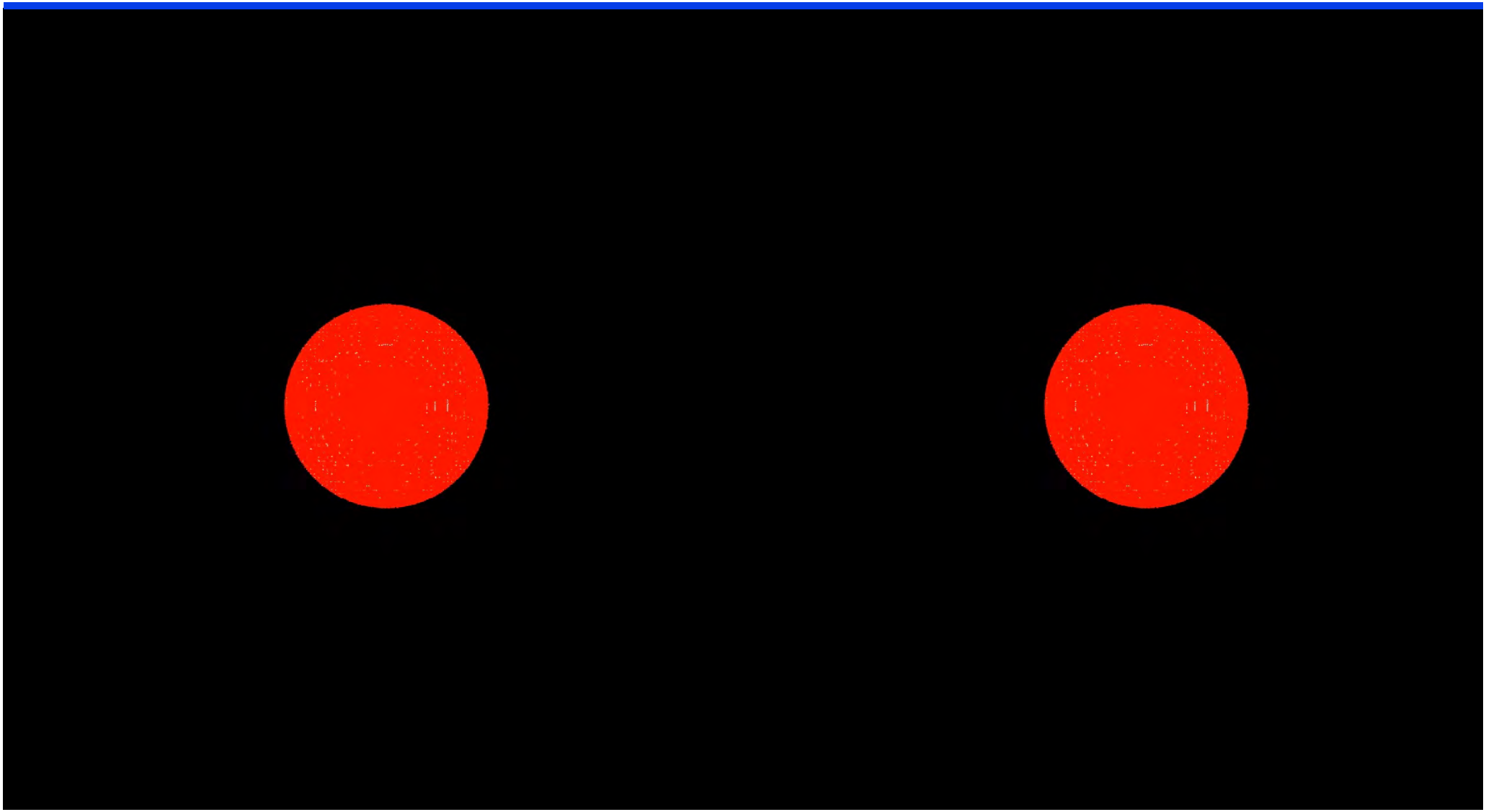
Expansion → Shell Broken → Oxidation Reaction

Jetting out of Al Core Atoms
Tcore = 9000K, t = 72ps



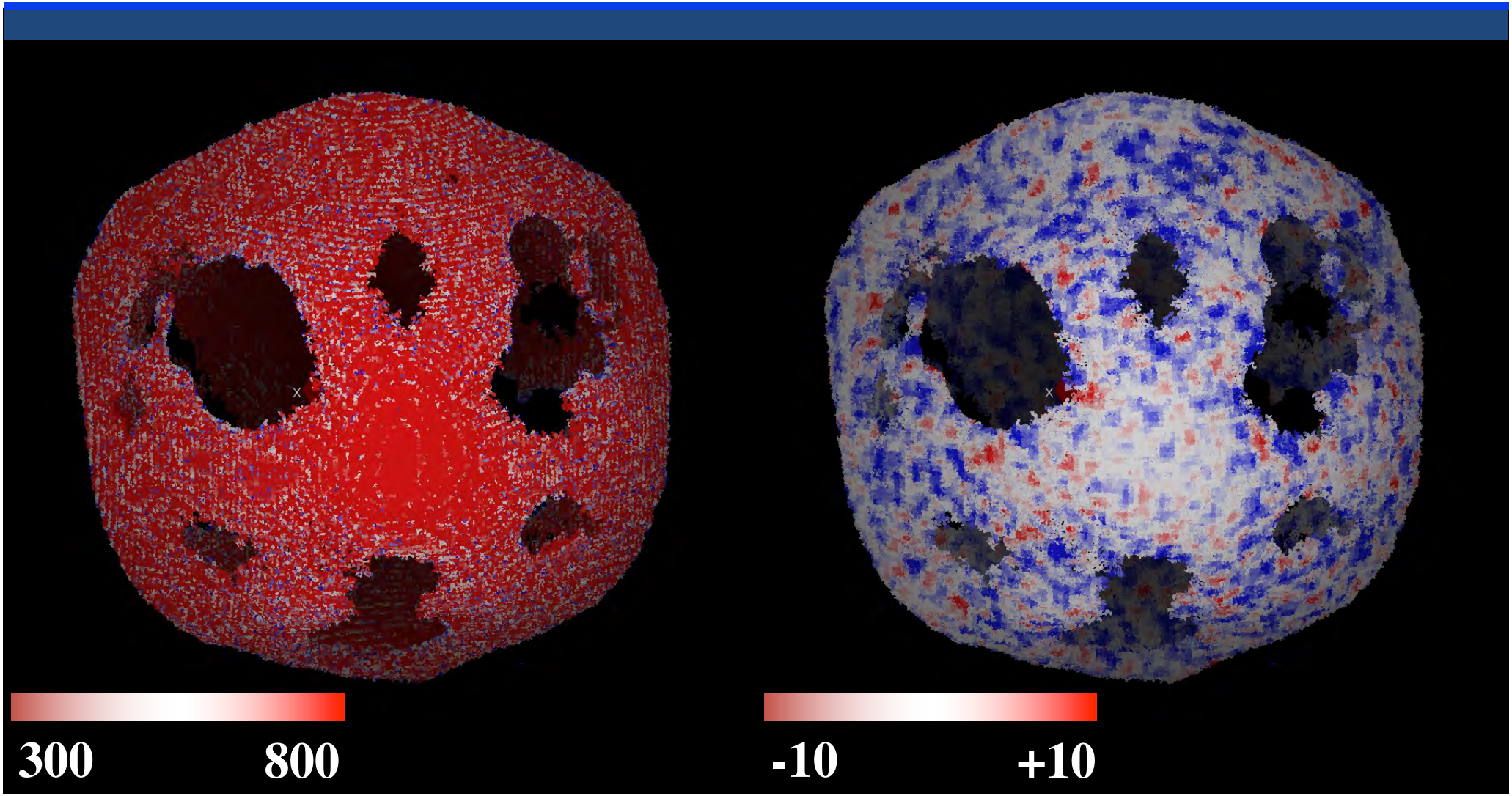
- More Al core atoms jet out from the weak areas of the shell

Jetting out of Al Core Atoms
Tcore = 9000K, 4 nm Shell



- More Al core atoms jet out from the weak areas of the shell

Structural Characterization of Nanoshell
S = 4nm, Tcore = 9000K



- **Density:** # of atoms / nm^3
- **Stress:** GPa

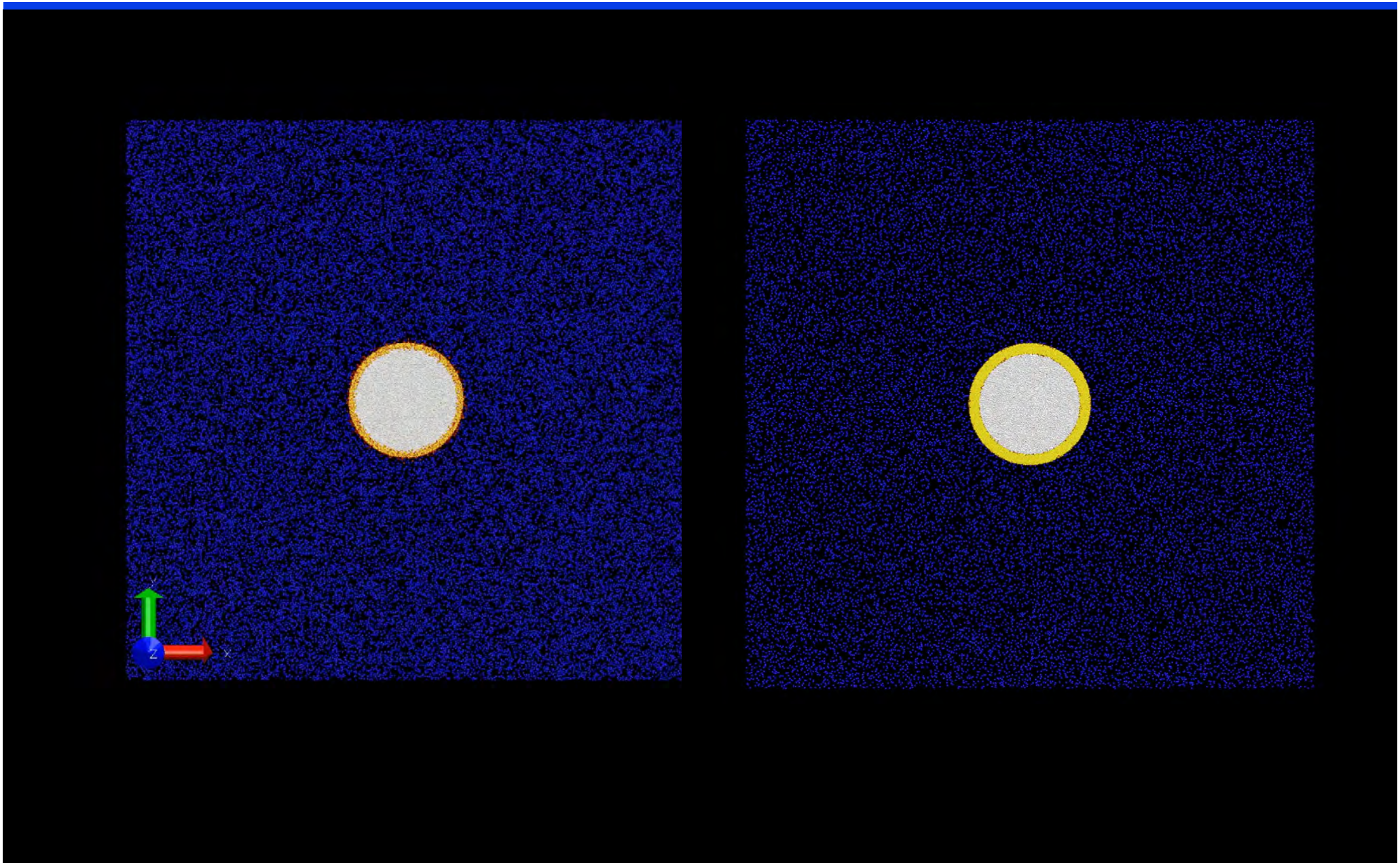
Nanoparticles with

4 nm (Crystalline) and

3 nm (Amorphous)

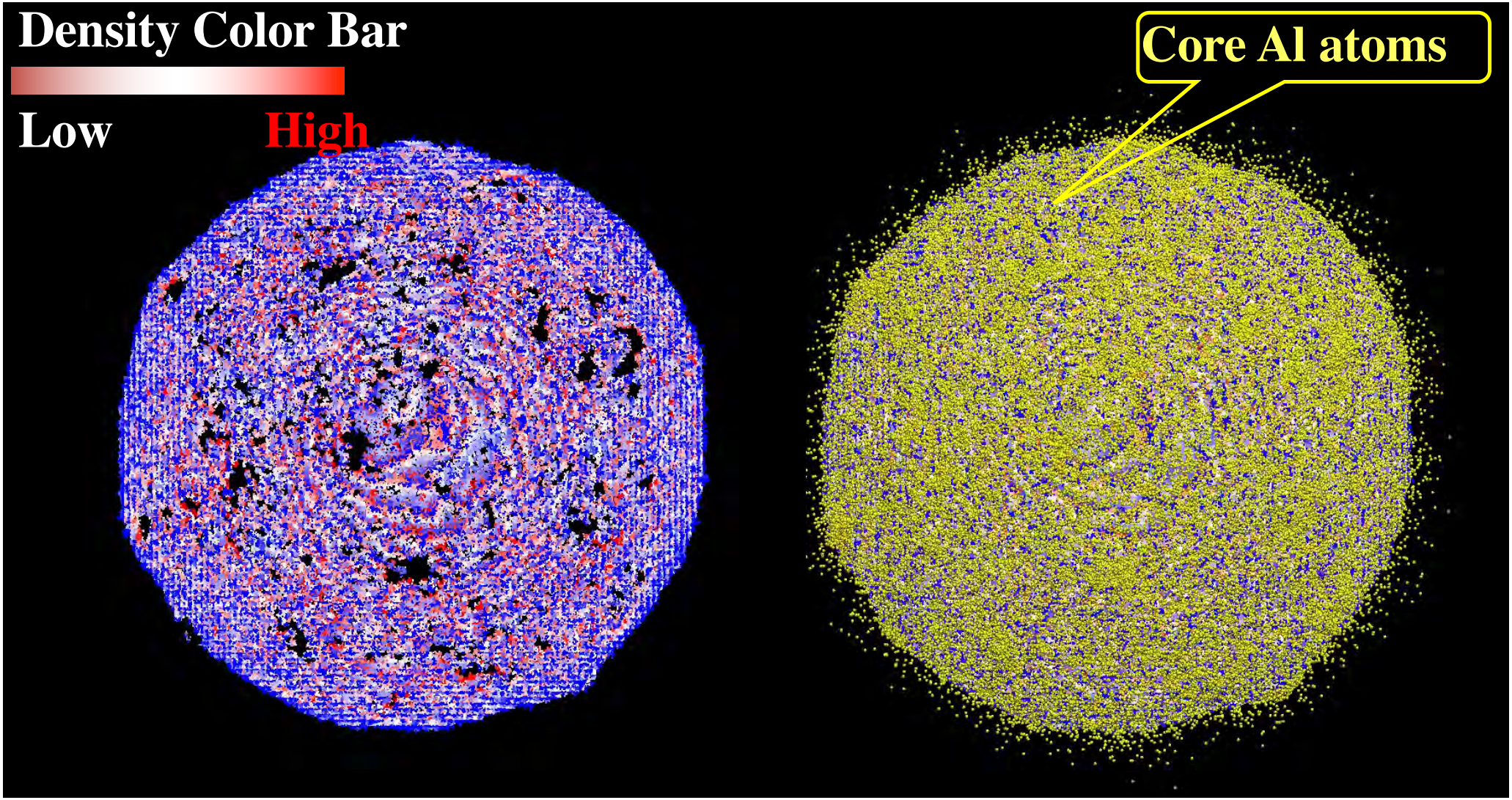
Alumina Shell

Amorphous and Crystalline Shells
Explosion: Tcore = 9000K



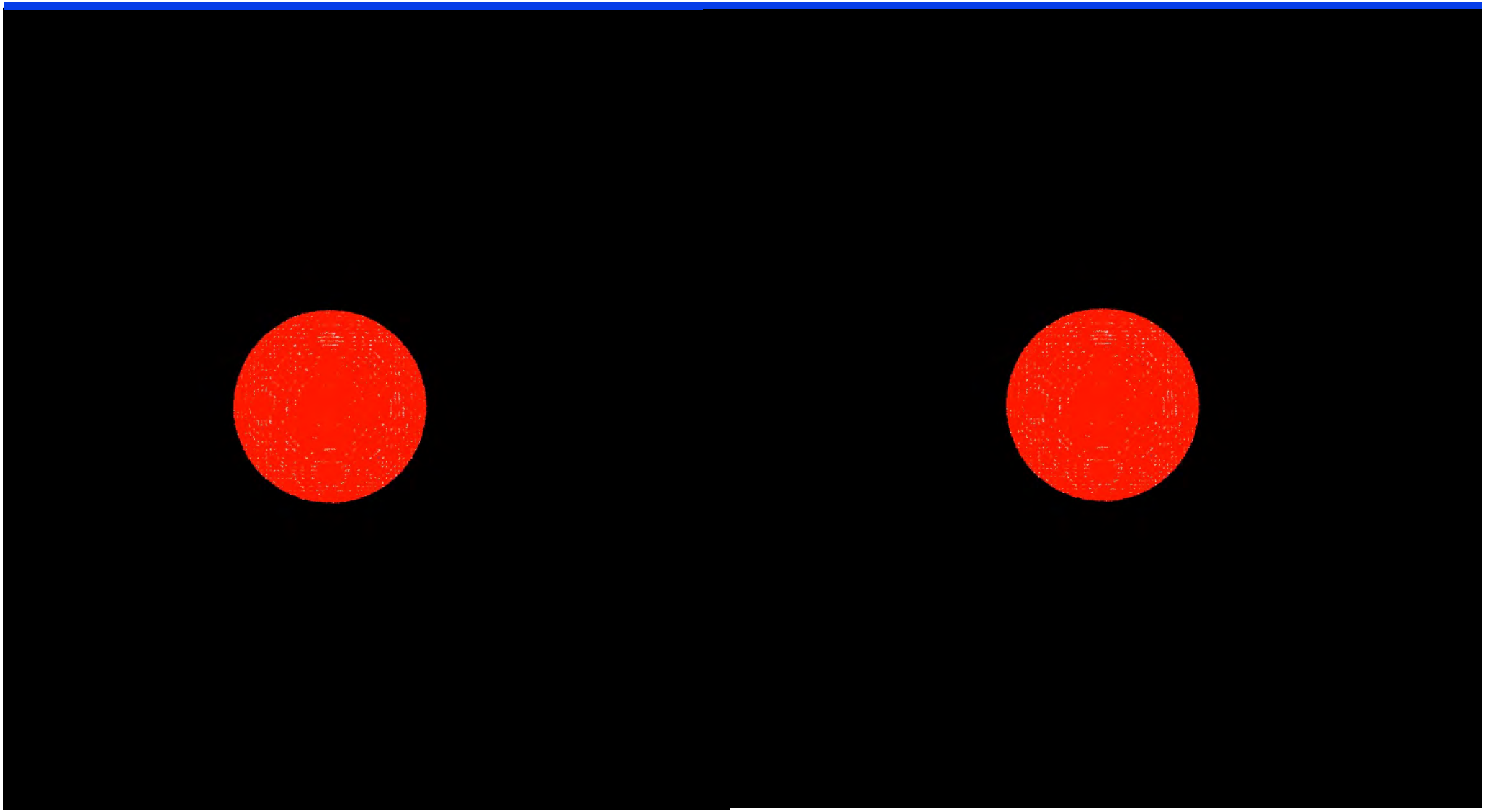
46 nm
Nanoparticle with
3 nm
Amorphous
Alumina Shell

Jetting out of Al Core Atoms
Tcore = 9000K, t = 60ps, Amorphous Shell



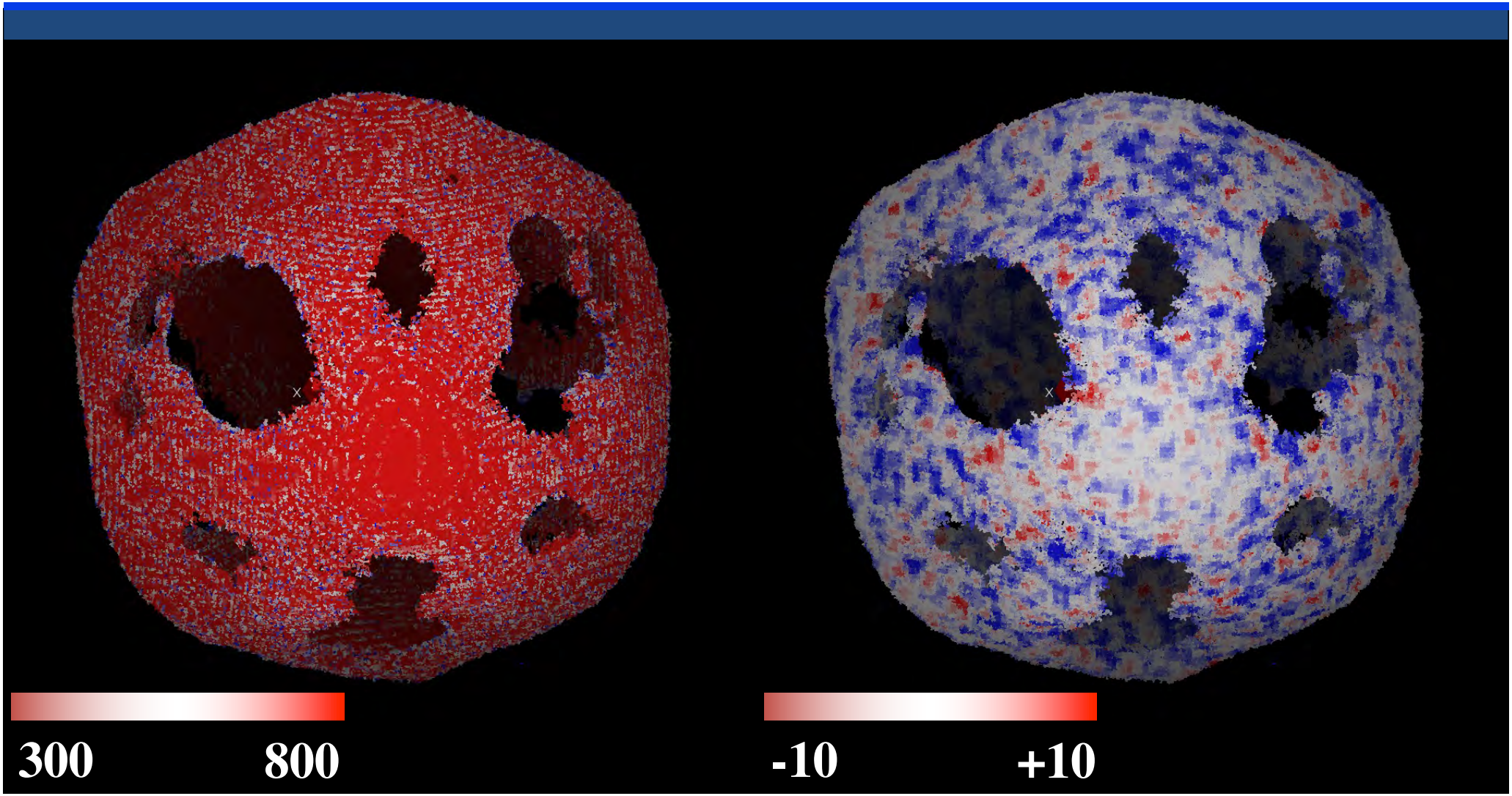
- Al core atoms jet out homogeneously from the shell

Jetting out of Al Core Atoms
Tcore = 9000K, Amorphous Shell



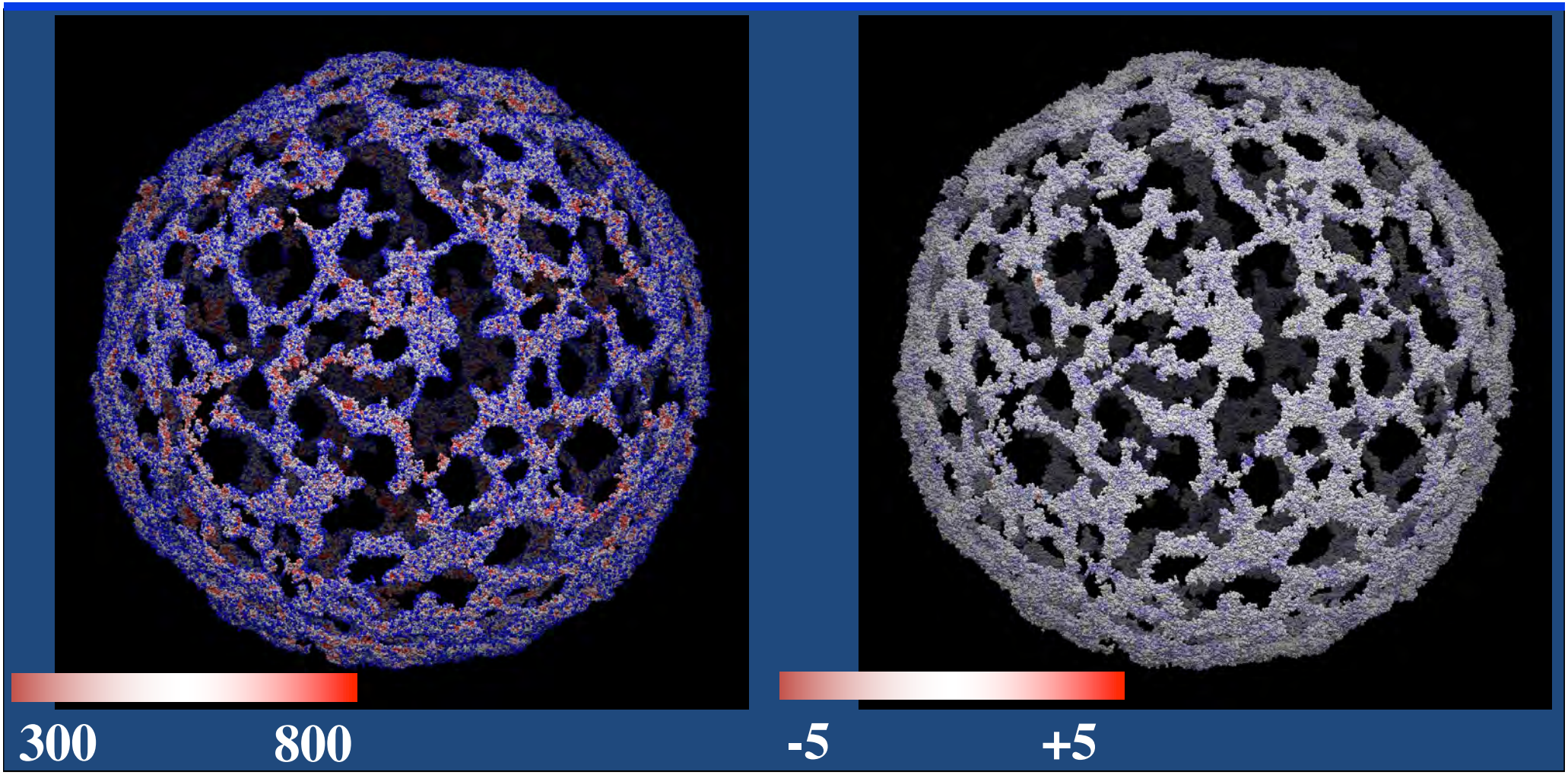
- Al core atoms jet out homogeneously from the shell

Structural Characterization of Nanoshell
Crystalline Shell, Tcore = 9000K



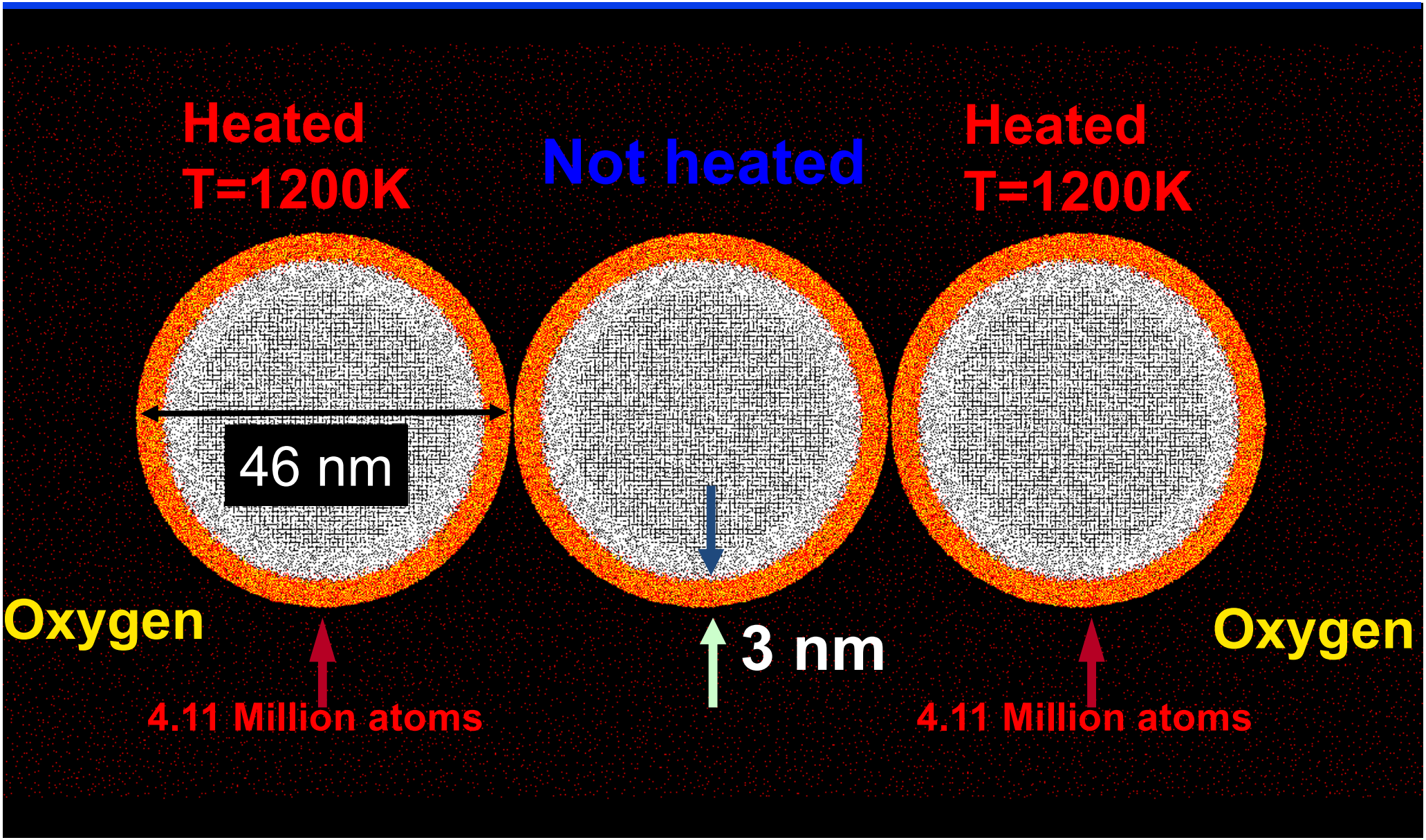
- **Density:** # of atoms / nm^3
- **Stress:** GPa

Structural Characterization of Nanoshell
Amorphous Shell, Tcore = 9000K

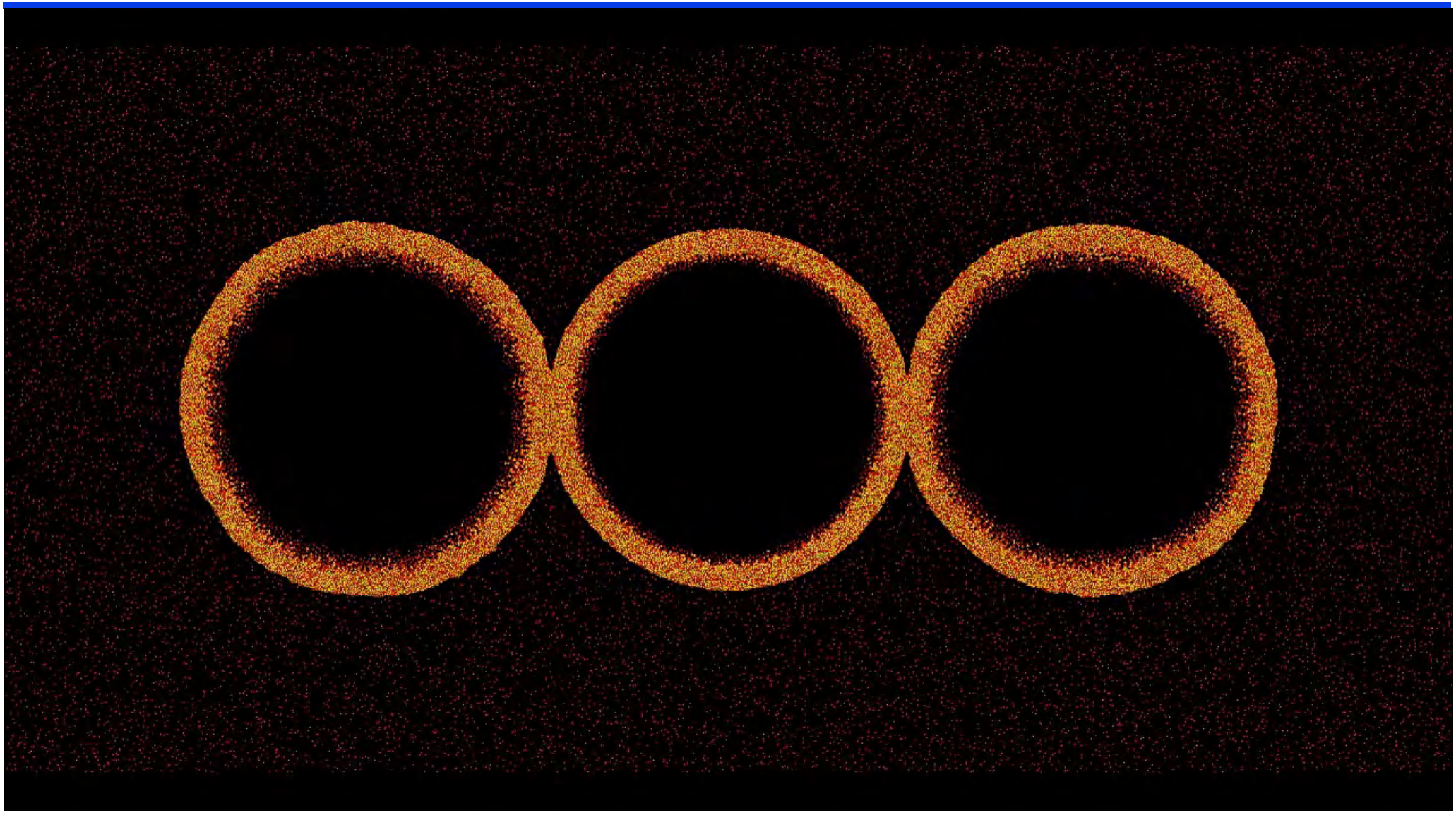


- **Density:** # of atoms / nm^3
- **Stress:** GPa

Three 46 nm Nanoparticles: Burning of the Center Nanoparticle

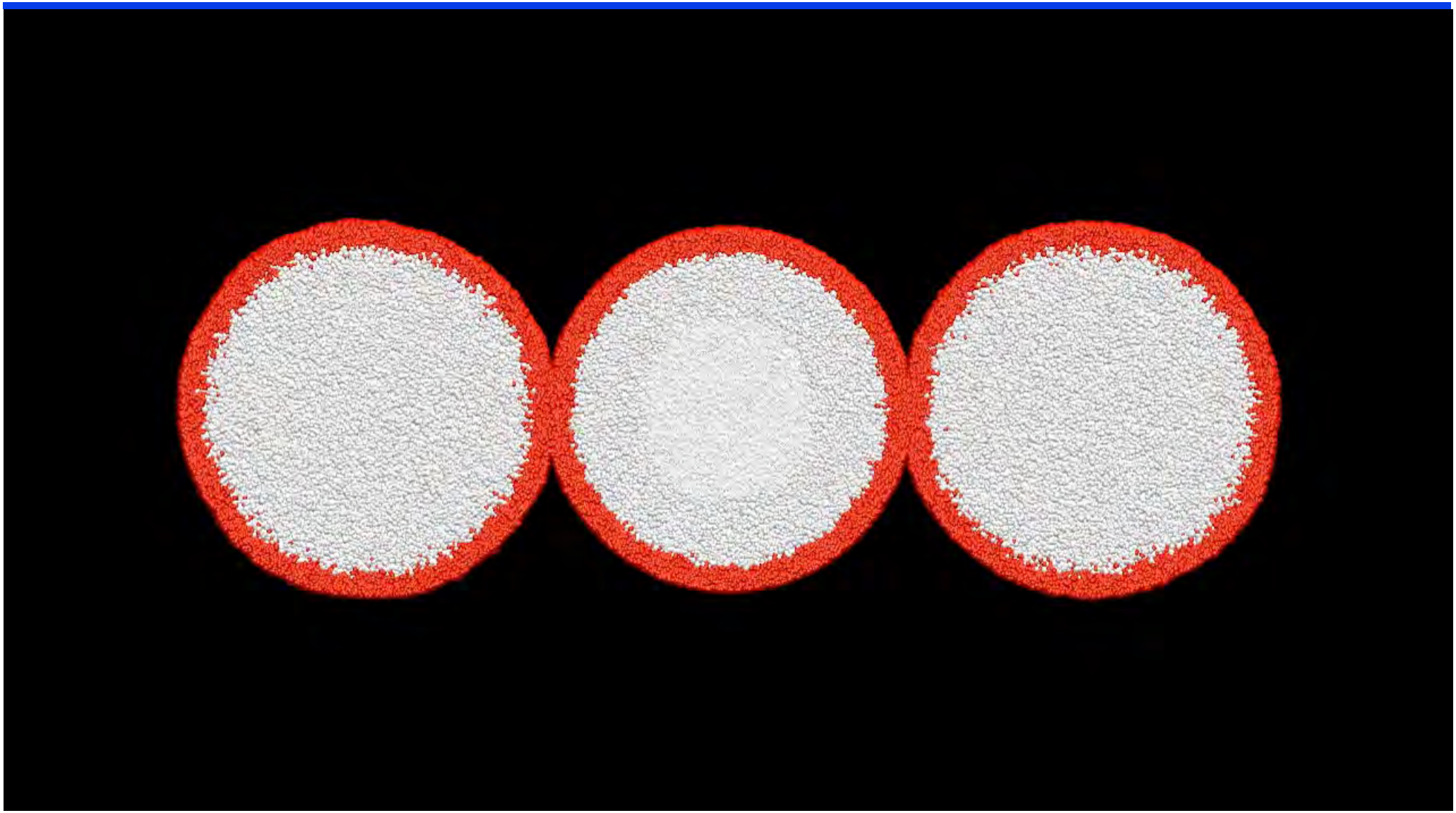


Oxidation of the Center Nanoparticle



Oxidation reaction (Al core is not shown)

Oxidation of the Center Nanoparticle Aluminum Ejections



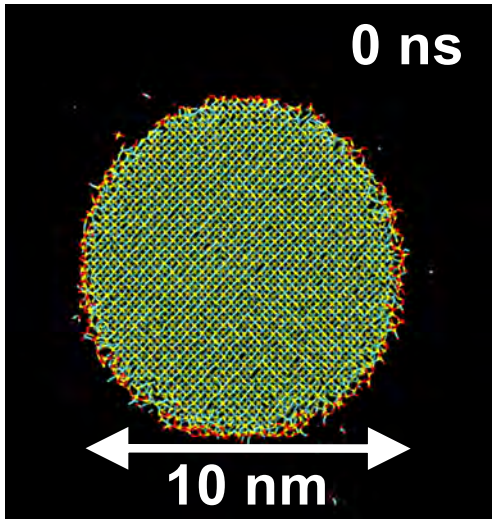
Aluminum ejections: core (white) and shell (red)

Computational Synthesis

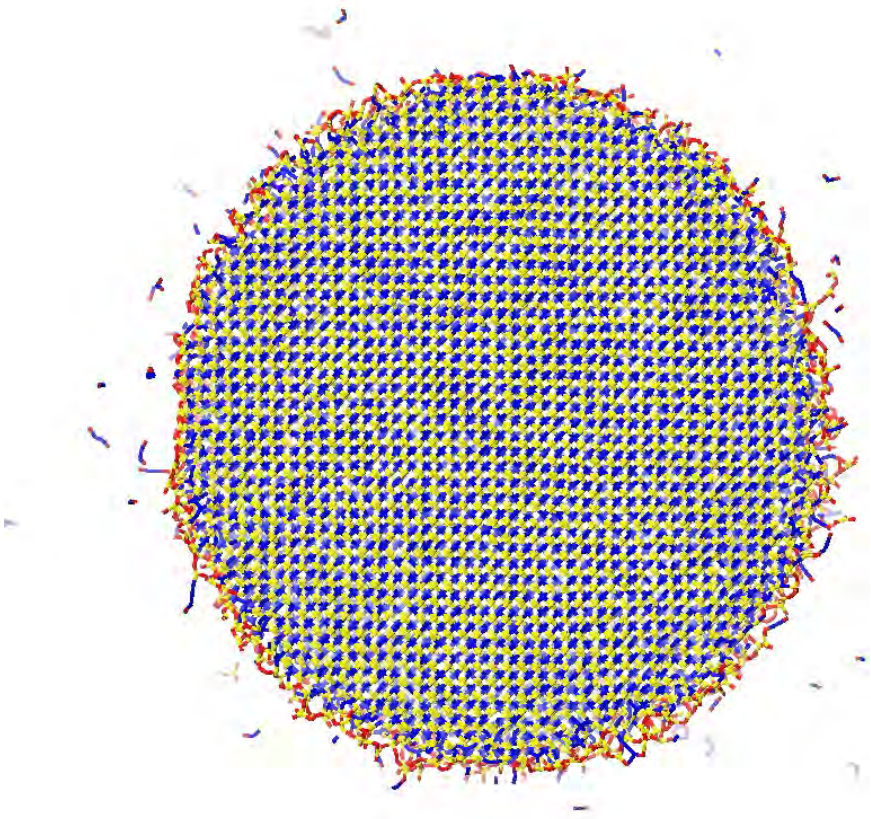
Graphitic metamaterial from high temperature oxidation of silicon carbide.

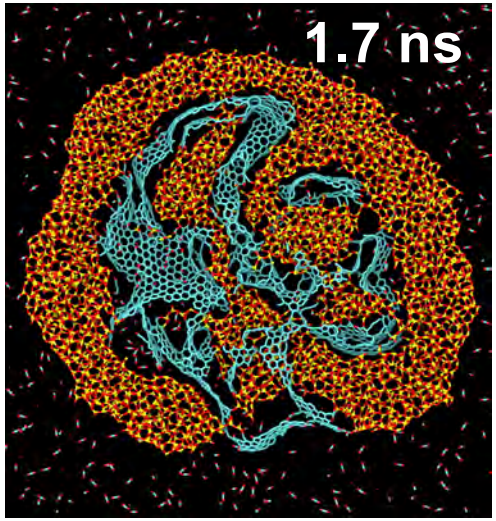
Oxidation of SiC Nanoparticle

- Reactive molecular dynamics (RMD) simulations: Diameter = 10 nm (100K atoms), 46 nm (10M atoms) & 100 nm (112M atoms) on 786,432-processor IBM Blue Gene/Q



Si, C, O
T = 2,800 K

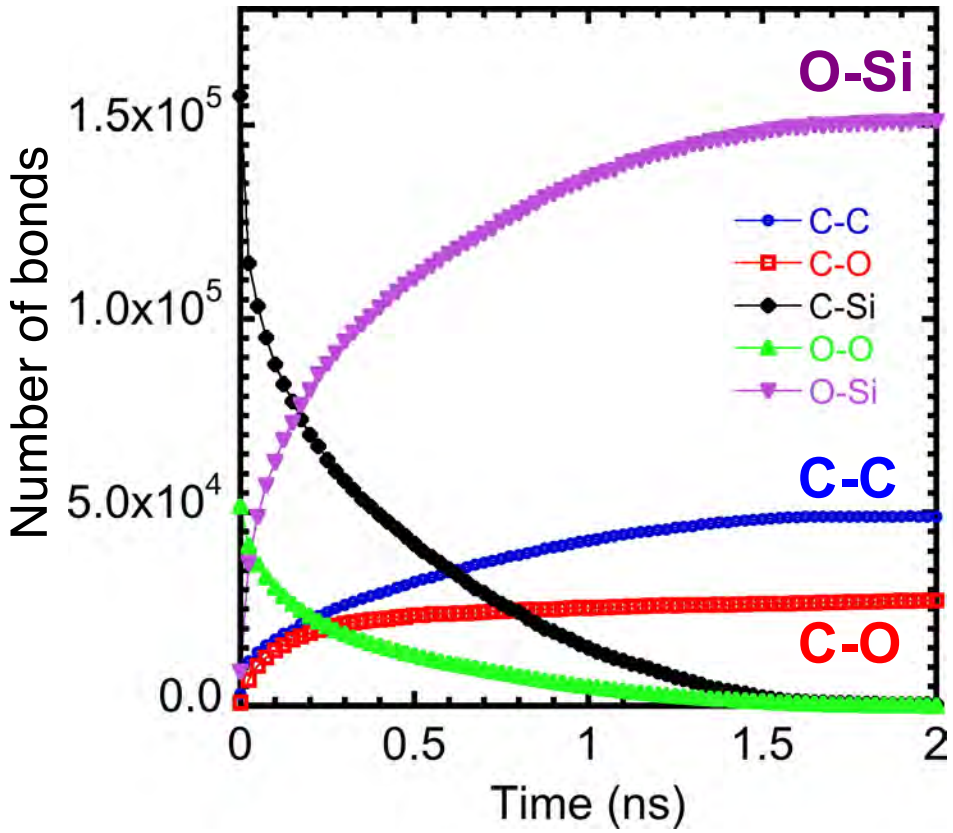


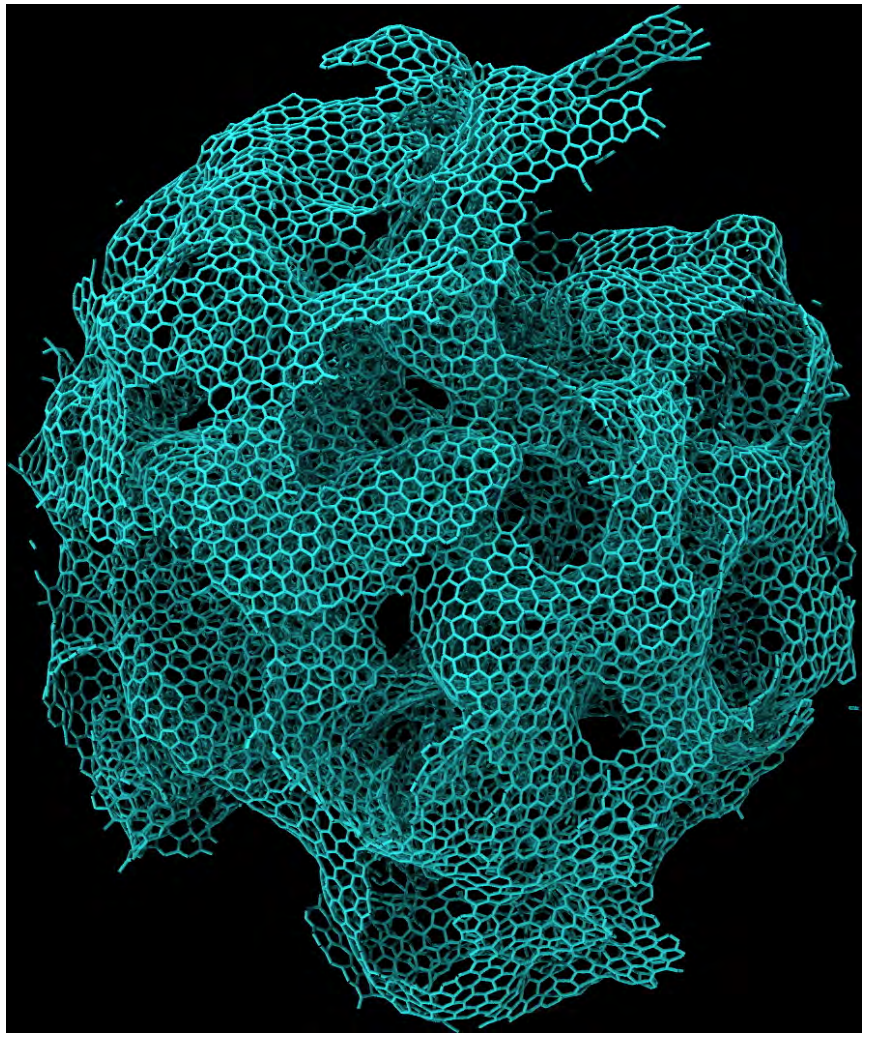


- Formation of nanocarbon, embedded within SiO_2 shell

Nanocarbon Production

- Much more Si-O bonds are formed compared with C-O
- C-C bonds are predominantly sp^2

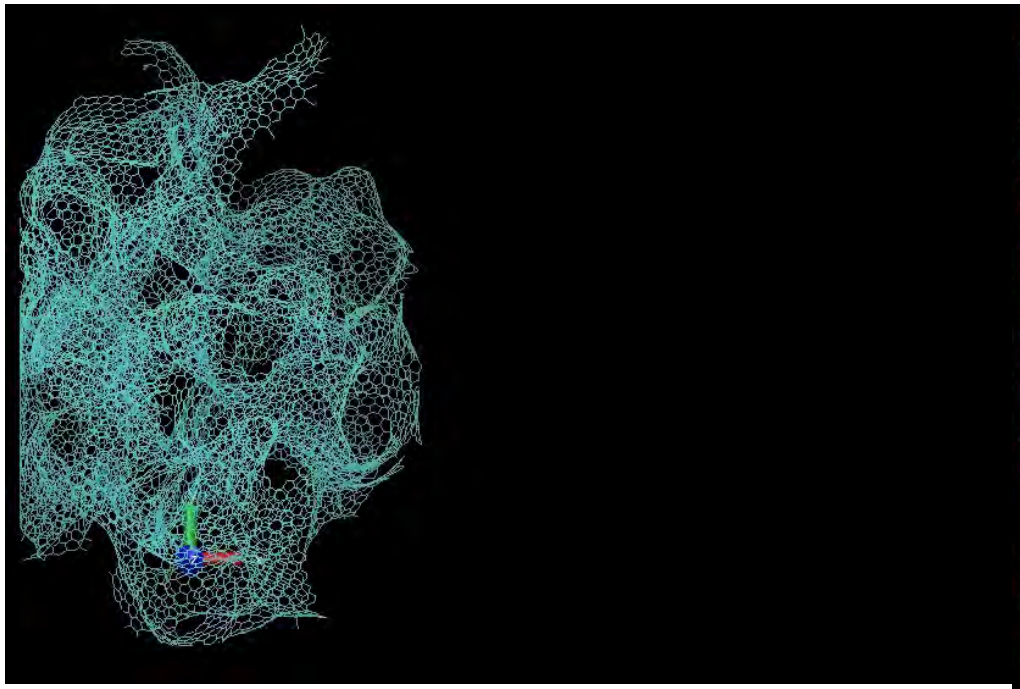




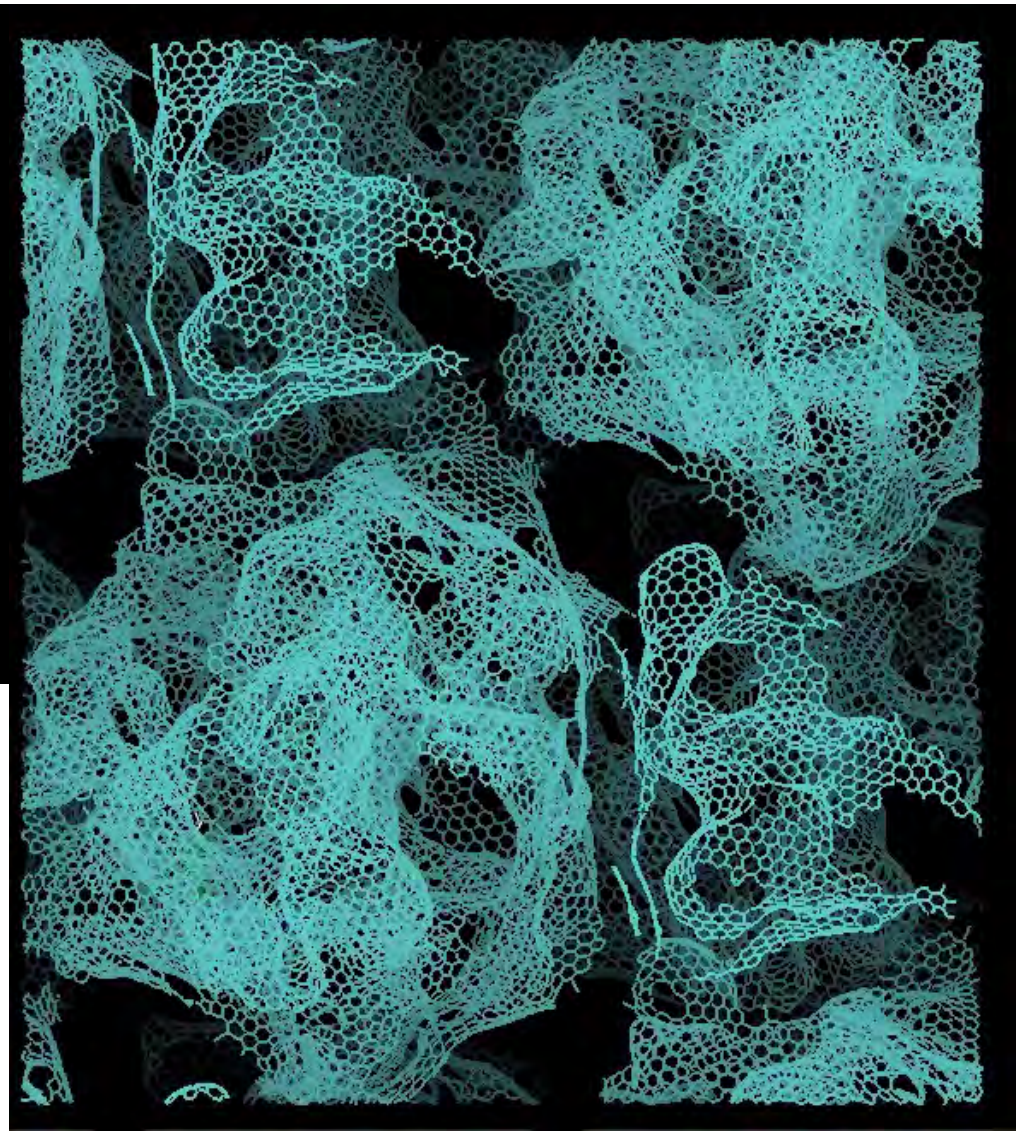
- Silica shell acts as a *nanoreactor* by transporting O reactants & protecting C products from harsh oxidizing environment

Mechanical Metamaterial?

- **A simple synthetic pathway to high surface-area, low-density nanocarbon with numerous energy & mechanical-metamaterial applications, including the reinforcement of self-healing composites**

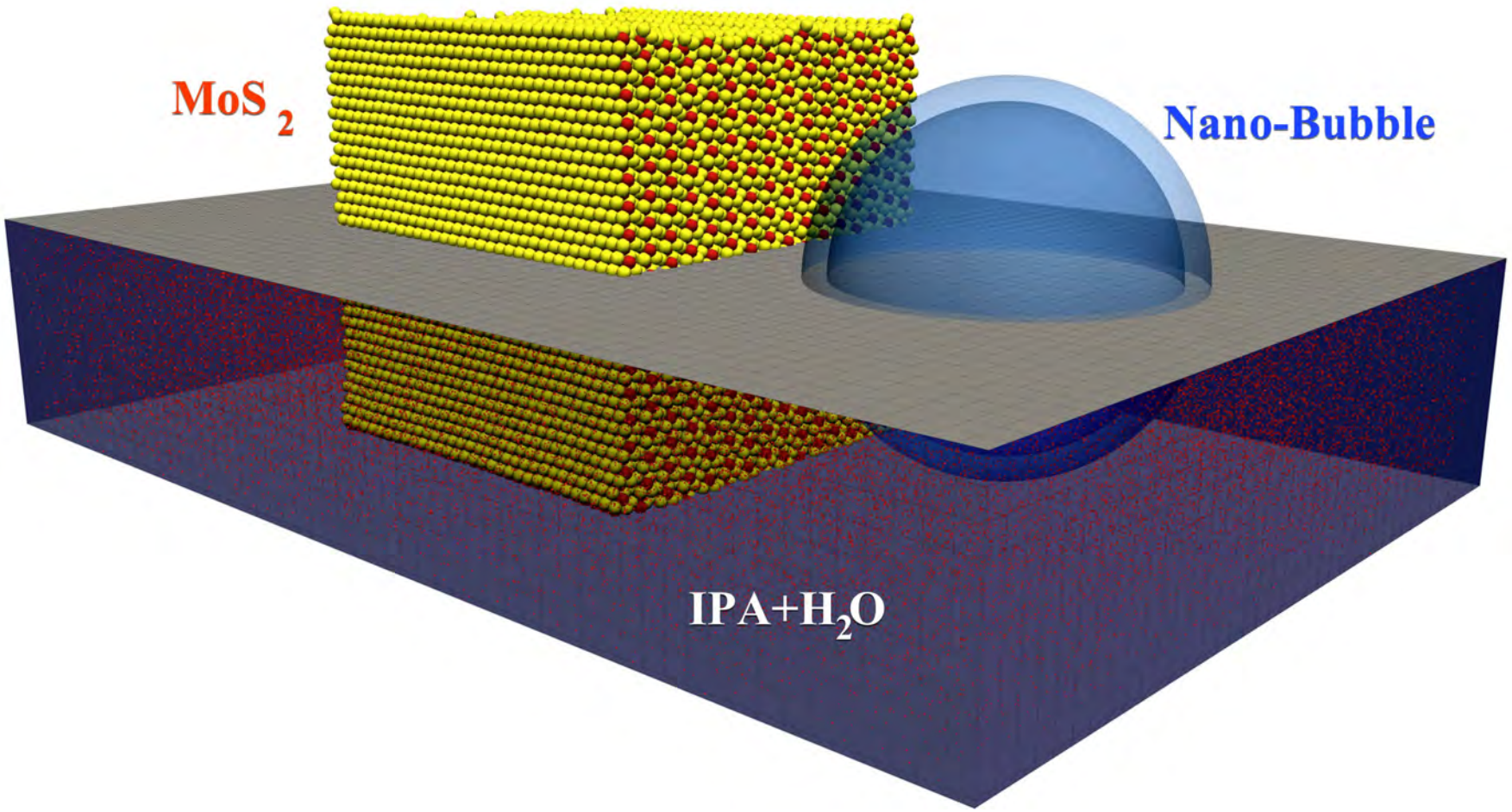


MetaCarbon
Under Shock Impact



MetaCarbon
Under Compression

Molecular Mechanism of MoS_2 Exfoliation



- Shear stresses on MoS_2 surfaces initiate exfoliation
- Shock waves reflected from MoS_2 surfaces enhance exfoliation

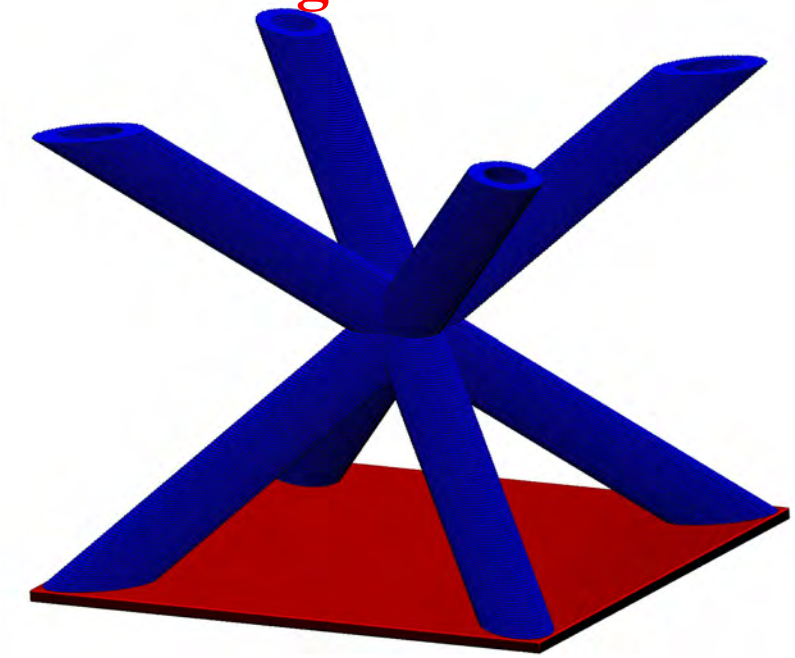
Ultralight Mechanical Metamaterials

Deformation of Cellular Architecture

Pankaj Rajak, 2:15PM, Today, Constitution B

Basic building block of cellular architecture

Kagome lattice



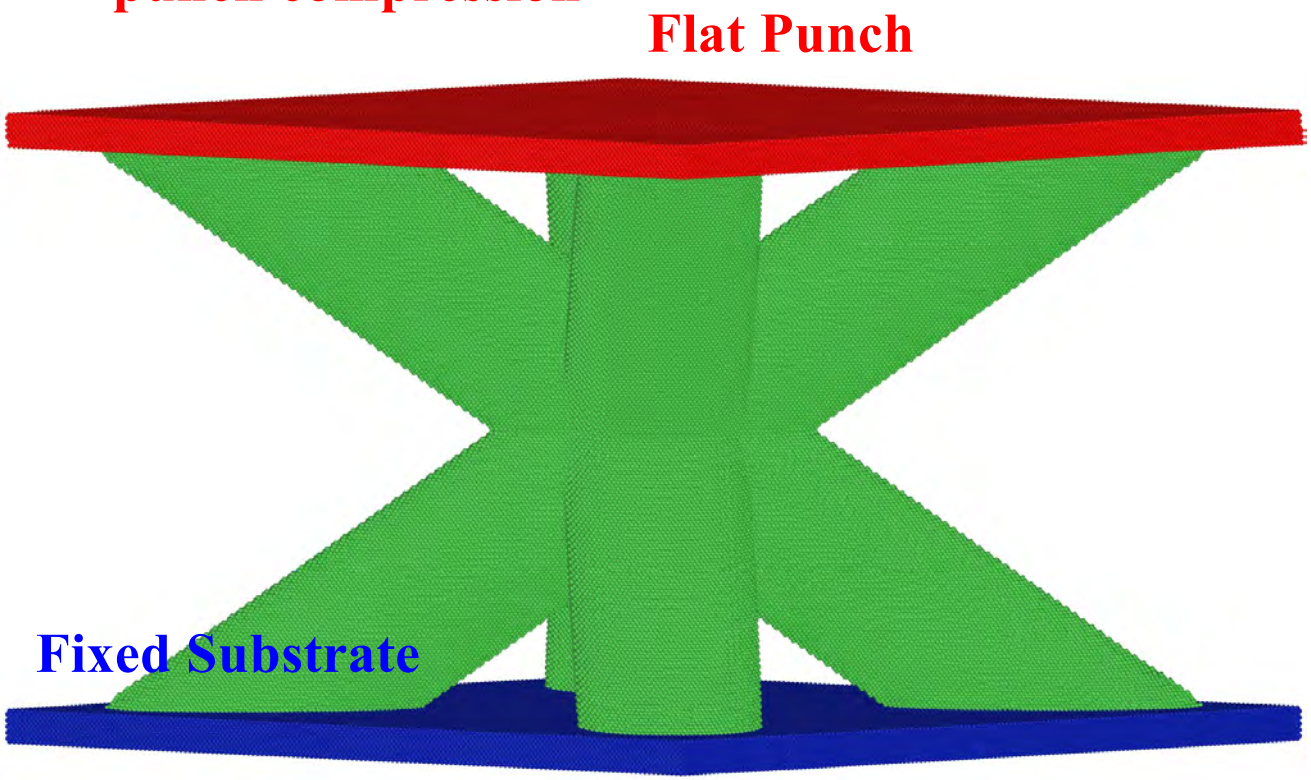
Octen truss

Deformation behavior of these structures at atomic level is not clean

To answer this question we have studied uniaxial compression of Nickel Kagome lattice using molecular dynamics simulation

Molecular Dynamics Simulation Setup

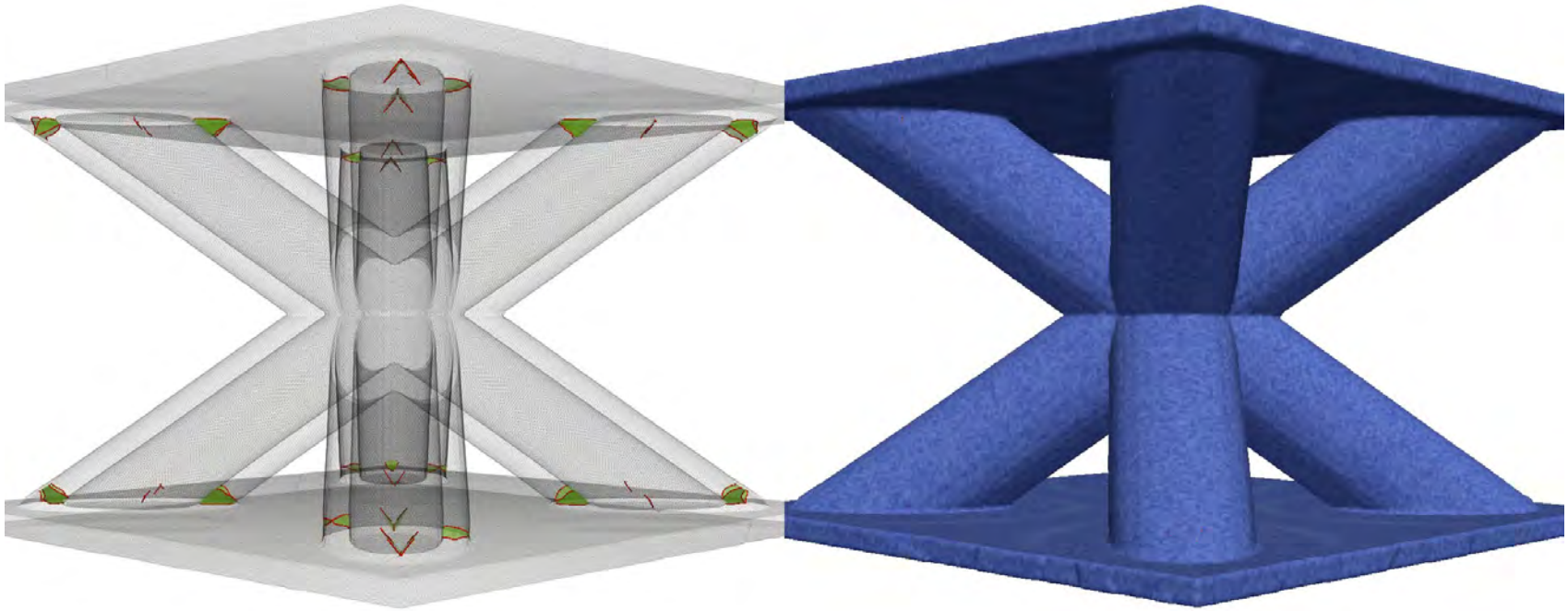
- Uniaxial Compression of Single Kagome structure is studied using flat punch compression



- Kagome structure made from hollow/solid Ni nanorod
- System size:550A*350A*0A, Ni nanorod diameter 10nm & thickness 2nm
- Total number of atoms: 1 million to 2.5 million

- Flat Punch is moved at a speed of 2m/sec and after each compression of 0.5%, system is relaxed for 400ps

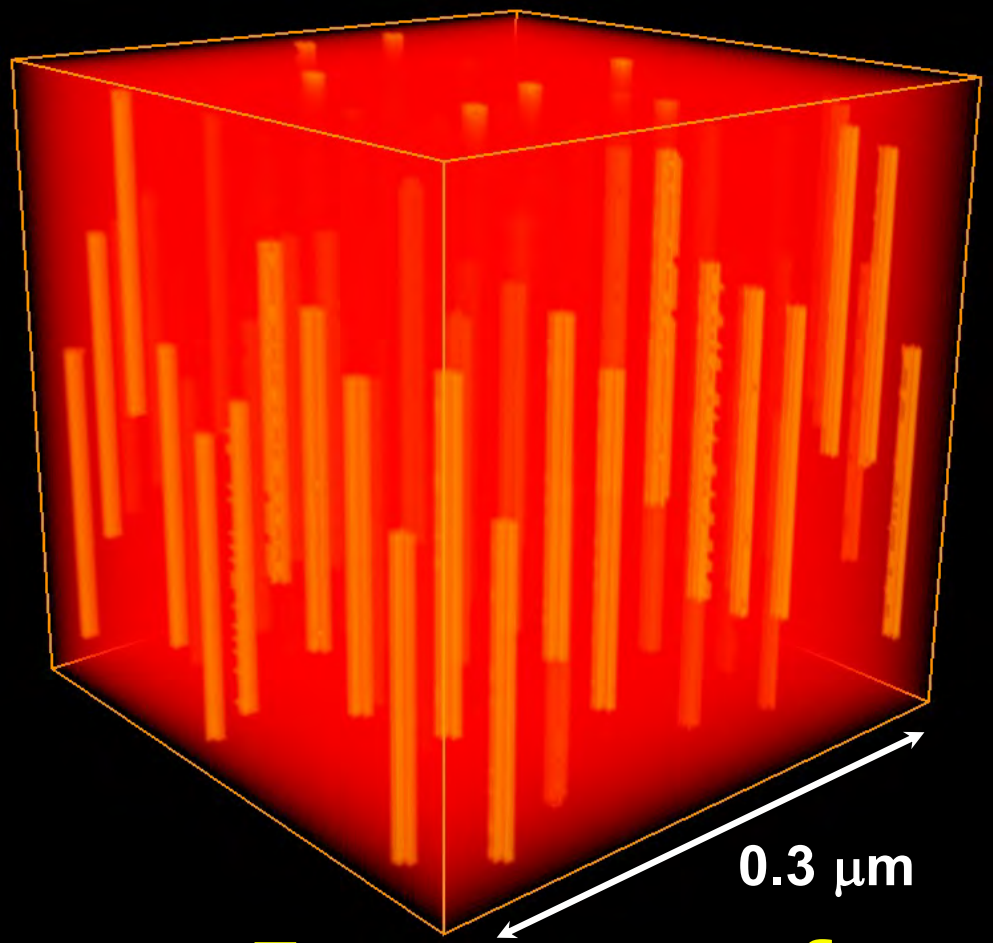
Conclusion

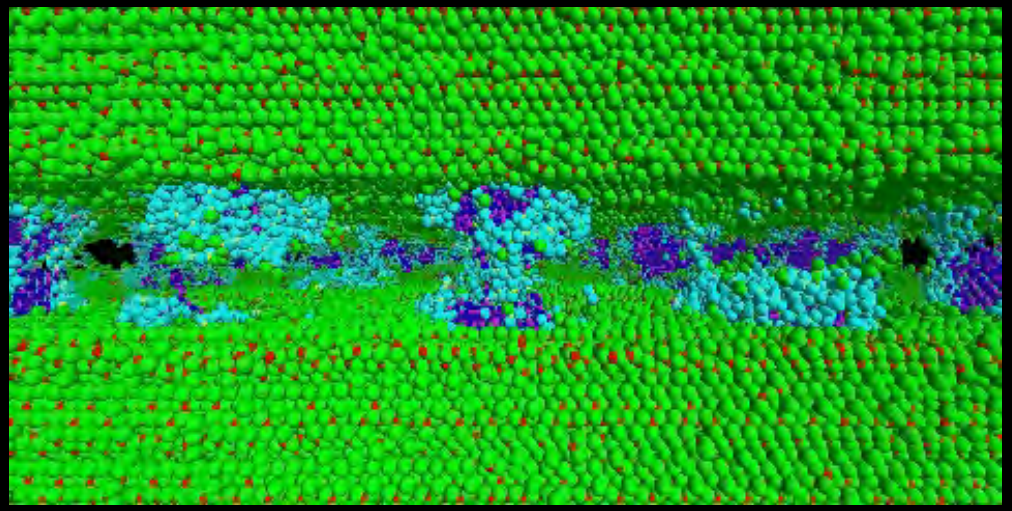


- Mechanical Collapse of single nanorod/nanotube happens at after 3.5% strain
- Yielding in solid kagome lattice happens at 2.5% strain while for hollow lattice after 3.9% strain
- All 8 beams in solid kagome lattice shows deformation after yield point which results in the formation of several slipped and twin region in the system
- Deformation happens near the node in hollow kagome lattice up to 11% strain and after that bending of the lattice is observed

Si_3N_4-Matrix SiC-Fiber Nanocomposite

1.5-billion-atom MD on IBM SP3

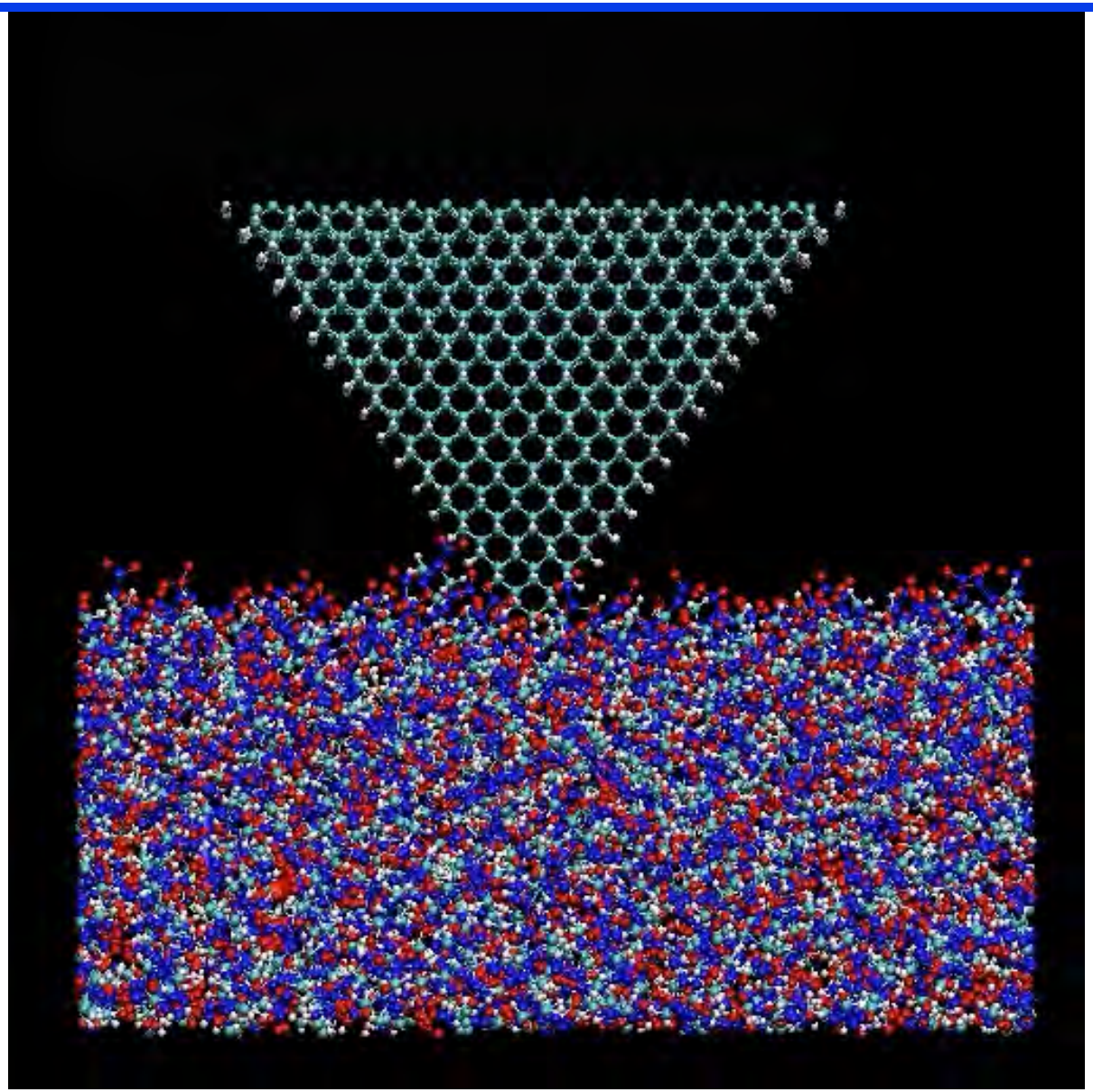


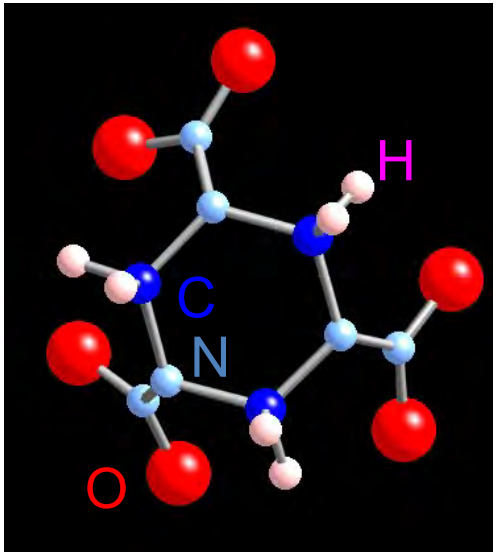


Color code: Si_3N_4; SiC; SiO_2

Fracture surfaces in ceramic-fiber nanocomposites: Toughening mechanisms?

Nanoindentation on RDX Crystal



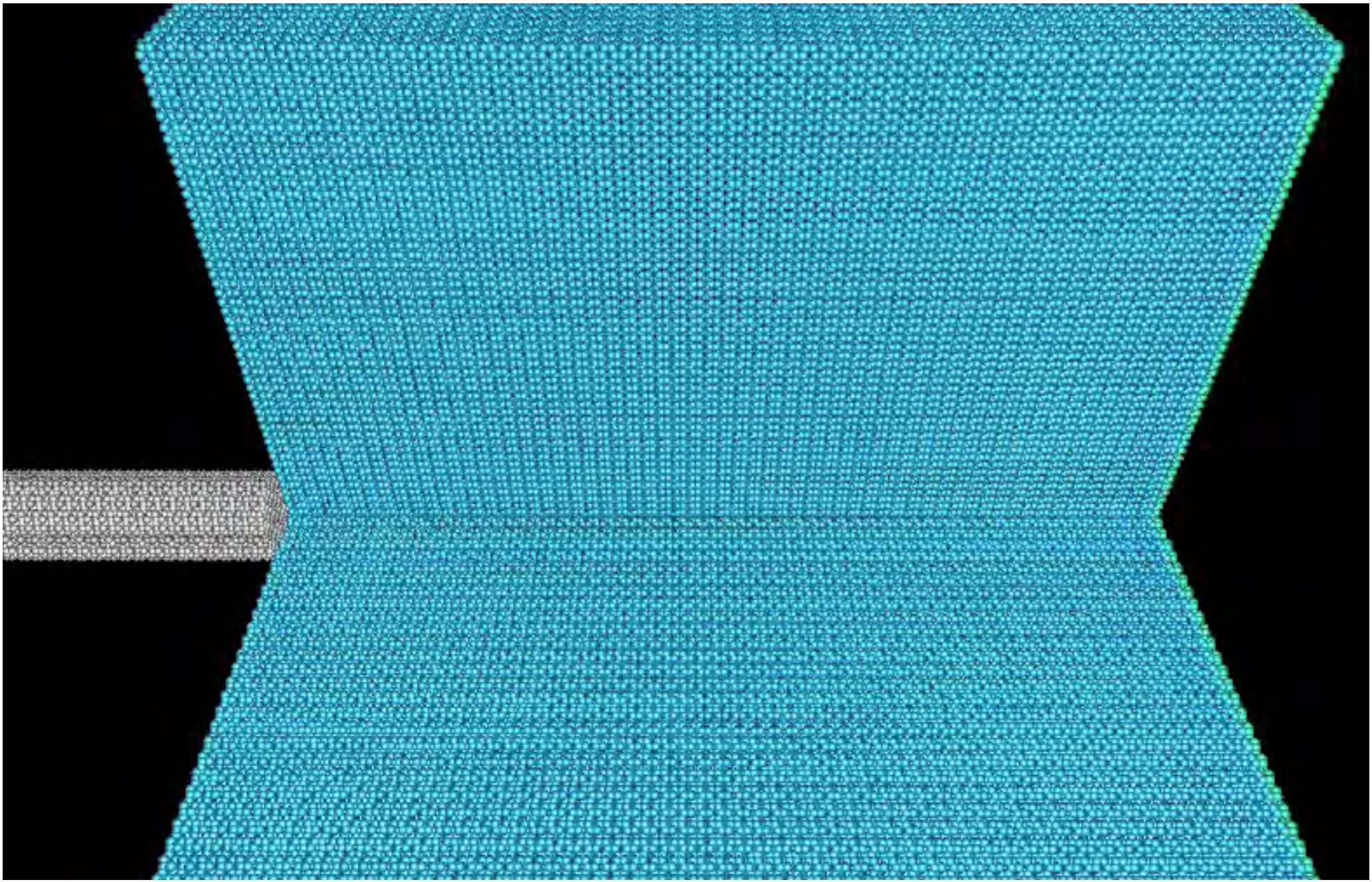


RDX molecule
$C_3N_6O_6H_6$

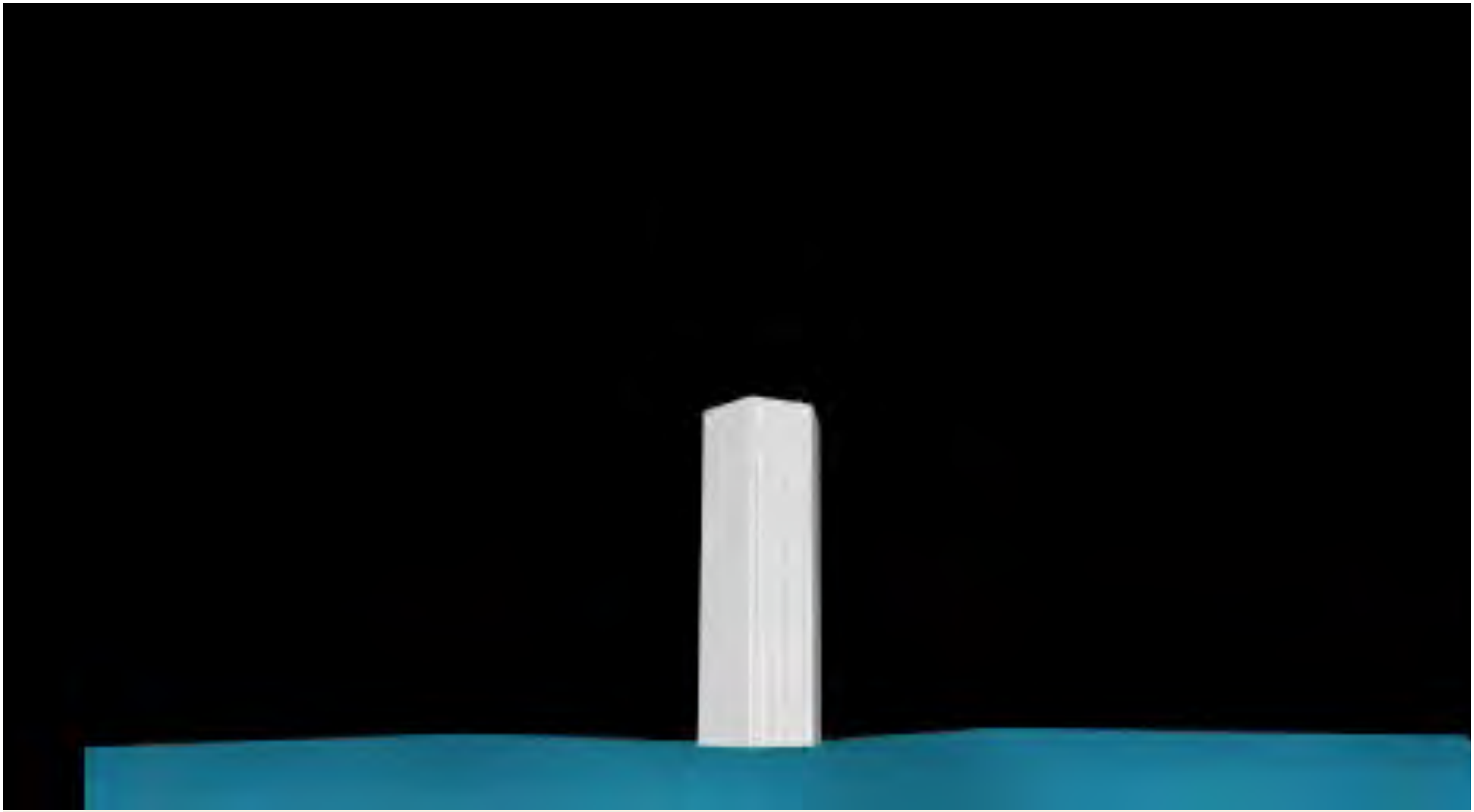
- Localized melting under a diamond AFM tip
- RDX molecules climb on the indenter surface

Hypervelocity Impact Damage

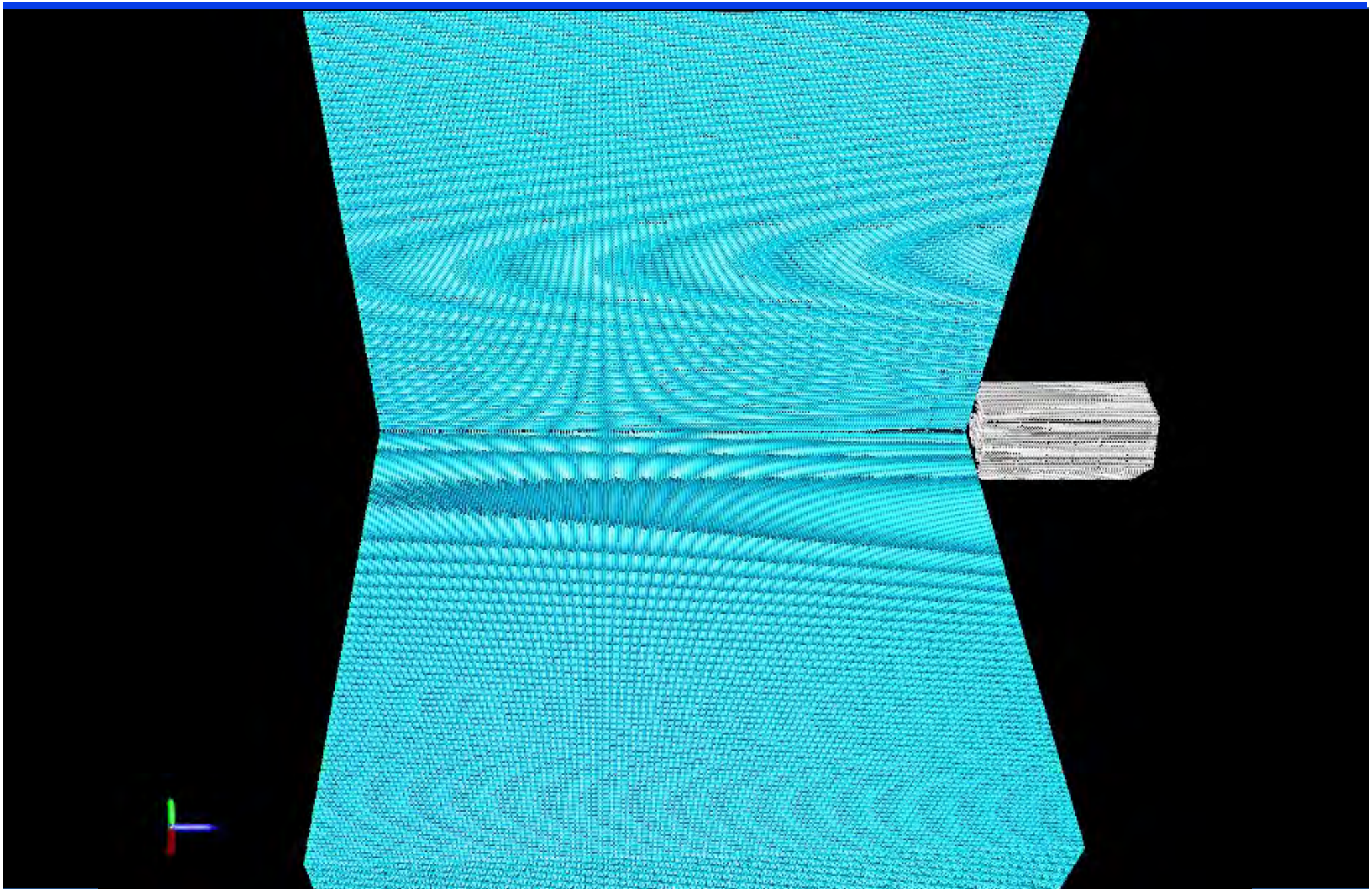
Damage from “Hard Impactor” in AlN Ceramic



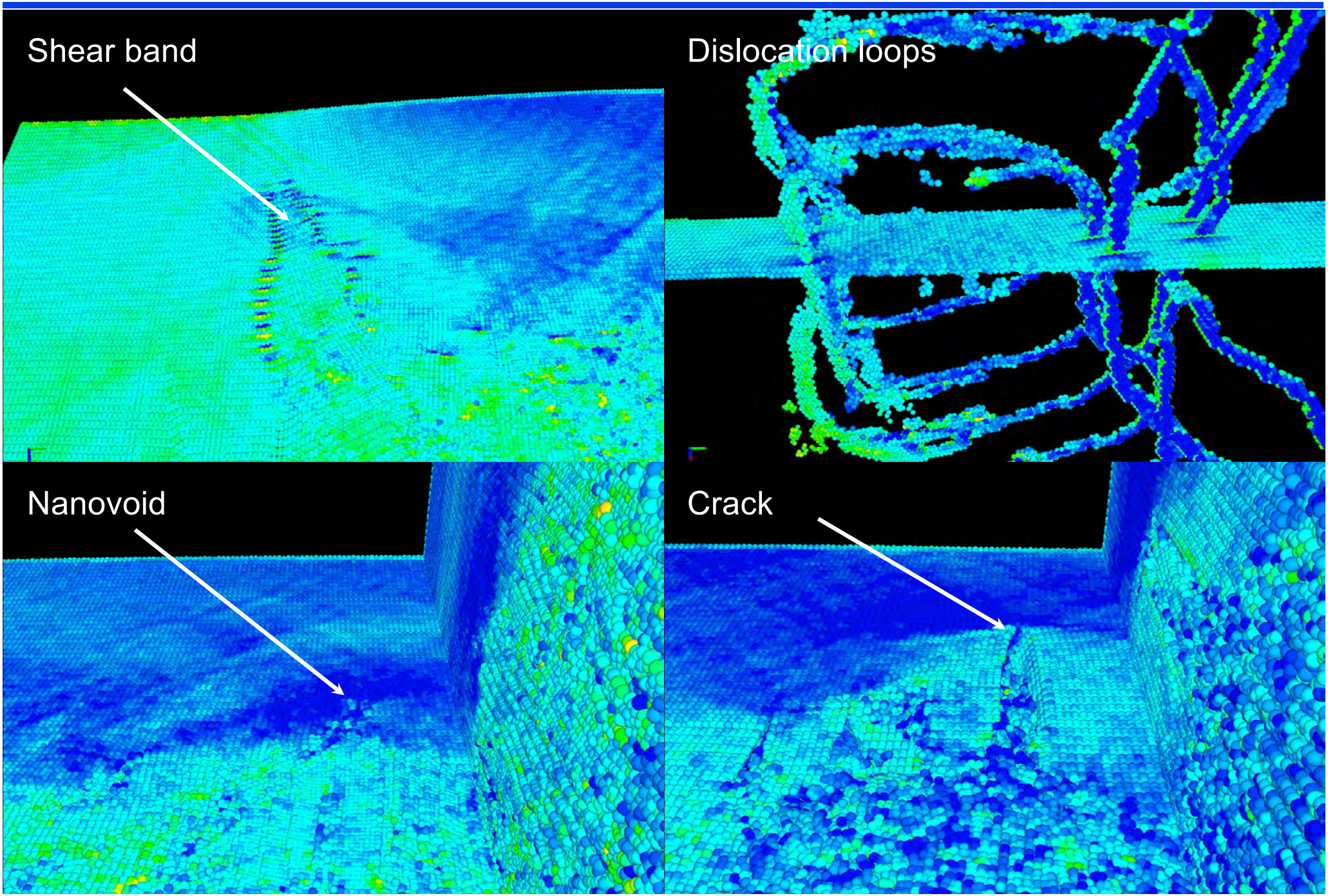
Damage Viewed from Behind the Impactor



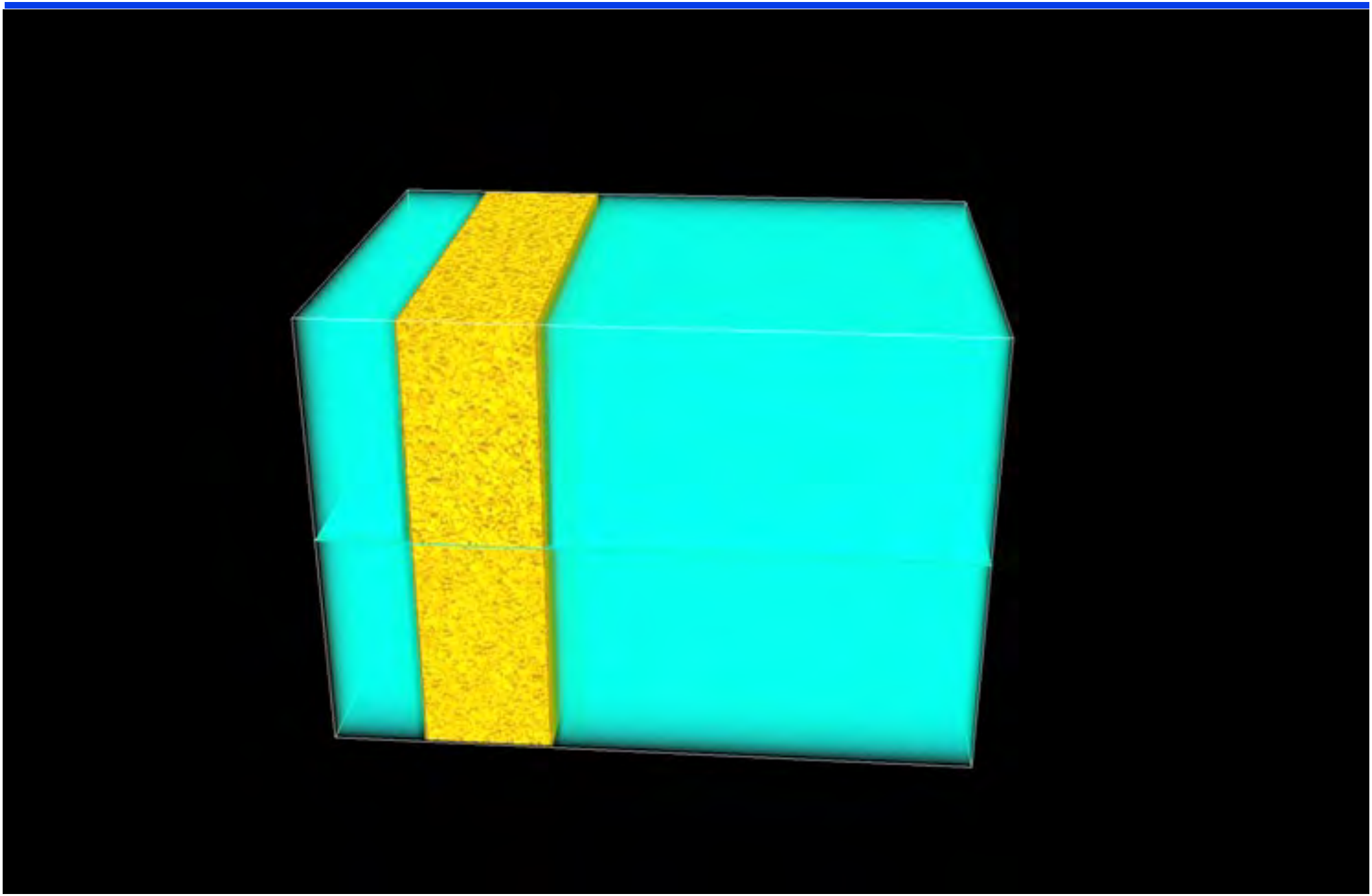
Damage from Real Impactor in AlN Ceramic



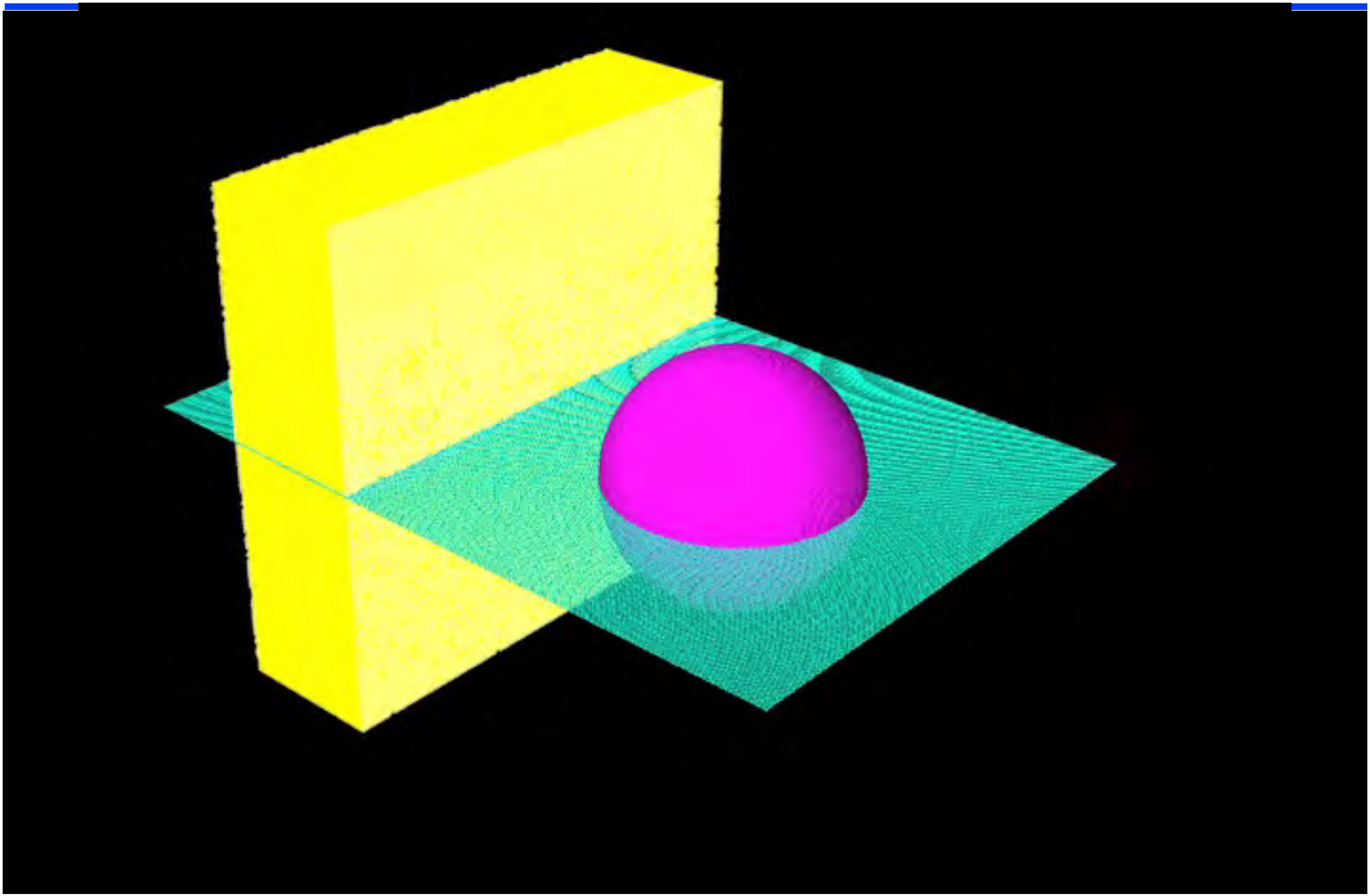
Summary of Shock Damage in AlN



One Billion Atom Reactive Simulation of Shock-induced Nanobubble Collapse (Empty)

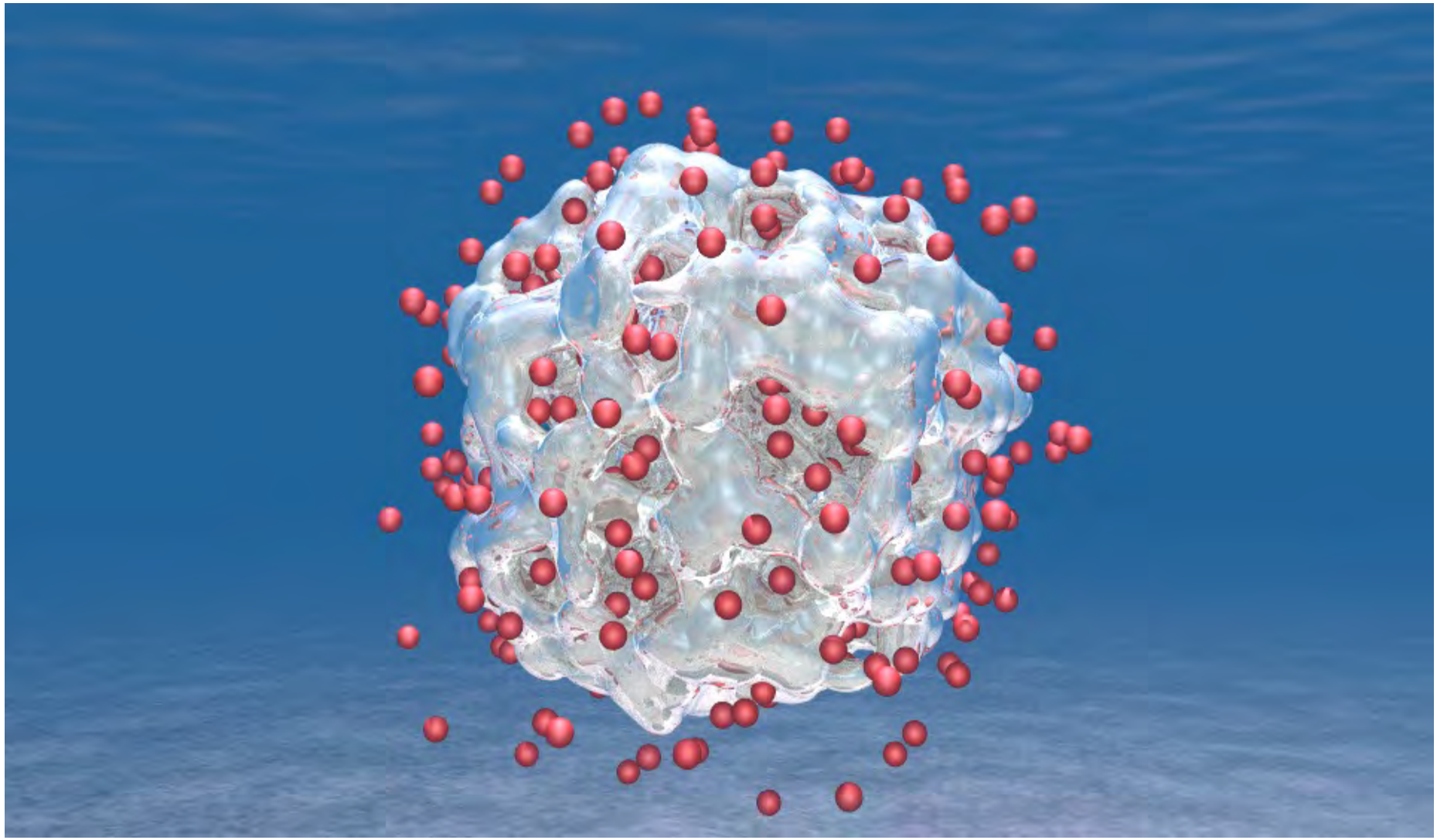


One Billion Atom Reactive Simulation of Shock-induced Nanobubble Collapse (Gas Filled)



H_2 Production from Water Using LiAl Particles

16,661-atom QMD simulation of $Li_{441}Al_{441}$ in water on 786,432 IBM BlueGene/Q cores



Thank you for your attention!

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