

Visualizations of Molecular Dynamics Simulations of High-Performance Polycrystalline Structural Ceramics

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Abstract

The Data Analysis and Assessment Center (DAAC) serves the needs of the Department of Defense (DOD) High Performance Computing Modernization Program (HPCMP) scientists by facilitating the analysis of an ever increasing volume and complexity of data [1]. Dr. Charles Cornwell is a research scientist and HPCMP user who ran nanoscale molecular dynamics simulations using Large-scale Atomic/Molecular Massively Parallel Simulator code (LAMMPS) from Sandia National Labs. The largest of the resulting data contained over 15 million atoms. The DAAC developed a novel method to visualize this unusually large-scale and complex data.

All of the molecular dynamics simulations and the analytics were processed using High Performance Computing (HPC) resources available to users of the DOD HPCMP.

Research Scope and Objectives

If it were not for their relatively low fracture-toughness and tensile strength, high-performance polycrystalline ceramics, such as SiC, would have significant potential as a replacement for aluminum and steel in structures. These twin weaknesses have been recognized for over a century [3].

Researchers are attempting to engineer state-of-the-art synthetic materials using mechanically designed principles found in nature, where the weak constituents were replaced with more advanced synthetically engineered materials. The goal of this research is to produce structural composite materials with mechanical properties that exceed both those of natural materials, as well as those of state-of-the-art synthetic materials [2]. Likewise, this research opens the door for an increase in potential material

combinations for reproducing the properties and behavior observed in nature.

Thus far, attempts to improve the fracture toughness and tensile strength of ceramics were almost all based on empirical approaches. The methodology and objective of this work is to couple experimental technologies with high performance computing simulations in an effort to complement experimental efforts to improve the fracture toughness and tensile strength of a SiC composite [3].

Recent developments in experimental techniques allow researchers to design, manipulate, and test the properties of materials with nanometer scale dimensions. Experiments at the nanoscale are difficult. Likewise, there are practical limits in the range of material parameters that can be explored, and the capability of instrumentation to provide a comprehensive picture of relevant phenomena, especially in the case of critical transient behavior such as chemical reactions, defect formation, and crack propagation. Advances in experimental, theoretical, and computational techniques, coupled with HPC resources, are changing the way materials scientists and engineers design new materials. This research guides experimentation by allowing a more rapid sweep of parameter space to reveal aspects of the relevant phenomena not accessible to direct measurement.

Visualization Process

The simulation results were used to produce still images and animations of the position of the atoms over time. Visualizing the simulation data from LAMMPS required the development of a custom program to extract the 3D position and the energy value of each atom. To represent each atom on a rendered image, a sphere was generated in VTK using the 3D position as the center point of the

sphere. In addition, aesthetics determined the radius of the spheres.

To create the appearance of a mesh, VTK primitive tubes, which represented the bonds between the atoms, were used to connect them. Atoms within 2.8 angstroms of each other were connected using a version of the k-nearest neighbor algorithm. This algorithm first sorted the atoms into buckets, based solely on their Cartesian position, which prevented the exponential increase in runtime complexity. Next, the straight-line distance between each atom in the bucket was calculated. The atoms located within the desired range were connected with a tube using VTK.

Colors were applied to the spheres and tubes based on the energy and stress values. The tubes were a special case because the ends of the tubes were colored the same as the atoms they were connecting, which, in some cases, required two differently colored atoms. VTK automatically colored the rest of the tube by smoothly blending from one end to another. After the color was applied, the geometry was appended into a PLY file (Stanford ASCII Polygon Format).

Using this process to prep the data for visualization worked well until the atoms numbered over 15 million, at which point the run-time of the analytics increased beyond an acceptable measure. A modification was needed; therefore, a new step was added that placed each atom into one of 100 possible lists. Each list contained atoms from inside a boundary that represented $\sim 1/10$ of the x and y domain ranges. Atoms along the boundaries were also included in adjacent lists to ensure the program created tubes between all qualifying atoms. Then, HPCMP systems processed each list according to the previously described custom program. The advantage of using HPC systems is that it allowed the program to run parallel on multiple cores and make full use of the large amount of RAM available. Likewise, using HPC systems reduced runtime to a few hours instead of a few days.

Visualization Results and Impact

Figure 1 shows the final result for a relatively small data set containing 143,536 atoms. In this simulation, the material was subjected to an external force that continued until the structure failed. The

spheres and tubes were colored by the stress applied in the horizontal direction.

Figure 2 represents a change in the processing steps. The simulation contained over 256,080 atoms, which required the use of cubes instead of spheres to reduce the polygon count. The number of polygons in each tube was also reduced.

Figures 1 and 2 were created by importing the PLY files into Autodesk's 3D Studio Max (3DS Max). Once the geometry was imported, a light was added to the scene, and an image was rendered and saved.

These images allowed the researcher to see the results of the simulations in a much higher quality than ever before. This is significant because high resolution images allow the entire result of the simulation to be seen at once, instead of smaller images where tiny details may go unnoticed. In addition, a movie was made from each set of results, which allowed the simulations to be viewed in high definition.

Visualizing the large simulation that contained 15,102,976 atoms presented a unique opportunity to render the final time step in ultra high definition. The goal was to view the image on a 4K monitor to allow the observer to see the results in as much detail as possible. Representing 15,102,976 atoms and their connecting tubes required over 350 million polygons. Normally, this is considered overkill because there are not 350 million pixels on the screen. In this case, high-resolution graphics are required to capture failure mechanisms that operate across multiple length scales covering three orders of magnitude. Material failure is initiated with bond breaking at the atomic level (10^{-10} M). Interactions between the structural elements are designed to produce toughening mechanisms that operate at the nanoscale (10^{-9} M). The evolution of these cracks produces fracture patterns at the microscale (10^{-6} M). The high-resolution graphics capture the synergy between these mechanisms across multiple length scales, and provide a better understanding of the failure mechanism and design requirements for advanced materials. Figure 3 shows the result. The red and green boxes identify two areas of interest discovered while viewing the image on a 4K monitor. The researcher verbalized how these details would have

been otherwise overlooked at normal rendering resolutions. The ultimate goal of the DAAC is to use our data analysis expertise to help our customers see things they would not have noticed in their data.

Why HPC Matters

Usually, material development has been exclusively build/test, then rebuild/retest to understand the behavior of the material and to achieve performance goals. Such physical experimentation is relatively slow and costly. For Dr. Cornwell, access to HPC systems allows the simulations to be performed at the nano-to-micro scale, where material response begins.

The HPC resources and high-resolution graphics improve the quality of research by extending the size and complexity of problems that can be solved with the aid of modeling and simulation.

HPC systems, also aid visualization efforts, that allow large data sets, which contain millions of points and polygons, to be processed and rendered quicker than ever before. The DAAC continues to improve on techniques and adopt new strategies that take advantage of the opportunities that HPC offers.

Conclusion

The results of this project demonstrate the potential benefit of an integrated computational experiment approach to materials development. Access to HPC resources improves the quality of research by extending the size and complexity of problems that can be solved with the aid of modeling and simulation [3], as well as aiding in the analysis and visualization of the resulting data.

References

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- [2] Wang, H., Chen, Y. & Rosen, D. W. (2005). A Hybrid Geometric Modeling Method for Large Scale Conformal Cellular Structures. ASME 2005 International Design Engineering Technical Conferences and Computers and Information in Engineering Conference. 3. ASME Proceedings | 25th Computers and Information in Engineering Conference.
- [3] Cornwell, C., "Molecular Dynamics Simulations to Guide the Development of High-Performance Polycrystalline Structural Ceramics", unpublished

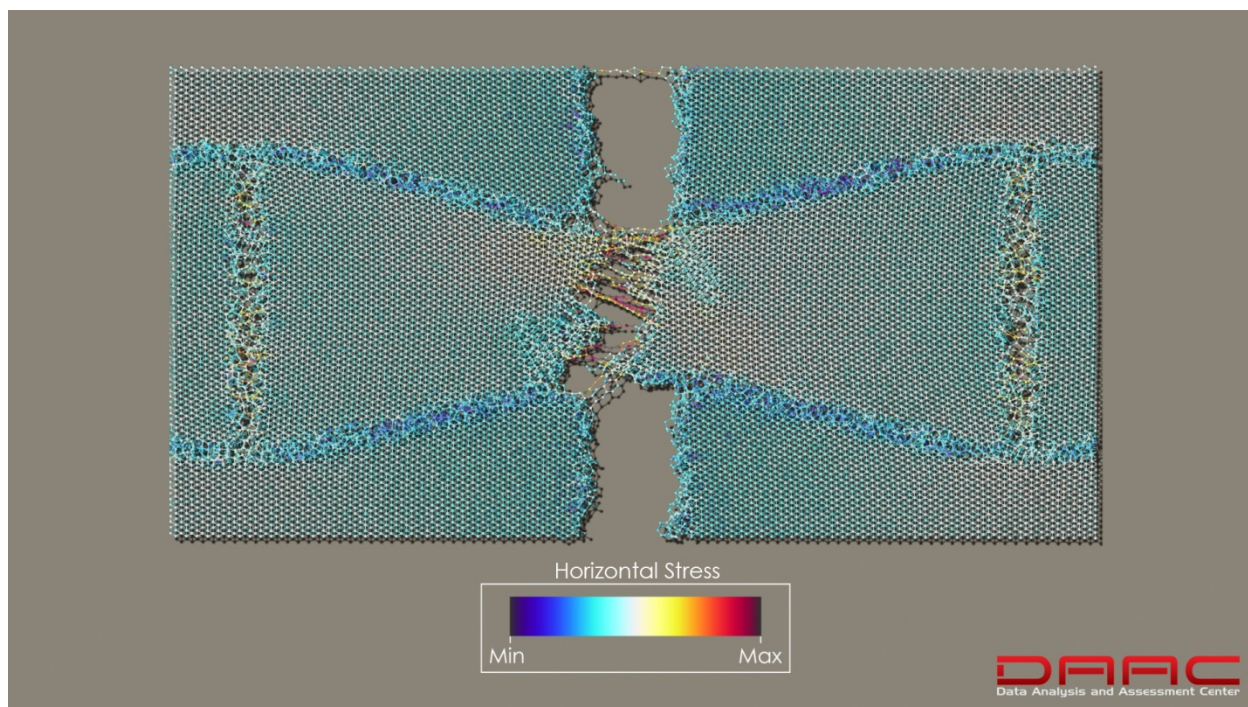


Figure 1: Structural Failure of Dovetail Geometry Pattern (Dimensions: 50.8 nm x 19.3 nm x 1.5 nm)

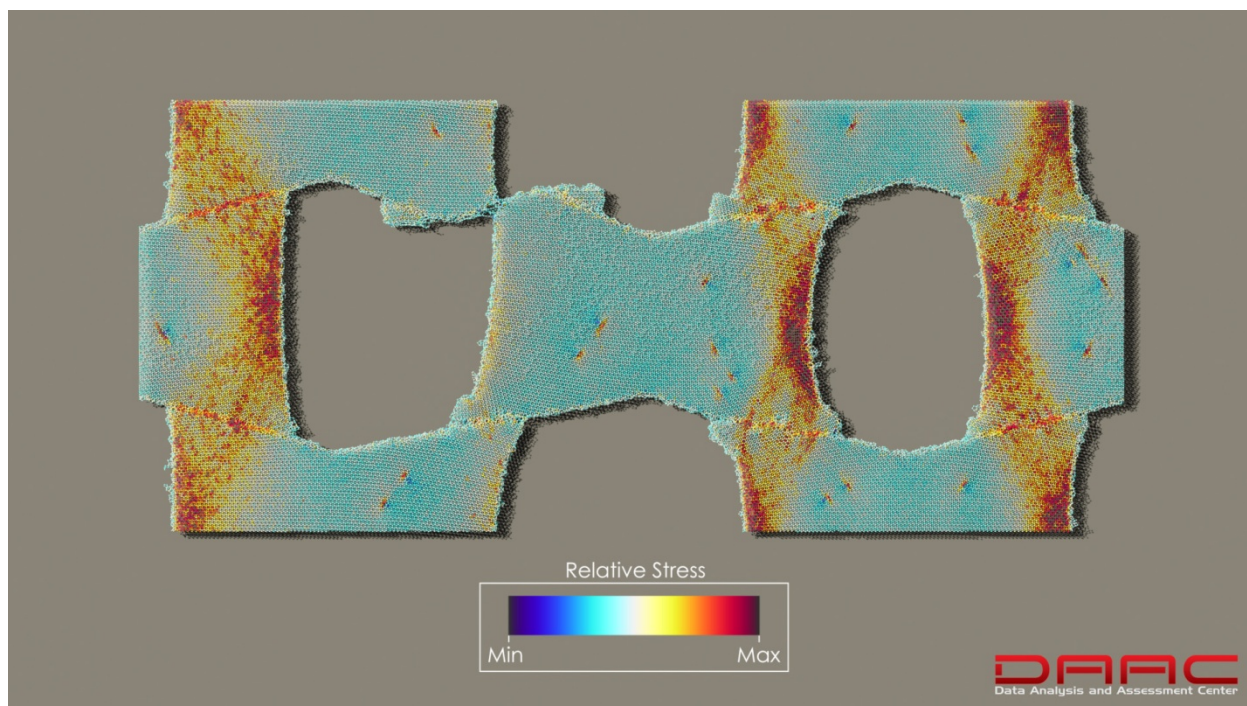


Figure 2: Structural Failure of Modified Dovetail Geometry Pattern
(Dimensions: 50.8 nm x 34.5 nm x 1.5 nm)

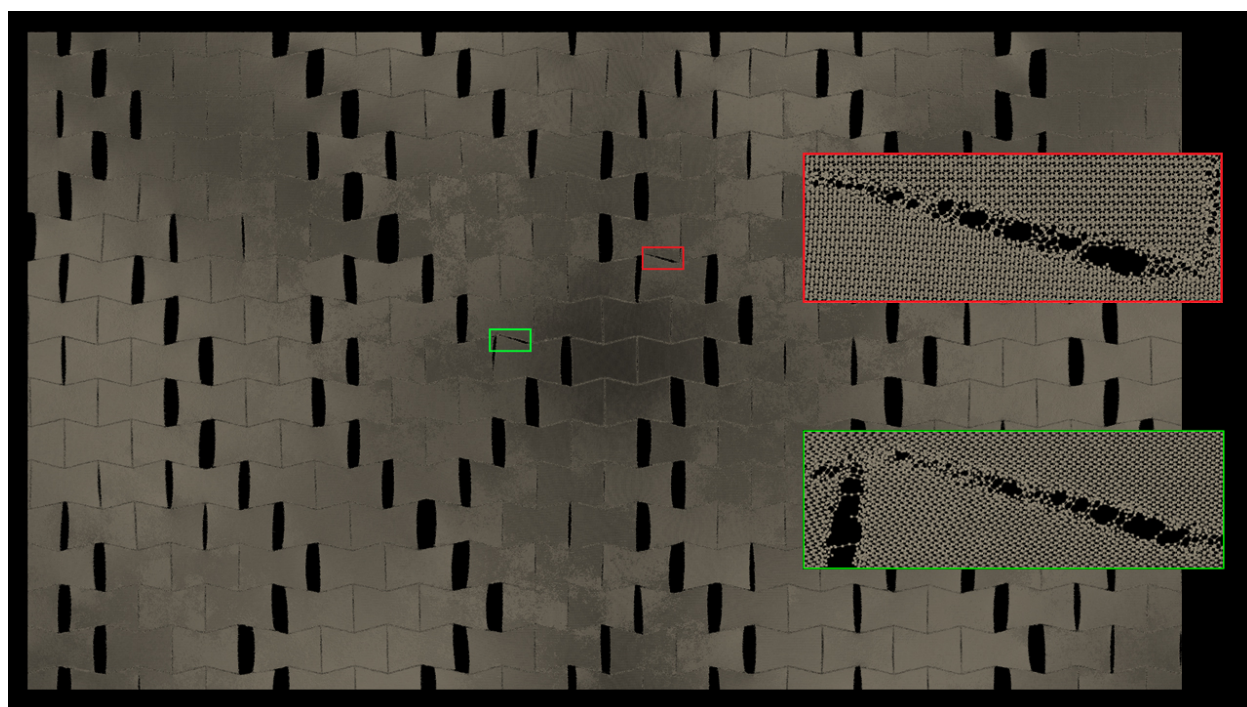


Figure 3: 16x HD Rendering of Large-Scale Simulation Revealing Previously Unobserved Behavior
(Dimensions: 406.4 nm x 254.4 nm x 1.5 nm)