Parallel Computing 55 (2016) 35–42

Contents lists available at ScienceDirect

Parallel Computing

journal homepage: www.elsevier.com/locate/parco

Visualizations of molecular dynamics simulations of high-performance polycrystalline structural ceramics

Christopher Lewis [a,*], Miguel Valenciano [a], Charles Cornwell [b]

[a] Department of Defense High Performance Computing Modernization Program (DOD HPCMP), Data Analysis and Assessment Center (DAAC), 3909 Halls Ferry Rd, Vicksburg, MS 39180, United States
[b] Information Technology Laboratory (ITL), Computational Analytics Branch (CAB), U.S. Army Engineer Research and Development Center (ERDC), Unites States

ARTICLE INFO

Article history:
Available online 27 October 2015

Keywords:
Visualization
High Performance Computing
Molecular Dynamics
Polycrystalline Structural Ceramics
LAMMPS
VTK

ABSTRACT

Initiated by the Department of Defense (DOD) High Performance Computing Modernization Program (HPCMP), the Data Analysis and Assessment Center (DAAC), serves the needs of DOD HPCMP scientists by facilitating the analysis of an ever-increasing volume and complexity of data [1]. A research scientist and HPCMP user ran nanoscale molecular dynamics simulations using Large-scale Atomic/Molecular Massively Parallel Simulator code (LAMMPS) from Sandia National Labs. The largest simulation contained over 70 million atoms (Fig. 7). Data sets this large are required to study crack propagation and failure mechanisms that span multiple length scales with atomic resolution. The DAAC developed new methods to visualize the time evolution of data sets this large. The size and complexity of the molecular dynamics simulations and the analytics required the use of DOD HPCMP High Performance Computing (HPC) resources.

Published by Elsevier B.V.

1. Research scope and objectives

Synthetic ceramics are generally strong but brittle and flaw-intolerant materials, rendering them unsuitable for most structural applications, while biomaterials composed primarily of brittle ceramics are able to achieve exceptional combinations of stiffness, strength and toughness. Nature combines materials into complex hierarchical structures to achieve exceptional mechanical properties. The increased demand for stronger and lighter materials is driving researchers to explore new methodologies to increase the toughness and overcome the brittleness of synthetic ceramic materials. In this paper we use a structural mechanics approach to analyze the properties of different nacre-like material designs for a material composed of silicon and carbon. Molecular dynamics (MD) is used to study the design parameters required to reproduce the mechanistic behavior observed in nacre and identify the parameters necessary to prevent unstable crack propagation in a synthetic silicon carbide (SiC) ceramic. We also investigate the relationship of the tensile strength of the grains and shear strength of the matrix on grain pullout and the strain hardening mechanism produced by the grain shape.

Natural processes for fabricating biological materials take place in aqueous solutions at room temperature using resources available in the environment. These processing requirements result in a large number of biological materials comprised from a comparatively limited range of elements. Nevertheless, many biomaterials exhibit remarkable mechanical properties despite the

* Corresponding author. Tel.: +1 601 634 3439.
E-mail addresses: Christopher.D.Lewis@erdc.dren.mil (C. Lewis), Miguel.A.Valenciano@erdc.dren.mil (M. Valenciano), Charles.F.Cornwell@erdc.dren.mil (C. Cornwell).

http://dx.doi.org/10.1016/j.parco.2015.10.008
0167-8191/Published by Elsevier B.V.

structural weaknesses of their individual components. Advances in micro- and nano-scale in situ experiments and computational techniques are shedding light on the delicate structure-property relationships required to reproduce the mechanistic behavior found in biomaterials [2–9]. Some underlying strategies are beginning to emerge that reflect general design concepts for achieving optimal performance from materials assembled from components with disparate and seemingly incompatible properties.

Researchers are attempting to engineer synthetic materials using design principles found in nature. Recent manufacturing techniques designed to produce synthetic nacre-like structures such as those designed through ice templating [10,7], thin film deposition [11,12], layer-by-layer deposition, and additive processing [13–16] techniques show the performance and behavior of nacre can be reproduced using a wide range of material combinations with varying degrees of success [17,13].

The design strategies for nano-micro-engineered synthetic materials are not constrained by the processing requirements of natural materials. Thus, synthetic material designs are free to explore a wide range of structure and material combinations that are not accessible to natural materials. A detailed understanding of the general design concepts and the structure-property-relationships responsible for the mechanistic behavior and mechanical properties observed in nature may result in new composite designs using synthetic materials. In some cases, it may be desirable to replace the constituent materials found in nature with synthetic engineered materials that are amenable to advanced manufacturing techniques. However, the choice of synthetic materials is much more extensive compared to natural materials. In many cases, it may not be possible or desirable to replicate the complex hierarchical structure of biomaterials. The goal is to determine structural arrangements and material combinations that can be achieved using advanced manufacturing techniques to produce structural composites with mechanical properties that exceed both natural and state-of-the-art synthetic materials [18].

The biological "brick-and-mortar" hybrid design is characterized by a layered structure consisting of strong inorganic platelets embedded in a soft, organic matrix. The properties of these materials can be tuned by manipulating the individual components to achieve performance and functionality that are inaccessible to monolithic materials. It is widely recognized that tablet sliding is a key mechanism in the toughness of nacre [19–22] and that the aspect ratio is used to strike a balance between the widely different strengths of the soft matrix and brittle mineral [23]. It has also been proposed that a strain hardening mechanism on the local scale is required to promote tablet sliding on a large scale. Strain hardening at the local scale is generated by the waviness of the tablet surfaces in natural materials [19]. Studies suggest that the "brick-and-mortar" structure allows large sliding deformation of tablets and suppresses the strain localization and crack propagation in the brittle inorganic platelets.

In this paper, we conducted a sensitivity analysis to gain insight into the causal relationships between crystalline structure, crystal size, grain boundary properties and the mechanical properties of the ceramic. A parametric study was performed using a two-dimensional representative volume element (RVE) consisting of a 2×2 arrangement of grains to analyze the parameters required to increase fracture toughness and strain hardening at the component level. The results were then tested on a larger system to determine the material response on a larger scale.

The simulations identify the design parameters and failure mechanisms necessary to reproduce the mechanistic behavior responsible for fracture toughness of a "brick-and-mortar" material composed of silicon and carbon. This research was able to identify the parameters that promote flaw tolerance and suppress crack propagation. The research also evaluated the parameters required to promote grain sliding and "dovetail-type" grain locking mechanisms necessary to suppress strain localization and spread crack formation over large volumes. The results indicate that there a number of designs that can produce strain hardening in the material and suggest additional designs that can be used depending on the level of control that can be obtained over the manufacturing process.

HPC simulations coupled with physics-based material models are having a significant impact on the design and performance of micro- and nano-engineered materials. Historically material development has been almost exclusively empirically based, with materials going through cycles of build/test, rebuild/retest to understand material behavior or to achieve performance goals. The tests are usually performed at the macroscale, whereas material response begins at the nano- to micro-scale. High-fidelity physics-based calculations coupled with HPC allow constitutive properties of materials to be determined based on the atomic and molecular structure of the material.

The atomic stress is calculated based on the virial theorem [24] and the equation for the i, j components (where i and $j = x, y$) of the symmetric stress tensor is given by:

$$\sigma_{ij} = \frac{\Sigma_k^N m_k v_{ki} v_{kj}}{V} + \frac{\Sigma_k^N r_{ki} f_{kj}}{V}$$

The time average of the atomic stress tensor summed over all the atoms in the system provides a bridge that links results of molecular dynamics simulations with structural mechanics. The maximum and minimum principal stress components are given by:

$$\sigma_p = \frac{(\sigma_{xx} + \sigma_{yy})}{2} \pm \sqrt{\frac{(\sigma_{xx} - \sigma_{yy})}{2} + \tau_{xy}}$$

and the maximum shear stress is given by:

$$\tau_{\max} = \sqrt{\frac{(\sigma_{xx} - \sigma_{yy})}{2} + \tau_{xy}}$$

The principal stress is used to evaluate the material performance as a result of variations in design parameters. Simulations of the RVE's were used to analyze the parameters required to increase fracture toughness and strain hardening at the component