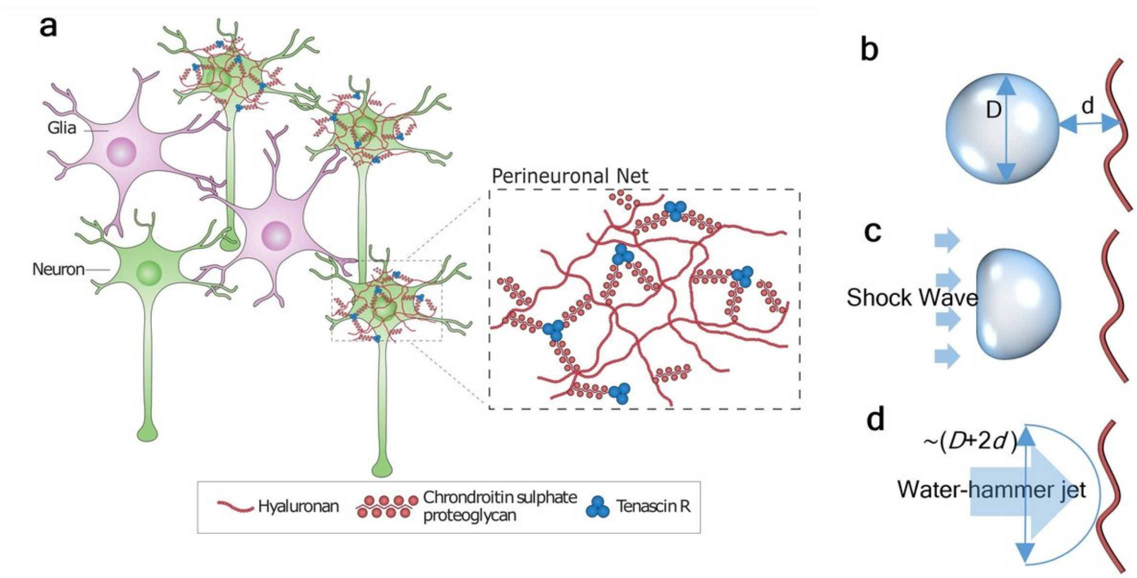
Researchers use simulations to study brain damage from bomb blasts and materials for space shuttles

January 24 2018



(a) Neurons surrounded by the ECM in the CNS. The region in ECM in the immediate vicinities of neurons are called Perinuronal Net (PNN). The components of PNN are shown in the magnified view (adapted from Fig. 1 of 37) (Permitted reprint) and (b–d) Schematic of pre-, during, and post-collapse bubble. Credit: University of Texas at Austin

Explosions produce unique patterns of injury seldom seen outside combat. They have the potential to cause life-threatening injuries and take a particular toll on the brain.

Ashfaq Adnan, an associate professor of mechanical engineering at The University of Texas at Arlington (UTA), and his postdoctoral associate Yuan Ting Wu published research findings in *Scientific Reports* in July 2017 revealing how battlefield blasts may cause bubbles in the brain's perineuronal nets which, in turn, may collapse and damage neurons.

"This study reveals that if a blast-like event affects the brain under certain circumstances, the mechanical forces could damage the perineuronal net located adjacent to the neurons, which could lead to damage of the neurons themselves," Adnan said. "It is important to prove this concept so that future research may address how to prevent cavitation damage and better protect our soldiers,"

Cavitation is the development of bubbles, much like those that form around a ship's spinning propellers. Existing scans cannot detect whether cavitation bubbles form inside the brain due to blasts or how these blasts affect a person's individual neurons, the brain cells responsible for processing and transmitting information.

Adnan's research used supercomputer-powered molecular dynamics simulations to study structural damage in the perineuronal nets (PNN) area in the brain. He then determined the point at which mechanical forces may damage the PNN or injure the neurons.

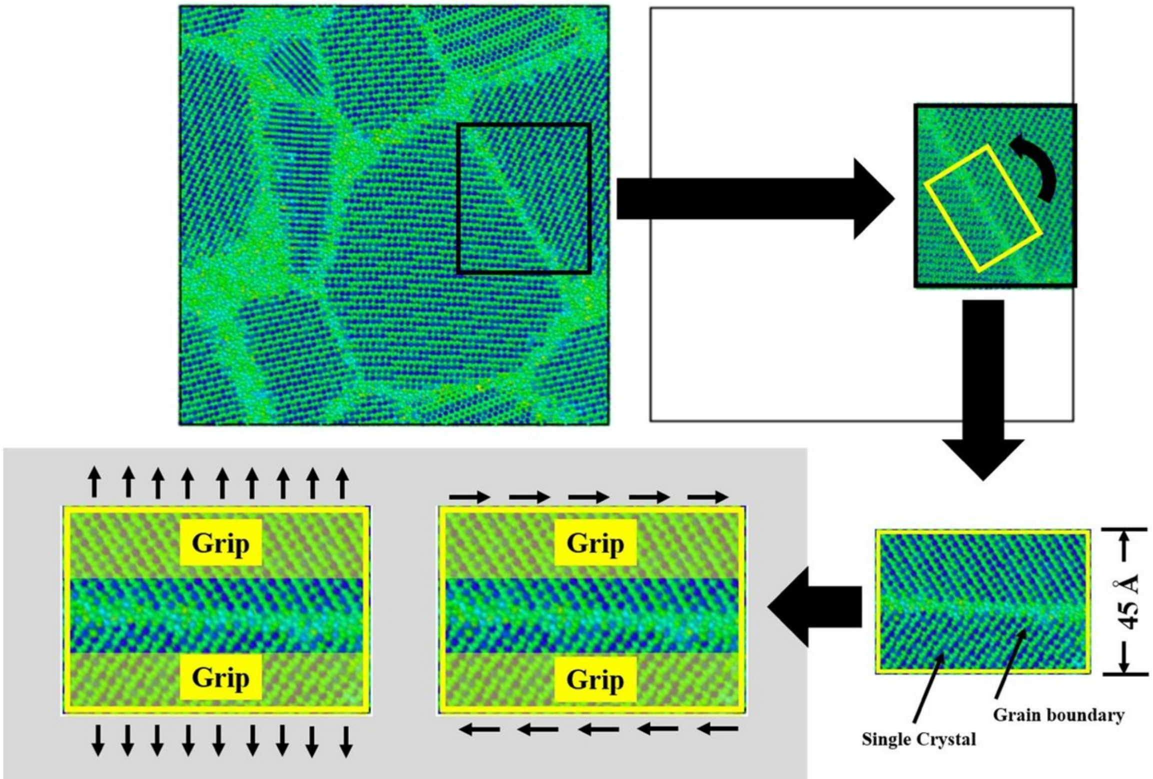
The research was supported by a grant through the Office of Naval Research's Warfighter Performance Department and UTA.

MODELING THE EFFECTS OF BOMB BLASTS

Understanding the details of the substructure of the PNN requires extremely high-resolution modeling, which were enabled by more than 1 million compute hours on the National Science Foundation-funded Stampede supercomputer at the Texas Advanced Computing Center (TACC). Adnan and his team were able to access TACC resources through a unique initiative, called the University of Texas Research Cyberinfrastructure (UTRC), which gives researchers from the state's 14 public universities and health centers access to TACC's systems and staff expertise.

The team ran 36 sets of simulations, each modeling the interactions of more than a million atoms, and used thousands of computer processors simultaneously.

"The study suggests that when a shock waves comes in the brain, the wave can reach the atomistic scale and interact with the water molecules, biomolecules and even the ions," Adnan said. "The science spans from the atomistic scale to the macroscopic scale—nine orders of magnitude larger. At different length scales, we have different physics and time-frames that we have to capture and we can't ignore one over the other. So, we have to model this complicated system in the most detailed way possible to see what's going on."



As tensile stress is applied across the ends of the nanocomposites, failure locations are visitable at the particle-matrix interaction and across the grain boundaries. This images confirms why presence of nanoparticle did not give any enhancement in strength. Credit: Ashfaq Adnan and Md. Riaz Kayser

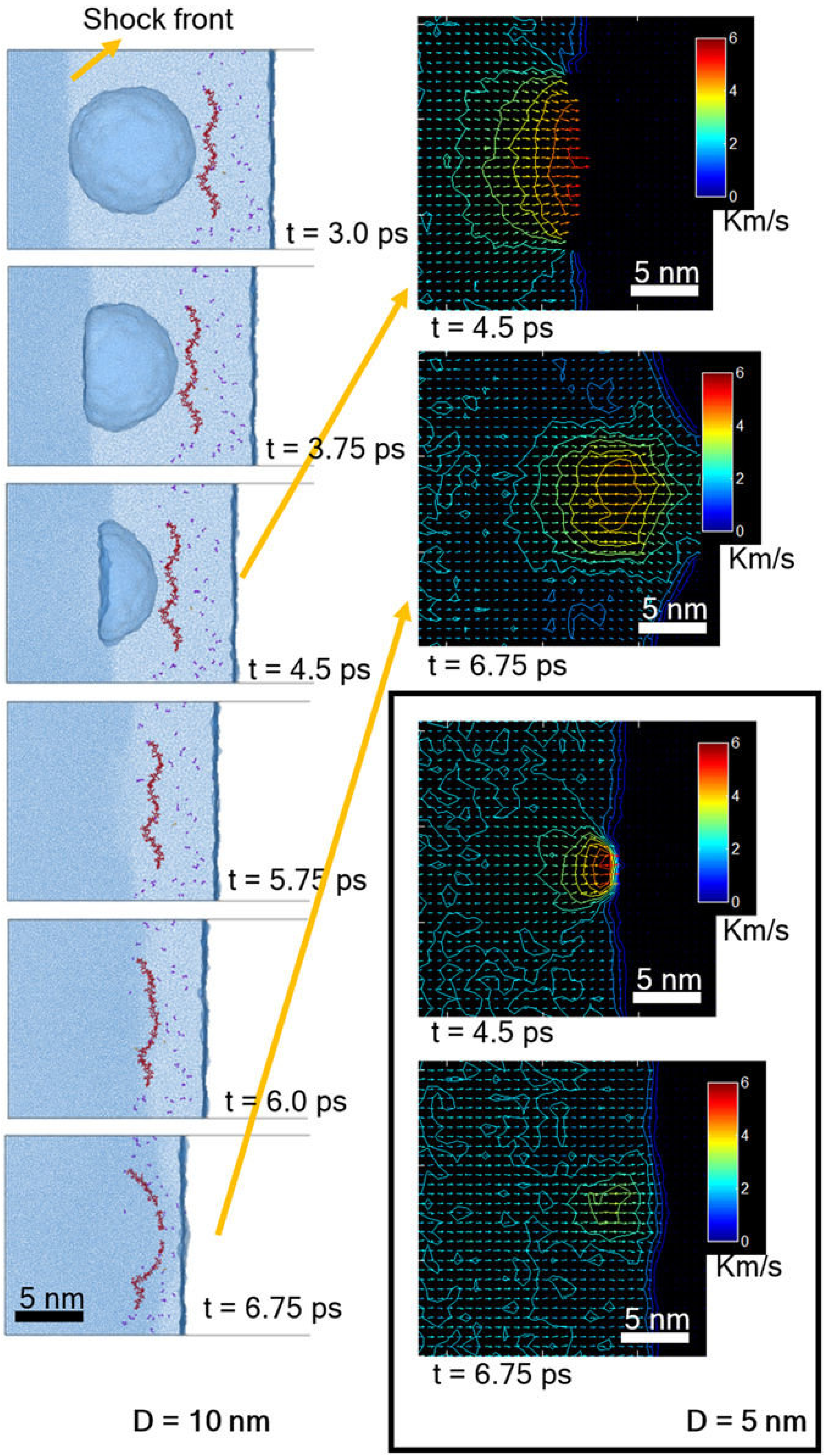
The team focused on the damage in hyaluronan, which is the net's main structural component. Their results show that the localized supersonic forces created by an asymmetrical bubble collapse may generate a phenomenon known as a "water hammer" - a powerful pressure wave - which can break the hyaluronan. The research improves current knowledge and understanding of the connection between damage to the perineuronal net and neurodegenerative disorders.

"Dr. Adnan's recently published findings offer important insight into how the brain is affected in combat scenarios," said Duane Dimos, UTA vice president for research. "Understanding the effects of blast injuries on the brain and knowing that cavitation occurs is an important step toward finding better ways to prevent traumatic brain injuries on the battlefield."

STUDYING SPACE SHUTTLE MATERIALS WITH SUPERCOMPUTERS

Parallel to his brain research, Adnan works on way to develop strong ceramic-based materials for advanced structural applications, notably for space shuttle reentry vehicles.

His computational designs of novel multiphase ceramic-ceramic and ceramic-metal materials are helping to better understand these materials, so new, better ones can be created.


Shock front
t = 3.0 ps
t = 3.75 ps
t = 4.5 ps
t = 5.75 ps
t = 6.0 ps
t = 6.75 ps
5 nm
D = 10 nm
Km/s
5 nm
t = 4.5 ps
t = 6.75 ps
D = 5 nm

Cavitation-collapse triggered by shock. Shock velocity?=?5.35?km/s, bubble radii?=?10?nm (top two) and 5?nm (bottom two). Scale for velocity color map is Km/s. Credit: Ashfaq Adnan and Yuan Ting Wu

In January 2018, Adnan and his PhD student Md. Riaz Kayser published a paper in the *Journal of the American Ceramic Society*, in collaboration with experimentalists from Missouri Science and Tech describing a molecular study of the mechanical properties of ZrB2 (Zirconium diboride) and ZrC-ZrB2 (a Zirconium carbide-Zirconium diboride nano-composite).

"These materials belong to a class of refractory ceramics called Ultra-High-Temperature Ceramics or UHTCs, one of only a few material systems that can be used for hypersonic vehicles," Adnan said. "The vehicles go at such high speed that they need to survive temperatures above 3600 degree Fahrenheit and most materials will just melt. UHTCs are the only materials that can survive under extreme conditions."

Though tough and heat-resistant, these metal-ceramic hybrids are fragile. In the Columbia shuttle disaster of 2003, a ceramic tile broke and came off and the material underneath melted, leading to the crash. Adnan's overall goal is to improve the properties of the material so they don't easily shatter.

"We revealed through our study that the conventional wisdom, that if you put a nanoparticle in the system you'd always get better results, is not necessarily guaranteed," he explained. "What we observed is that the strength of grain-boundary materials at the nanoscale are weaker than any other part of the material. As such, the presence of nanoparticles doesn't improve their strength. The paper is about finding the fundamental reason behind why nano-reinforcement isn't always very effective. We need to design our manufacturing process to get the best out of the nanoparticle infusion in ceramic materials."

Though this line of research seems a far cry from simulations of brain-damaging bomb blasts, it is actually much more similar than it first appears.

"My interest is in the behavior of materials at the atomic scale. The tools that I use are the same, it's just the application that are different," Adnan said. "We have the experience in our group and among our collaborators that allows us to be highly diversified and multidisciplinary."

More information: Md. Riaz Kayser et al, Grain boundary driven mechanical properties of ZrB2 And ZrC-ZrB2 nanocomposite: A molecular simulation study, *Journal of the American Ceramic Society* (2018). DOI: 10.1111/jace.15443

Yuan-Ting Wu et al. Effect of Shock-Induced Cavitation Bubble Collapse on the damage in the Simulated Perineuronal Net of the Brain, *Scientific Reports* (2017). DOI: 10.1038/s41598-017-05790-3

Provided by University of Texas at Austin

Citation: Researchers use simulations to study brain damage from bomb blasts and materials for space shuttles (2018, January 24) retrieved 2 May 2024 from https://phys.org/news/2018-01-simulations-brain-blasts-materials-space.html