PHYS.ORG

Roadrunner supercomputer simulates nanoscale material failure

October 29 2009

Very tiny wires, called nanowires, made from such metals as silver and gold, may play a crucial role as electrical or mechanical switches in the development of future-generation ultrasmall nanodevices.

Making nanodevices work will require a deep understanding of how these and other nanostructures can be engineered and fabricated as well as their resultant strengths and weaknesses. How mechanical properties change at the nanoscale is of fundamental interest and may have implications for a variety of nanostructures and nanodevices.

A major limiting factor to this understanding has been that experiments to test how nanowires deform are many times slower than computer simulations can go, resulting in more uncertainty in the simulation predictions than scientists would like.

"Molecular dynamics simulations have been around for a long time," said Arthur Voter of the Theoretical Division at Los Alamos National Laboratory. "But the simulations have never before been able to mimic the atomistic tensile strength of nanowires at time scales that even come close to experimental reality."

Using the "parallel-replica dynamics" method for reaching long time scales that Voter developed, members of Voter's team adapted their computer code to exploit the Roadrunner supercomputer's hybrid architecture, allowing them to perform the first-ever simulation of a stretching silver nanowire over a period of a millisecond, or onethousandth of a second, a time that approaches what can be tested experimentally.

"Bigger supercomputers have made it possible to perform simulations on larger and larger systems, but they have not helped much with reaching longer times -- the best we can do is still about a millionth of a second. However, with the parallel-replica algorithm, we can utilize the large number of processors to 'parallelize' time," said Voter. "Roadrunner is ideally suited to this algorithm, so now we can do simulations thousands of times longer than this."

With this new tool, scientists can better study what nanowires do under stress. "At longer time scales we see interesting effects. When the wires are stretched more slowly, their behavior changes -- the deformation and failure mechanisms are very different than what we've seen at shorter time scales," said Voter.

Through these simulations, Voter and his team are developing a better understanding of how materials behave when they are reduced to the size scale of a nanometer, or one-billionth of a meter. "At this scale, the motion of just one single atom can change the material's mechanical or electrical properties," said Voter, "so it is really helpful to have a tool that can give us full atomic resolution on realistic time scales, almost as if we are watching every atom as the experiment proceeds."

Source: Los Alamos National Laboratory (news : web)