System X: An Advanced Tool for Material Science and Engineering

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Virginia Tech students now have one of the world's most powerful research tools in their own backyard. In the winter of 2003, Virginia Tech researchers took major strides in supercomputer innovation when their high-profile supercomputer was ranked the third-fastest computer. It was given the name "System X" because it was the first academic supercomputer to pass 10 teraflops, or 10 trillion floating point operations per second. In addition to processing data at high speeds, it is also the cheapest available supercomputer.

Figure 1. System X

System X was initially made of 1100 off-the-shelf Apple Power Mac G5 desktop computers. Presently it consists of the same number of Xserve G5s replacing the normal G5 desktops as shown in Figure 1. These computers have had their memory and speed increased, allowing more accurate predictions to be made in a shorter time.

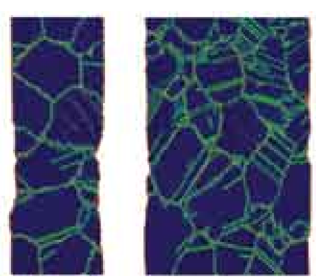
Materials Science and Engineering (MSE) is one of the fields addressing problems using advanced tools such as System X. One of the main reasons for using these computational resources is that experimental studies cannot provide precise information about the mechanisms that govern different phenomena at the atomic scale. Dr. Diana Farkas is one of the leading MSE professors conducting research projects at the atomic and molecular level with this supercomputer. "Before System X existed, we performed simulations in materials with a hundred thousand atoms—now we can work with hundreds of millions," said Dr. Farkas. Simulation and modeling have reached a much higher level of accuracy in tackling practical problems in materials engineering and other sciences.

One of the applications developed by Dr. Farkas' group has been the simulation of tensile tests on nanocrystalline nickel wires. This work was performed at different strain rates and at room temperature, reaching deformation levels up to 36%. Under these conditions, researchers were able to study the grain growth process by monitoring the evolution of the volume of individual grains for the different strain rates. The results clearly showed that grain growth is fundamentally driven by the stress. These virtual experiments were performed using a conventional molecular dynamics algorithm, and the interaction between the atoms was modeled using an empirical interatomic potential. Figure 2 shows the simulated nanowires after 0, 90, and 270 ps
and for deformations of 0, 12, and 36% strain, respectively for a strain rate of 1.33 x 10^9 s^{-1}. The various grains are color coded, showing significant grain growth as the deformation proceeds.

(a) (b) (c)

Figure 2. Nanowires after (a) 0, (b) 90 and (c) 270 ps tensile deformation for a strain rate of $1.33x10^9 s^{-1}$.

Mechanical test simulations on nanocrystalline metals were performed in tension and compression. MSE student Joshua Monk, one of the members of Dr. Farkas' group, said "these simulations have helped in the studies of both the size effect for a 10 nm grain size and the asymmetry of tensile/compressive strength." Figure 3 shows details of dislocations, stacking faults and grain boundaries (green). The blue pixels represent the perfect structure atoms; red represent the surface atoms. This study shows a clear difference in necking performance for the 8- and 18-nm tensile tests. For larger samples, it is energy-efficient to emit dislocations, but at a smaller size, grain boundary sliding is preferred.



(a) (b)

Figure 3. Tensile tests for (a) 8 nm and (b) 18 nm radii

In addition, virtual experiments performed by Edward Parker and Peter Gaudreau, MSE students, revealed that mechanical properties of nickel nano-thin films may be different at thicknesses less than 100 nm. These simulations suggest that hardness of the film increases as the film thickness decreases. More information about this significant study can be found in the research article on page 24.

System X has provided researchers an opportunity to perform precise studies of very complex phenomena, especially at the atomic level. These studies are used to establish new trends and correlations that guide designers in the search for novel materials. These achievements are examples of what can be carried out with System X and are the motivation for having such a system. In the coming years, System X will have new capabilities for expanding the frontiers in science and engineering.