NEWSLINE

Published weekly for employees of Lawrence Livermore National Laboratory *Friday, September 23, 2005* *Vol. 30, No. 37*

Laboratory team's research points to a new method for making super hard materials

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Research conducted by a team of scientists led by the Laboratory suggests a new way of making super hard materials under high pressure conditions. The research offers a glimpse at harder materials that could one day be used in fusion energy production, spacecraft shielding and safer automobile frames, as well as other applications.

The findings, under the title "Ultra-Hard Nanocrystalline Metals by Shock Loading," are reported in the Sept. 16 edition of *Science* magazine.

"This marks the first time anyone has been able to do actual shock experiments on nanocrystalline metals and, at the same time, carry out numerical simulations in supercomputers to interpret the results" said Eduardo M. Bringa, a materials scientist at the Laboratory and the principal investigator on the team.

Until now, understanding of how nanocrystalline metals deformed at very high strain rates had been limited to computer simulations. For their research, Lab scientists introduced shockwaves via the Lab's Janus laser.

Their findings point the way to making materials harder than anything previously achieved.

In general, metallic materials used in everyday applications are made of small "grains" joined by grain boundaries. When the grain size is reduced to less than 100 nanometers, the material is considered

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"nanocrystalline." (As a reference point, human hair has a thickness of a few microns; one micron equals 1,000 nanometers.)

Nanocrystalline materials have extraordinary properties, such as enhanced hardness. However, when the grain size becomes extremely small, the grains slide over each other as the material deforms, causing the material to become softer.

"It's sort of like stepping into sand," said Bruce Remington, a laser physicist at the Lab and a participant in the research. "The material is solid but you still sink into it."

The Lab-led team studied what happened when a shock wave was passed through samples of nanocrystalline nickel and copper. In addition to the experiments, they carried out simulations using up to 4,000 processors in LLNL computers. These are the largest simulations of nanocrystals to date. The shock waves, produced by a high-intensity laser, move faster than the speed of sound and generate pressures nearly one million times larger than atmospheric pressure.

"This high pressure increases the friction among grains and decreases the sliding," Bringa said. "By turning off the mechanism that softens the grains, we create a material that, being hard to begin with, is even harder during and following the shock wave application."

Remington cautioned the research remains in an early phase, but said such research could point the way to harder materials that could be used in shielding military vehicles, protecting spacecraft from damage caused by interplanetary dust particles, or safer bumpers and automobile frames. The materials also could have applications in inertial confinement fusion experiments.

In addition to Bringa and Remington, Lab team members include Alfredo Caro, Yinmin (Morris) Wang, Maximo Victoria, James McNaney and Ben Torralva of Materials Science and Technologies Division within Chemistry and Materials Science; and Raymond Smith of the Physics and Advanced Technologies Directorate. Helena Van Swygenhoven from the Paul Scherrer Institute in Switzerland also contributed.

"I feel very lucky to be part of a gifted team of scientists polling their talent to understand nanocrystals," Bringa said. "It was truly emotional when things clicked in place and we realized that we could understand something extremely complex based on relatively simple ideas."

Bringa said the team has not yet been able to measure what happens during the shock wave transit, which lasts nanoseconds, "but we have studied how the material changes after shock loading." As part of this ongoing project, Bringa said the team will continue collaborating with worldwide experts in order "to improve our understanding of these interesting nanocrystalline materials." Plans are in place to do the first time-resolved measurements at the Janus laser, to refine the understanding of the shocked nanocrystalline samples.

"Ultimately, however, we hope to conduct such experiments at the extraordinary pressures accessible on the 2-MegaJoules NIF (National Ignition Facility) laser currently being built at LLNL," Remington noted. "We would like to see just how hard such materials can become, when we 'pull out all the stops' on the applied pressure. If we were surprised with the results from the Janus laser, all bets are off when we throttle up by another factor of 100 in pressure on NIF. This is a very exciting time for this new scientific frontier of 'extreme materials science'."