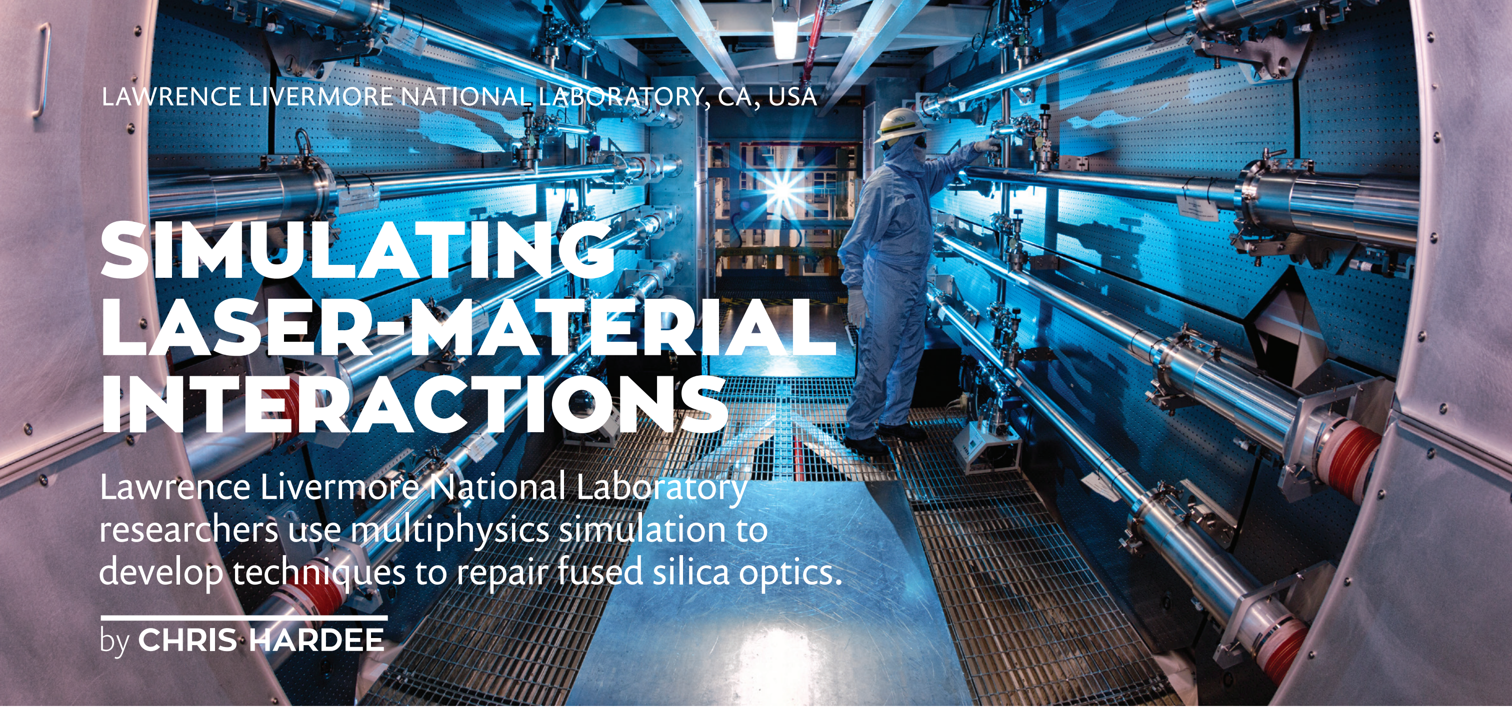

LAWRENCE LIVERMORE NATIONAL LABORATORY, CA, USA

SIMULATING LASER-MATERIAL INTERACTIONS

Lawrence Livermore National Laboratory researchers use multiphysics simulation to develop techniques to repair fused silica optics.

by **CHRIS HARDEE**

Tunable and precise, lasers are used extensively in everything from common household devices to state-of-the-art research facilities. Prominent everyday uses include automotive parts, barcode scanners, DVD players, and fiber-optic communications. Lasers are, perhaps, less well known as precision heat sources. However, it is this particular characteristic that makes them a very effective tool for material processing applications, where they are used to manipulate or alter specific substances such as glass, metals, or polymers with nanometer-scale accuracy.

Understanding the interaction of lasers with materials is the key to designing and optimizing laser systems for any application. It is these complex laser-material interactions that Manyalibo Matthews, deputy group leader in the Materials Science Division of the Lawrence Livermore National Laboratory (LLNL), studies. His research pertains to the repair and maintenance of fused silica optics in the most expansive laser system in the world.

➔USING LASERS TO REPAIR HIGH-POWER SYSTEM OPTICS

California-based LLNL oversees the National Ignition Facility (NIF), home to the world's largest and most energetic laser. The giant machine—with 192 separate beams and 40,000 optics that focus, reflect, and guide those beams—can amplify emitted laser-pulse energy by as much as ten billion times and direct it towards a target about the size of a pencil eraser. The laser produces temperatures, pressures, and densities that are similar to those found in the cores of stars, supernovae, and large planets. Astrophysics and nuclear researchers use the giant laser to better understand the universe, utilizing such technologies as inertial confinement fusion (ICF), where hydrogen fuel is heated and compressed to the point where nuclear fusion reactions take place.

However, repeated use of this powerful laser can damage the optics within the system. "The optics can be quite expensive," says Matthews. "The high-power laser light generated by the NIF can damage some of the fused silica optics, creating little pits in the surface—similar to the ding you get when a rock hits your car's windshield. We do everything we can to repair and recycle the damaged ones." An example of two damaged optic surfaces before and after repair is shown in Figure 1.

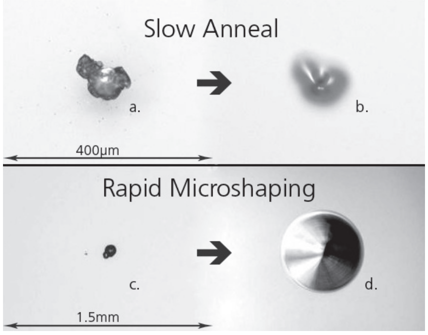

FIGURE 1. Examples of optics damaged by repeated exposure to high-peak-power laser pulses. Damaged optic surfaces are shown in (a) and (c) and the corresponding repaired site is shown in (b) and (d). A slow annealing process was used to repair the damaged site in (a), while the rapid microshaping technique currently employed at NIF was used to repair the site in (c) so that it is optically benign.

Although the energy deposited by repeated laser use is damaging to the optics over time, lasers can also aid in their repair. In contrast to the giant laser system in the NIF, which spans three football fields, the lasers used to repair damaged optics are smaller, tabletop systems that are integrated with beam- and pulse-shaping components to produce a damage mitigation system. Matthews' recent research at LLNL focuses on novel techniques for optic repair and more broadly encompasses laser interactions with fused silica or glass[1].

➔SIMULATING LASER-GLASS INTERACTIONS

Matthews and his team have used simulation to explore three techniques for repairing damaged optics: infrared (IR) pulsed laser microshaping/micromachining, slow annealing, and laser chemical vapor deposition (L-CVD)[2].

In a first research cycle, they focused on the basic underlying physics and material science of how fused silica behaves when exposed to laser light at varying temperatures.

There were several milestones in their temperature-tiered campaign: The first was to understand the thermal-elastic response of the material up to the glass transition temperature of 1,300 K, where fused silica exhibits a sudden increase in elastic response and becomes less resistant to flow. They continued by examining the molecular relaxation of glass under viscous flow between the glass transition and the evaporation point at ~2,200 K. The final objective was to investigate the evaporation and redeposition of the material over temperatures between 2,200 and 3,400 K.

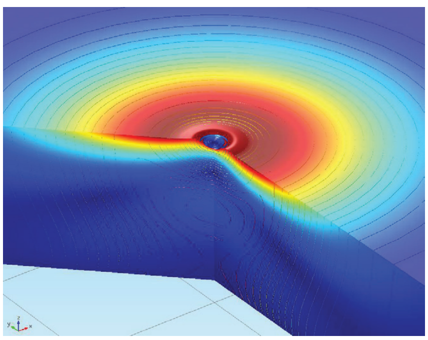

FIGURE 2. Simulation results showing Marangoni flow of laser-heated glass. This effect occurs when laser heating leads to gradients in temperature-dependent surface tension, which causes material to flow radially outward, forming what looks like ripples or layers.

To explore specific techniques for repairing the damaged optics, Matthews turned to the COMSOL Multiphysics® software. "I decided to use COMSOL to get a better understanding of what was going on," says Matthews. "All the necessary physics were already available in the software, so I could readily try out ideas and avoid the time and effort that would be needed to develop my own code from scratch."

According to Matthews, COMSOL has been instrumental in helping them understand how lasers interact with fused silica, as well as in refining their specific repair methods. "A high-power laser system can't tolerate much surface roughness in the optics. Controlling flatness to such high standards required extensive simulation," he says. His simulations include heat transfer in fluids, chemical reactions, and structural mechanics, as well as mass transport and fluid flow.

➔IR-PULSED LASER MICROSHAPING

While the simple approach of slow annealing was first used to mitigate optic damage (see top panels of Figure 1), experimentation and simulation showed that surface rippling caused by thermocapillary flow, or Marangoni shear stress, leads to unwanted light modulation when such surfaces are placed into a laser beam. A simulation showing the laser-induced temperature profile and material displacement due to Marangoni shear stress is shown in Figure 2.

To counter this effect, Matthews and colleagues explored the use of shorter (10's of microseconds compared with minutes) laser pulses to precisely "machine" away material into a shape that is less prone to downstream light modulation when placed in the laser system. In Rapid Ablation Mitigation (RAM), an IR laser is used to heat the substrate just beyond the evaporation point, which precisely removes a small amount of material, leaving behind a smooth, fractureless surface. This nano-ablation of material is repeated thousands to millions of times to produce a smooth, conical-shaped pit, which is "optically benign" in that it does not produce downstream light modulation (see bottom panel of Figure 1).

"Despite the long history of IR-laser processing of silica optics," Matthews says, "few attempts have been made to understand the energy coupling and heat flow in order to optimize the process. We were able to answer many of these questions by simulating a wide range of laser parameters and material properties in COMSOL."

Results from the simulations for temperature and material behavior in the ablated regions compared well with the team's experiments. "What we learned in our research is far-reaching," Matthews says, "and can be applied beyond the repair of damage in our high-energy, pulsed-laser systems to virtually any system that requires laser polishing, annealing, and microshaping of silica surfaces[1]."

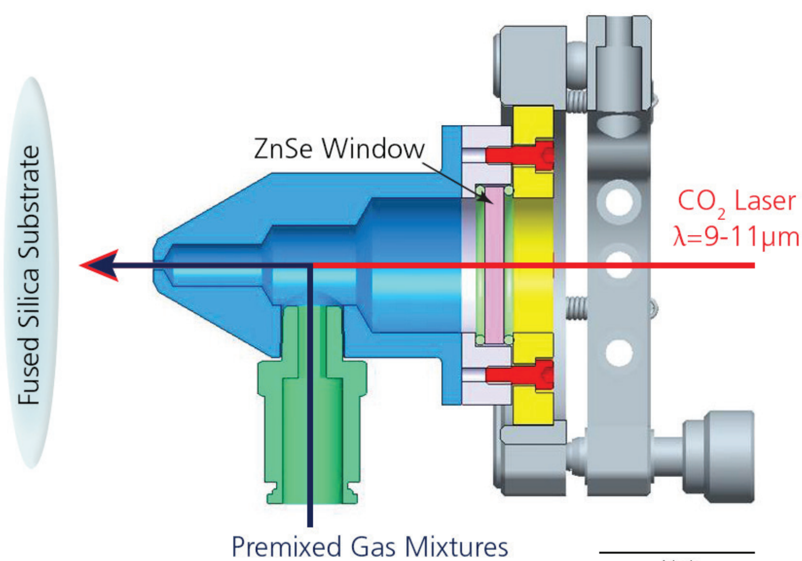

FIGURE 3. Schematic showing the optically coupled gas nozzle used for laser-based CVD processing, which allows gas flow to enter through a lateral port while IR laser light enters axially through a ZnSe window.

➔LASER CHEMICAL VAPOR DEPOSITION FOR LARGE REPAIRS

The third approach the LLNL team studied for repairing damaged optics was laser-based chemical vapor deposition (L-CVD). In this additive process, a silica precursor gas is "flowed" onto the surface through a nozzle. A focused CO_2 laser beam, coupled into the nozzle through a window (see Figure 3), decomposes the precursor and deposits solid SiO_2 glass into the damage pit. L-CVD is being explored to repair large defects on optic surfaces with nanoscale precision that are difficult to fix using IR microshaping or other subtractive approaches. Ultimately, the optic performance can be entirely restored.

"Using simulation, we experimented with how beam intensity, position, and pulse duration affected the amount of material deposited onto the optic," explains Matthews. Simulation can determine the concentration and flow of the silica as it decomposes, as well as the location of deposited material (see Figure 4).

The team found that the laser power was a critical process parameter for avoiding the unwanted features that are common in many L-CVD deposition profiles, such as the well-known "volcano" feature.

"To date, we know of no other approach that additively repairs damage by replacing lost material with high-grade substrate material," says Matthews. "Successful application of such a method could reduce processing costs, extend optic lifetime, and lead to more damage-resistant optics for high-power laser applications in general. In addition, L-CVD can offer advantages over conventional methods for other material systems beyond silica glass. The ability to simulate the transient flow, reaction, and heat transport are critical to exploring new applications."

➔FROM GLASS REPAIR TO MANUFACTURE

While the L-CVD process is still exploratory for optics refurbishment, the team has implemented CO_2 laser-based surface microshaping at NIF, optimized using multiphysics simulation, as part of the facility's optics mitigation program. Through 2014, over 130,000 damage sites have been repaired using IR microshaping and other techniques, and the optics are continuously being recycled back into the NIF, enabling its routine use.

Their laser-material interaction research, however, does not stop at optics repair. Mathews and his team are also supporting a laboratory-wide Additive Manufacturing Initiative by further developing an additive process for 3D printing known as selective laser melting (SLM)[3]. "I'm really excited about this research," says Matthews. "Figuring out how to optimize the 3D printing system could have a huge impact on this rapidly growing industry, which could benefit tremendously from a model-based approach, which was largely trial-and-error in the past." ❖

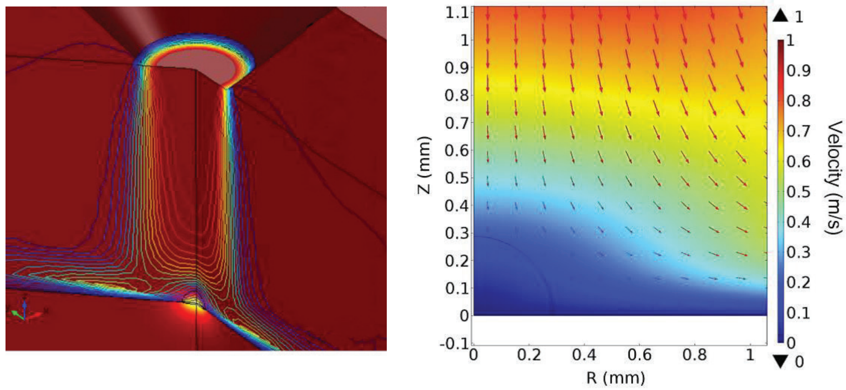

FIGURE 4. Simulation of velocity and temperature fields for L-CVD. Left: Velocity contours associated with the L-CVD precursor flow from a 3 mm diameter nozzle and the temperature field induced by laser heating at the air-glass interface. Right: Velocity streamlines of the vaporized silica where diffusion-dominated transport of the glass in the lower left corner can be seen (dark blue).

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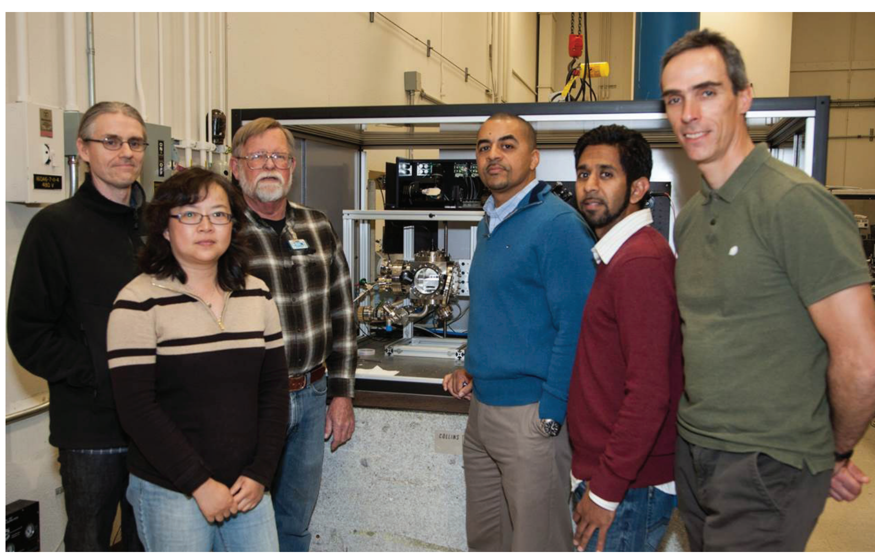

Optical damage mitigation and laser materials processing research team at LLNL (from left to right): Gabe Guss, Nan Shen, Norman Nielsen, Manyalibo Matthews, Rajesh Raman, and Selim Elhadj. The apparatus in the background is used to study the dynamics of metal powder melting under high-power laser irradiation, a topic important to the field of metal-based additive manufacturing (3D printing).