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## Materials, physics and chemistry

We have developed decontamination foam that may be tomorrow's best first response in a chem-bio attack. The foam begins neutralizing both chemical and biological agents in minutes. Because it is not harmful to people, it could be dispensed on the disaster scene immediately, even before causalities are evacuated. In laboratory tests at Sandia the foam destroyed simulants for the most worrisome chemical and biological agents. Confirmatory live agent tests have successfully been done by the Edgewood Chemical and Biological Center and at a university research center. (6800) (E/CISBU)

Sandia researchers in Center 15300 have combined self-focused optical pulses from a femtosecond terawatt laser with adaptive optical compensation techniques to produce a new controllable laser propagation regime in atmosphere which exhibits enhanced brightness without diffractive divergence. The resulting laser channel is attributed to a dynamic self-guiding process that couples self-focusing, ionization, and group velocity dispersion to modify the refractive index of air at high intensity. This technology development, funded by LDRD and WFO, is expected to have important ramifications for remote sensing and directed energy. (15300) (ETSBU, LDRD)

We developed the Polychromator, a microelectromechanical system (MEMS) programmable diffraction grating combined with an optical processor, that is used for the remote sensing and rapid identification of chemical species under battlefield conditions. The Polychromator was developed with DARPA funding and in partnership with Honeywell (MEMS fabrication), and MIT (device design and actuation method). This technology received a 1999 Industry Week Technology of the Year award. (1700, 1800) (S&T SMU)

A team developed new computational methods for coupling microstructure and micromechanical materials response simulations. Its integrated approach to spanning length and time scales in computational materials science resulted in the first fully coupled microstructure/ micromechanics simulations -- the most realistic simulations of microstructure and micromechanics ever. The approach also provided the first direct links between mesoscale simulations and real microstructures and responses. The results are important for many problems of relevance to Sandia, including thermomechanical fatigue of solder joints and fracture in brittle materials. (1800, 9100, 9200) (S&TSMU)

A chemical synthesis process has been developed and patented for preparation of PZT 95/5 -- a key material in the active ceramic components of ferroelectric neutron generator power supplies. Because of the new material's high level of performance during explosive functional testing, the lab-scale powder synthesis and billet fabrication processes are being scaled to production size for in-house production. Beginning in FY2002, chem-prep PZT 95/5 will be used in all ferroelectric neutron generator builds, including the new small neutron generator currently in development for several weapons systems. (1400, 1800, 2500) (NWSBU)

We developed a new apparatus for chemical dynamics studies based on femtosecond lasers and on extensions of the ion imaging technique invented previously at Sandia. This new photoion/photoelectron coincidence experiment will permit measurement of the fine details of molecular dissociation and isomerization processes in real time (10-1210-13 seconds). These molecular-level processes are critical steps in combustion chemistry, often dictating flame ignition, propagation, and acceleration in combustion devices. This research supports the nation's goal for clean, efficient energy production from combustion systems. (8300) (E/CISBU)

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