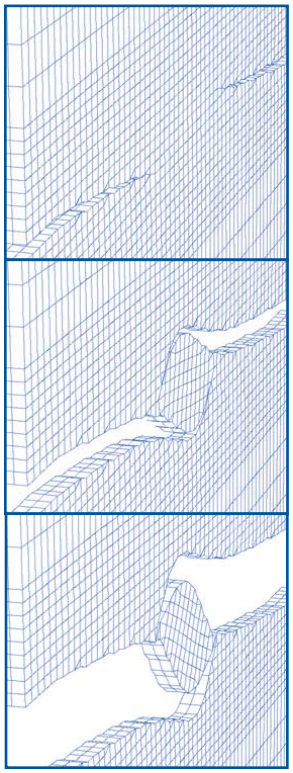
Identifying the cracking point of laminates



Composite laminates — engineered materials made from two or more distinct properties — can be found everywhere, from asphalt-concrete roads to the shell of the space shuttle.

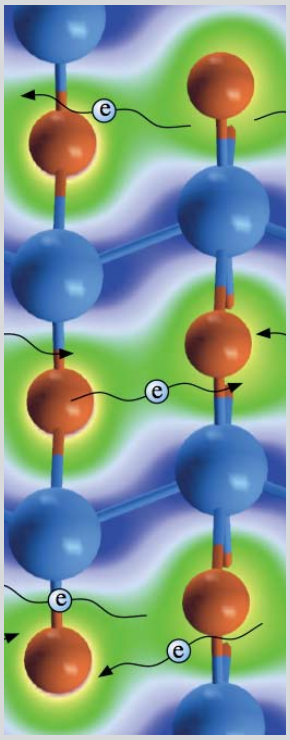
Normal stresses and impacts, as well as fabrication defects or misalignments of the composite fibers, can cause the laminate to separate at the junction point between the two layers. This condition, called delamination, is one of the predominant modes of damage to these materials.

University of Cincinnati aeronautical engineer Ala Tabiei, Ph.D., is using the resources at the Ohio Supercomputer Center to develop a better method for simulating how a laminate cracks and separates, within the non-linear, explicit finite element software DYNA3D. He is developing numerical methods to determine the dynamic energy released, measure stress factors on the crack under certain conditions and capture when a crack begins to expand. He's also implementing a method to recalculate the fracture model, which will allow researchers to simulate crack growth when the material is significantly stressed.

"Our goal is to develop an automated, dynamic fracture procedure that can be used to simulate delamination failure between adjacent layers of laminated composites," Dr. Tabiei said. "To effectively use laminate composites, researchers need to consider the characteristics that cause the material to fail. We think this new numerical model, when completed, will be a valuable tool for industries such as aerospace, automotive and construction." ■

Project lead: Ala Tabiei, Ph.D., University of Cincinnati
Research title: An automated dynamic facture procedure for finite element simulations of delamination failure in laminated composites

Bonding lithium and beryllium under pressure



The stalwart computing power of the Ohio Supercomputer Center recently played an integral role in a groundbreaking discovery by Cornell University scientists.

By combining theory and computational modeling, the researchers predicted that the lightest known metals in the universe, lithium (Li) and beryllium (Be), will bond under high levels of pressure and form stable — and possibly superconductive — alloys. Under normal conditions, Li and Be repel each other. Unexpectedly, they also found that the combination creates a quasi two-dimensional electron gas sandwiched between the Li layers of the LiBe alloy.

"While I searched for stable high-pressure structures using the random search method, my colleague used chemical information to determine likely stable bond arrangements for LiBe," said Richard Hennig, Ph.D., a Cornell University professor in materials science and engineering. "OSC's queuing system enabled us to simultaneously run large numbers of density functional calculations within a few weeks time. This is a great benefit over other supercomputing centers."

The research, supported by the National Science Foundation, appeared in the Jan. 24, 2008, issue of the journal *Nature*.

"The Ohio Supercomputer Center was my first choice for computing the structures at each composition and pressure," Dr. Hennig said. He previously used OSC extensively for ab-initio and quantum Monte Carlo calculations of defects in semiconductors and phase transformation in transition metal alloys as a post-doctorate researcher under Ohio State University Physics Professor John Wilkins. Their on-going collaborations grant Dr. Hennig access to OSC's supercomputers from Cornell. ■

Project leads: Roald Hoffmann, Ph.D., & Richard Hennig, Ph.D., Cornell University
Research title: Emergent reduction of electronic state dimensionality in dense ordered Li-Be alloys
Funding sources: National Science Foundation & the Petroleum Research Fund of the American Chemical Society