Materials can come from the mind, not just the mines

February 4 2008

Dr. Julia E. Medvedeva, assistant professor of physics at Missouri University of Science and Technology, believes materials can come from the mind, not just the mines.

Medvedeva is examining how such properties as optical transparency or electrical conductivity depend on how the atoms are put together on the microscopic level. Such in-depth understanding of underlying physical phenomena allows her to design new materials with properties required for a particular application.

“Right now, we are experiencing a materials revolution,” Medvedeva says. “Advanced materials have already transformed the lives of millions of people around the globe. Now, supercomputers facilitate the progress toward even more high-tech innovations.”

Until recently, scientists concentrated on understanding materials that exist in nature or are prepared in a laboratory. Now, the advent of ever-more-powerful supercomputers and the development of state-of-the-art computational approaches make it possible for researchers to simulate new materials and manipulate their properties based on knowledge of the atomic composition and the spatial arrangement of the atoms.

Such computational “experiments” allow Medvedeva to speed up the search for materials with optimal performance for a specific application – something that could have taken years to achieve using trial-and-error experimental techniques.

In particular, Medvedeva is interested in a unique class of materials called transparent conductors, which share the seemingly contradictory properties of being optically transparent, like glass, and electrically conductive, like metal. Transparent conductors are vital components in many devices, including solar cells, smart windows, flat-panel and flexible displays, invisible, or “see-through,” electronics and gas sensors. Despite the multitude of applications and the growing demand for such devices, only four materials are known to be good transparent conductors – doped zinc, indium, cadmium and tin oxides. Of the four, only two are used commercially.

Although relatively simple compounds, all of the known transparent conductors require sophisticated preparation techniques to achieve optimal balance between sufficient optical transparency and useful electrical conductivity. There are other drawbacks to these

compounds, as well. Due to the increased demand, some of the oxides have become expensive. For example, the cost of indium rose 10-fold from 2002 to 2006. Besides, indium and cadmium are highly toxic.

With financial support from the National Science Foundation (NSF) and the Petroleum Research Fund of the American Chemical Society, Medvedeva is working to develop new transparent conductor materials that are more efficient, easier to fabricate, less expensive and environmentally friendly. Medvedeva’s preliminary research shows that with proper preparation calcium, aluminum or silicon oxides, the most abundant substances in the Earth’s crust, can be made electrically conductive while maintaining their superior optical properties. Further studies of these materials are underway.

To help with this effort, Medvedeva has also received computational grants that give her access to national supercomputer facilities, the National Energy Research Scientific Computing Center and TeraGrid

Cluster, supported by the Department of Energy and NSF.

Source: Missouri University