CU team gets $1.7 million for research on new materials

The research team that received an NSF grant for simulation and modeling of materials that could be used in semiconductors are, from left, Paulette Clancy, associate professor of chemical engineering; Michael Teter, adjunct professor of physics; Fernando Escobedo, assistant professor of chemical engineering; Michael Thompson (on the rock), associate professor of materials science and engineering; George Malliaras, assistant professor of materials science and engineering; and Edwin Kan, assistant professor of electrical engineering. *Charles Harrington/University Photography*

By David Brand

The integrated circuits of the future could possibly be made with a substrate of silicon with a thin film of polymer containing the transistors and the interconnections dropped on top. The idea is novel, but as yet the marrying of two such dissimilar materials is poorly understood.

The future applications of such new types of semiconducting materials could be such things as light-emitting diode displays and flexible laptop screens, leading to an era of cheap and highly portable "throwaway electronics."

To try to understand the underlying science behind these potentially new types of semiconductors, the National Science Foundation (NSF) has awarded $1.7 million to a Cornell research team led by Paulette Clancy, associate professor of chemical engineering.

Clancy

The award is among $50 million in recent NSF grants for broad-based research through the agency's Knowledge and Distributed Intelligence Initiative (KDI). The awards are for projects as varied as knowledge networking in biocomplexity, earthquake computer modeling and case studies in intellectual property.

This is the second KDI grant within a year for Cornell research. Last October the Cornell Theory Center received a $1.5 million, three-year grant for a project called "multiscale modeling of defects in solids" that will enable researchers to create computer simulations that show how defects at the atomic level can lead to changes at increasingly larger scales, up to the visible cracks seen in the everyday world.

The 31 grants to 24 institutions in 20 states "are a solid foundation for NSF's new initiative in information technology for the 21st century," said Richard Hilderbrandt, NSF program manager for the multidisci-plinary awards.

The Clancy group's award is for simulation and modeling of organic and inorganic noncrystalline materials that could be used in semiconductors. The electronics industry has a long history in dealing with crystalline silicon, with its ordered arrays of particles, but less well understood is amorphous silicon, the material used for such purposes as solar cells. Amorphous silicon has the local order of crystalline material but looks disorganized on a broader scale.

Understanding the structure of polymers is even less understood. Experimental routes to the structure of polymers are difficult to find, and they are hardly easier to model on a computer. Compounding the problem, it is also difficult to make computer models of sandwiches of the two materials.

As Clancy and her team investigate the problem, they plan to look at the structural differences from several different approaches. "Even though this is supposed to be a modeling and simulation program," she said, "we felt that without the experimental verification we wouldn't feel comfortable pressing forward with the modeling."

That is why Clancy and her team already are looking forward to the future applications of these new types of semiconducting materials, such as disposable electronics. On the applications side of the research, Edwin Kan, assistant professor of electrical engineering, will be making single electron devices, called nanodots, from the new materials. To get to that stage, two experimenters will be investigating both sides of the organic-inorganic "sandwich" -- with George Malliaras, assistant professor of materials science and engineering, testing the organic polymers and Michael Thompson, associate professor of materials science and engineering, focusing on the inorganic silicon.

On the computational side, Michael Teter, adjunct professor of physics, will be developing novel quantum mechanical codes that combine great accuracy with computational speed. Clancy and Fernando Escobedo, assistant professor of chemical engineering, will be using these and other models to predict the materials' molecular structure. Kan will, in turn, take the results from these models and predict the materials' behavior in practical applications.

There will be another highly practical spinoff from this research: education at the middle- and high-school levels. Clancy and her team plan to work with local teachers and Cornell graduate students to develop modules on growing crystals and on crystal structure aimed at grades six through eight. "We want to fire up these young people's enthusiasm for science," Clancy said.

Teachers in the Ithaca area interested in participating in the program are urged to contact Clancy at pqc1@cornell.edu.

September 30, 1999