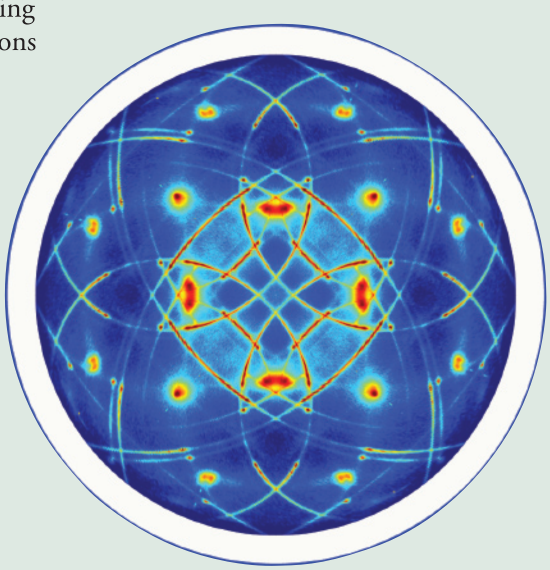
NSLS Users Discover a New Material Texture Type

Researchers working at the National Synchrotron Light Source have identified a new way in which the orientation of the tiny grains that make up various materials can be classified. There were previously only three known types of grain orientation, and the discovery of a fourth type may have broad impact on technology research and the study of materials and crystals.

The results appeared in the December 11, 2003 issue of *Nature*.

At the microscopic level, most manufactured and naturally occurring materials, such as metals, are made of crystalline grains – tiny regions of ordered, symmetrical arrays of atoms or molecules. In the field of materials science, the way these grains fit together to form the overall material is referred to as the material's "texture."



A pole figure of the NiSi thin film.

Until this discovery, there were three texture types, known as "random," "fiber," and "epitaxy" textures. To get a sense of these textures, picture a bucket of children's building blocks to represent the individual grains. If the blocks are dumped onto a table, the resulting jumbled pile, containing blocks in messy layers and many different positions, simulates a random texture. If the blocks are instead placed in layers such that the bottom face of each one is parallel to the table, but neighboring blocks are not parallel to each other, the configuration resembles a fiber texture. Finally, if the blocks are carefully placed in a series of neat, parallel stacks, like a three-dimensional checkerboard, an epitaxial texture is represented.

In materials science research, materials often take the form of "thin films" that are less than one-millionth of a meter thick. To be studied, these thin films must be produced on the surface of another material, called the "substrate." The region where the substrate meets the thin film is called the "interface." In our block example, the table acts like a substrate, and an interface exists between it and the blocks.

Keeping all this in mind, the new texture type, named "axiotaxy," is similar to fiber texture. However, instead of sitting flat on the table, each "block" is tilted upwards at the same angle, as if resting against an invisible sloped surface. This causes a special relationship to form between the orientation of the grains in the thin film and the substrate.

"The mechanism that causes the formation of this new type of texture is unique, and may help us to better understand the physics of thin film growth and phase transformations in thin films," said Christophe Detavernier, a materials scientist at the IBM T.J. Watson Research Center in Yorktown Heights, New York and the University of Ghent, Belgium. He is a member of the research group that discovered the new texture at the NSLS.

In the continuing development of portable electronics, such as cell phones, handheld computers, and digital music players, the study of thin films is crucial to creating the tiny electrical circuits that make these devices work. Therefore, gathering more knowledge of texture is just as important.

"The effect of texture on a material's physical properties is exploited in technology development in order to produce materials with specific characteristics," explained Detavernier.

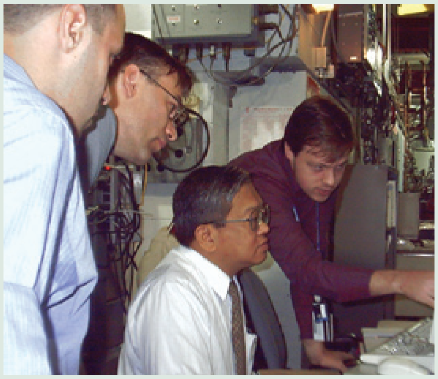
"We focused on a class of materials called silicides that are used in integrated circuits. As the aggressive trend in miniaturization continues in silicon-based devices, controlling the properties of silicides becomes challenging. Therefore, understanding and controlling texture becomes critical in certain cases."

Authors Jean Jordan-Sweet and Ahmet Ozcan.

Details of the Discovery

The researchers discovered the new texture while studying a thin film of a nickel/silicon compound, called nickel silicide (NiSi). Starting with a substrate of pure silicon, they formed a NiSi thin film by depositing a small amount of pure nickel on the silicon substrate. During an annealing treatment, in which the sample was heated to 550 degrees Celsius in a furnace, a solid-state reaction occurred between the nickel and silicon. This caused all of the nickel to be consumed and a NiSi layer to form on the substrate.

Working at NSLS beamline X20A, the researchers shined x-rays at the film from several different angles and, using a computer, analyzed the pattern the rays created as they emerged from the material. The resulting image, known as a "pole figure," represents the distribution of the grain orientation in the film.



From left, IBM Researcher Cyril Cabral, Jr., Author Christian Lavoie, T.C. Chen (IBM Vice President, Silicon Technology), and Christophe Detavernier.

The researchers knew they had found a new texture when they noticed that their pole figures did not resemble those produced by materials with random, fiber, or epitaxy textures, or any combination of them (since many films contain elements of all three textures). They are now looking for axiotaxy in other thin films.

— Laura Mgrdichian