Combinatorial Tools for Materials Science

Combinatorial methods are increasingly used by industry for the discovery and optimization of materials for use in electronic, optical, and magnetic applications as well as for designing chemical and biological sensors and for creating molecular patterns. We have developed tools for the fabrication of thin film libraries and characterization of thickness and optical properties. We introduce combinatorial near edge x-ray absorption fine structure as a new tool for the rapid, non-destructive determination of the chemistry (including bond concentration) and molecular orientation of chemically heterogeneous surfaces.

Peter K. Schenck and Daniel A. Fischer

We have developed combinatorial tools that can be applied to a broad range of materials: a pulsed laser deposition (PLD) system for thin film library fabrication; a rapid throughput, spatially-resolved spectroscopic reflectometer for mapping thickness and refractive index; and a combinatorial near edge x-ray absorption fine structure (NEXAFS) tool.

PLD is a versatile, rapid method for growing thin films that has the following advantages: complex target compositions are possible; congruent vaporization leads to stoichiometric material transfer; high energy process; low substrate temperatures; and high deposition rates. Our deposition chamber utilizes a dual-beam, dual-target configuration designed for the fabrication of compositionally graded films. Thickness and optical property assays are performed on the film libraries using a semi-automated spectroscopic reflectometry apparatus.

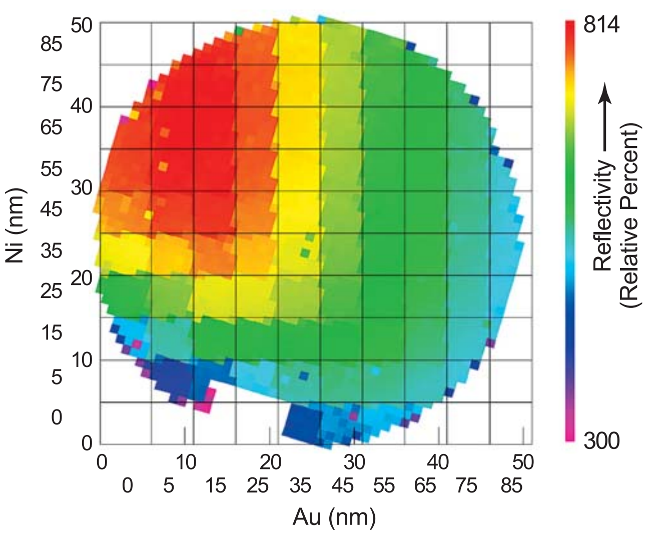

Figure 1: Reflectivity (450–500 nm, relative to sapphire) of Ni-Au interconnects on GaN after heating to 400 °C.

$BaTiO_3$-$SrTiO_3$, Au-Ni, and Au-NiO film libraries have been deposited and characterized using these tools. In addition, combinatorial library films of Ni-Au interconnects (88 compositions) on GaN have been characterized before and after annealing (as shown in Figure 1).

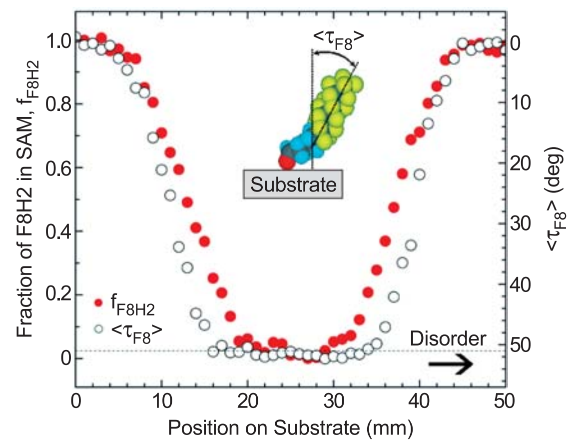

Figure 2: *Fraction of F8H2 in the SAM (f_{F8H2}) (closed circles) and the molecular orientation (open circles).*

Combinatorial NEXAFS is used to simultaneously determine molecular orientation and bond chemistry of planar, chemically heterogeneous surfaces. Information on the chemistry and molecular organization of chemical groups on surfaces is needed, for example, to shed light on the behavior of monomolecular templates and surface modifiers and to characterize new classes of catalysts. We illustrate the power of the combinatorial NEXAFS method by simultaneously probing the concentration and molecular orientation of semifluorinated $F(CF_2)_8(CH_2)_2SiCl_3$ (F8H2) molecules in self-assembled monolayer (SAM) gradients on flat silica substrates as shown in Figure 2.

Notable Outputs: Invited paper in *Chemistry in Britain*, May 2003 (pgs. 45–47), “Blazing a Trail.” Cover of *Applied Physics Letters*, January 13, 2003 (pgs. 266–268) and press release, January 17, 2003, Brookhaven National Laboratory, “Scientists Develop Technique to Determine Molecular Structure of Heterogeneous Surfaces.”

Contributors and Collaborators

M. Vaudin, J. Kim, J. Blendell (Ceramics Division, NIST); A. Davydov (Metallurgy Division, NIST); E. Bretschneider (Uniroyal Optoelectronics); J. Genzer, K. Efimenko (North Carolina State University)