Crystallographic Nanotechnology Research

Carroll K. Johnson
Chemical & Analytical Sciences Division, Oak Ridge National Laboratory,
Oak Ridge, TN 37831-6197
and Department of Mathematics, University of Tennessee,
Knoxville, TN 37996. e-mail: ckj@ornl.gov .

Nanoscience is a field currently well funding through the National Nanotechnology Initiative, http://www.nano.gov , which includes most of the major U.S. funding agencies. A principal nanotechnology problem is the assembly of various nanoparticle sized (i.e., 10 – 10,000 angstroms in one or more dimensions) subunits to form superstructures with engineered physical and chemical properties. A future generation computer, for example, may have component density well outside lithographic mask printing capabilities, and use electronic circuits based on quantum properties unique to nanoparticles, http://www.darpa.mil/ito/solicitations/cbd_01-11.html .

Ideally, one would like to have the subunits self-assemble like the growth of a crystal, and is currently an active research area. About two nanotechnology conferences per month are scheduled for 2001. One of the better-documented series is the Foresight Conference on Molecular Nanotechnology, http://www.foresight.org/Conferences/MNT8/Papers .

How well will crystallography fit into that strange new research environment? The answer should be: very well! Small molecule modulated structure and quasicrystal studies are revealing nature's secrets for growing systematically imperfect crystals, while macromolecule studies of biological systems are revealing nature's methods for self-replication of arbitrarily complex patterns, energy efficient catalysis, and biocomputation feedback, http://www.darpa.mil/ito/solicitations/CBD_01-26.html .

Mathematical modeling of these systematically imperfect nanocrystal complexes will require modification of the classical perfectly imperfect crystal symmetry and diffraction theory to include crystallographic detail at nanoparticle boundaries and interfaces. We suggest that can be handled most conveniently with groupoids, which are a component of our plan for future crystallographic topology of nanomaterials research, as outlined in a white paper at http://www.ornl.gov/ortep/topology/preprint.html .

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