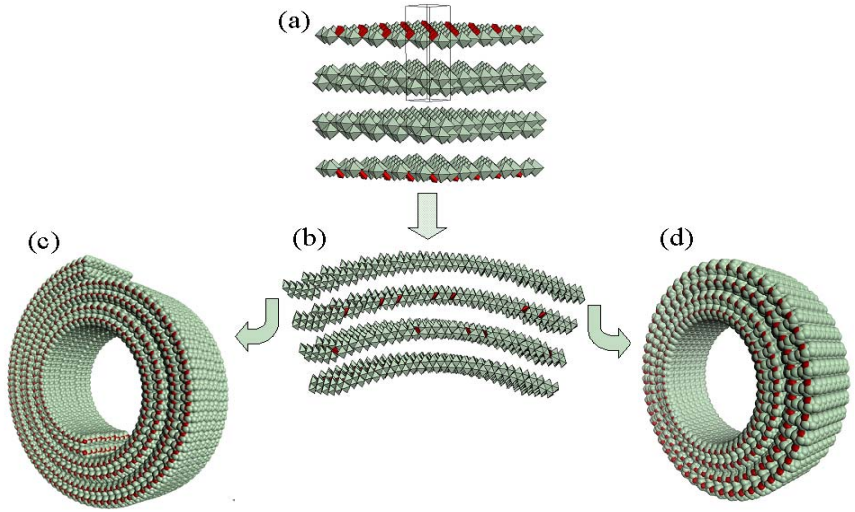
NIRT-Atomic Scale Structure of Nanoparticles

DMR-0304391

PI: Simon J. L. Billinge (MSU), *Co-PI's:* M. G. Kanatzidis (MSU), V. Petkov (CSU), M. F. Thorpe, (ASU)

The properties of materials depend sensitively on their atomic-scale structure. This is also true of nanoparticles, which also have unique properties because of their nanometer size. Solving the atomic-scale structure of nanostructured materials is notoriously difficult. This interdisciplinary group of researchers is tackling this problem using recently developed methods of collecting and analyzing high-energy x-ray and neutron data, the atomic pair-distribution-function (PDF) method.



Example of the atomic scale structure of V_20_5 nanotubes obtained from our recent PDF study. This showed bent bilayers of VO_6 octahedra as the basic building unit of these nanoparticles. These could form into nanoscrolls (c) or closed nanoparticles (d) apparent in TEM images

V. Petkov *et al., Phys. Rev. B* **69**, 085410 (2004).

Materials physicists endeavor to understand why materials have the properties they do; for example, why can you see through a window but not through the wall? This fundamental understanding allows us to engineer new and better materials. A material's properties depends sensitively on how the atoms arrange themselves in the material. Carbon is a great example. In one atomic arrangement (graphite) the material is black, soft and electrically conducting. Take the same atoms (just carbon) and arrange them differently into the diamond structure and you have a material that is extremely hard, transparent and electrically insulating (diamond). The properties completely changed by rearranging the atoms. A prerequisite to understanding material properties, therefore, is to have a thorough knowledge of the atomic-scale structure. X-ray, diffraction and crystallography has been a workhorse for studying atomic scale structure since 1911 when it was discovered. However, the new interest in nano-materials presents a problem: traditional crystallographic methods no longer work for structures with this nanometer-length-scale. This NIRT collaboration has been developing novel methods for collecting and analyzing data from state-of-the-art x-ray and neutron national facilities to study the atomic scale structure of nanostructured materials. Combining these modern, high-power, sources with advanced computing methods allows us to learn quantitative information about the arrangement of atoms in nanomaterials with unprecedented detail. The above nugget gives just one example of how we can unravel the structure of nanoparticles using these new methods.

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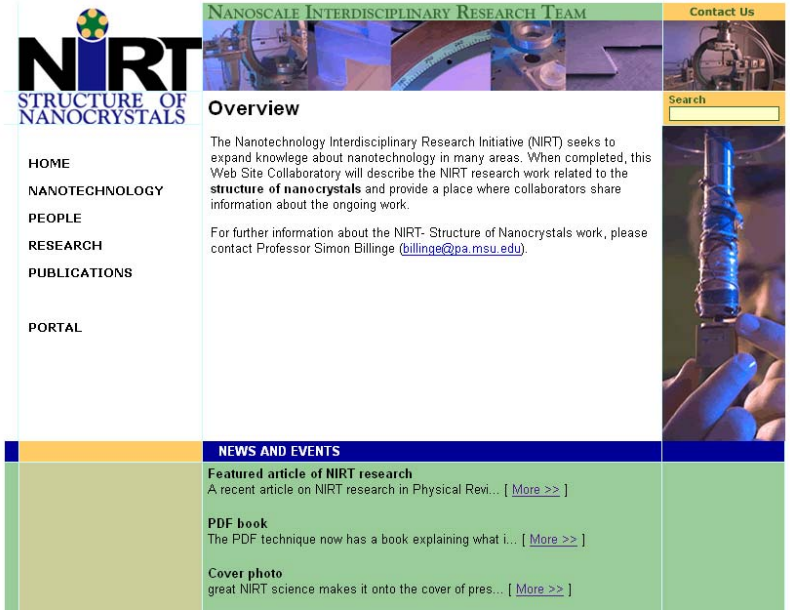
Collaboration: This collaboration brings together 5 senior researchers (the PI's plus H. Foley at PSU) and their groups in 4 institutions and three distinct disciplines (theoretical and experimental physics, chemistry and chemical engineering) as well as a number of external collaborators. Such interdisciplinary groupings are necessary to solve problems in nanoscience and provide a rich working environment for graduate students, post-docs and undergraduates. So far, 6 grads, 5 undergrads and two post-docs have been directly involved in the research



A collaboratory web-page is under development to help researchers in the collaboration share data and results in a secure but convenient way, and to publicize the results of the collaboration for a wider audience. Software developed by the collaboration will also be downloadable from here.