Structure of Nanocrystals

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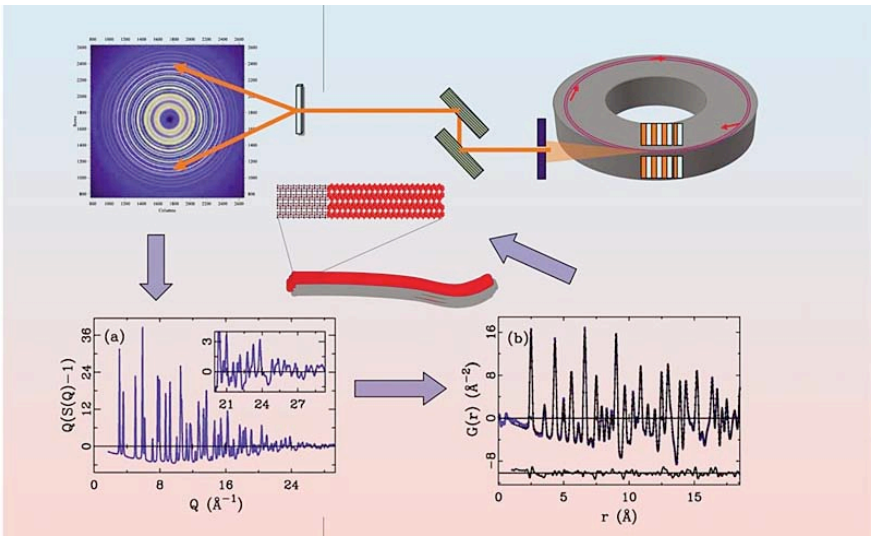
A quantitative knowledge of atomic scale structure is a prerequisite to understanding material properties in general. However, the atomic structures of nanoparticles and nanostructured materials are not accessible by conventional methods used on crystalline materials because, by their very nature, nanostructured materials are not periodically long-range ordered. This is an important unsolved problem in nanoscience. We are developing methods of "nanocrystallography" to solve the atomic scale structure of nanomaterials using x-ray and neutron scattering methods. These methods are quantitative, bulk average, probes that complement imaging methods such as scanning-probe and transmission electron microscopies that give spatially resolved images of small parts of a sample and are limited to surfaces or thin-sections.



The approach makes use of high-quality x-ray or neutron scattering data from powerful modern national user facilities such as the Advanced Photon Source at Argonne National Lab., combined with advanced computing and novel modeling methods to extract the structural information. The approach is illustrated schematically in the Figure. The scattering data are carefully processed and modeled resulting in quantitative information about the atomic arrangement in nanostructured materials. More details, including recent publications and research highlights, can be found at the NIRT-Structure of Nanocrystals website [1] and in recent overviews of the subject [2,3].

The Structure of Nanocrystals NIRT is a collaboration between physicists who are developing and applying these methods, with chemists and chemical engineers making novel nanostructured materials. We are particularly interested in collaborating with researchers with interesting structure questions from partially ordered and nanostructured materials.

References

[1] For further information about this project link to **http://nirt.pa.msu.edu/** or email **billinge@pa.msu.edu**
[2] S. J. L. Billinge and M. G. Kanatzidis, **Beyond crystallography: the study of disorder nanocrystallinity and crystallographically challenged materials**, *Chem. Commun.* , 749-760 (2004).
[3] T. Egami and S. J. L. Billinge, **Underneath the Bragg peaks: structural analysis of complex materials**, Pergamon Press Elsevier, Oxford England, 2003.