Paolo Scardi, Struct Chem Crystallogr Commun, 3:2
DOI: 10.21767/2470-9905-C1-001

Paolo Scardi

University of Trento, Italy

Static and dynamic atomic disorder in nanocrystalline systems

Much is known about the effect of size and shape of metal nanocrystals on their catalytic activity. Size effect may appear obvious for the direct relation with the total surface area exposed to the environment, whereas shape is a major factor controlling selectivity of the catalytic reaction. Palladium nanocrystals, for example, can catalyze a variety of oxidation reactions, but the yield of the process is strongly influenced by the exposed nanocrystal facets: Better O_2 activation occurs on (100) than on (111) facets, for the differences in the O-O bond stretch and spin charge density. As a consequence, Pd nanocubes are much more effective than nanooctahedra in oxygen-related catalytic reactions. The different, generally lower coordination of surface atoms reflects in an excess surface energy, which in many metals gives shorter bond distances between surface atoms, causing an average shrinking of the nanoparticle. The atomic displacement influences electronic properties, leading to d-band center modification and, in general, surface properties differing from corresponding bulk materials. Change in bond distances is largest on the surface, gradually decreasing toward the nanoparticle core; therefore, the displacement field is inhomogeneous and depends on nanocrystal size and shape. In addition to the static component, dynamic displacement in nanocrystals is also peculiar: Phonon confinement arises from the finite size, capping longest possible phonon wavelengths, while additional effects are due to the amplitude of thermal vibration, changing toward the surface for the decreasing coordination. The present contribution shows how X-ray spectroscopies can shed light on the behavior of metal nanocrystals, influenced by complex relations between size, shape, surface atomic coordination and bond distances. Atomistic approaches are indispensable to go beyond the limits of traditional crystallography, clearly inappropriate to deal with small crystals. In particular, we show how X-ray diffraction, applied to powders of nanocrystals with definite shape and little size dispersion can provide detailed information on atomic disorder.

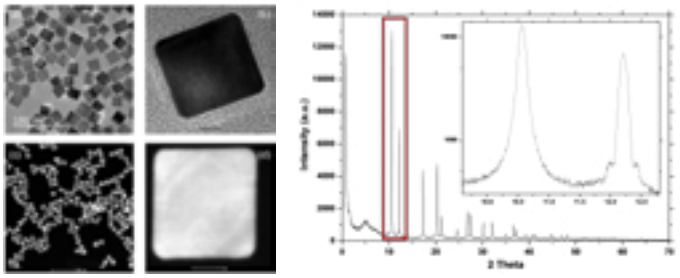

Figure-1: Pd nanocubes (left) and corresponding XRD powder pattern (right).

Biography

Paolo Scardi is a Full Professor of Material Science and Technology and Head of the PhD School in Civil, Environmental and Mechanical Engineering at the University of Trento, Italy. He is the author of more than 250 papers and his main interest concerns diffraction and crystallography with applications to materials science. His recent work focuses on thin films and highly deformed materials, photovoltaic devices, residual stress analysis and atomistic modeling of nanocrystalline materials.

Paolo.Scardi@unitn.it