

Structure of Nanoparticles by Pair Distribution Function Analysis

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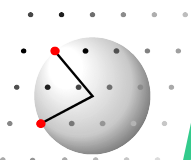
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Representative for the
International Union of Crystallography, IUCr
www.iucr.org

No standardized procedures exist at our university or for IUCr

Size and atomic structure
AND technique used to derive these figures

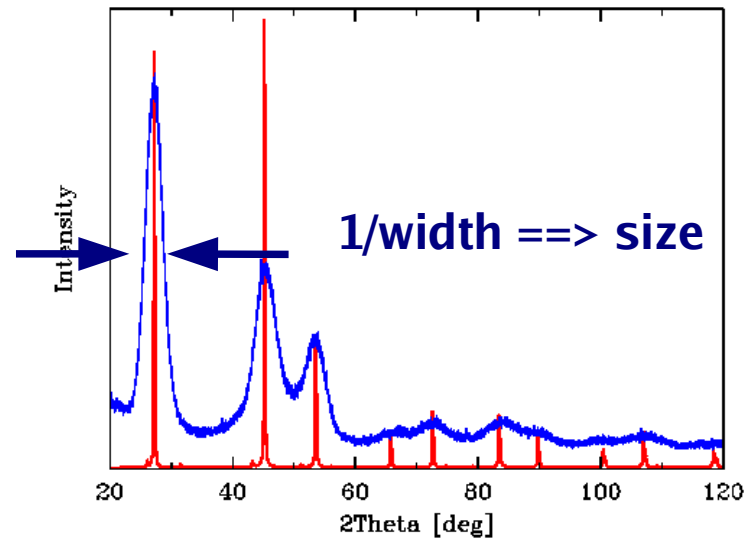
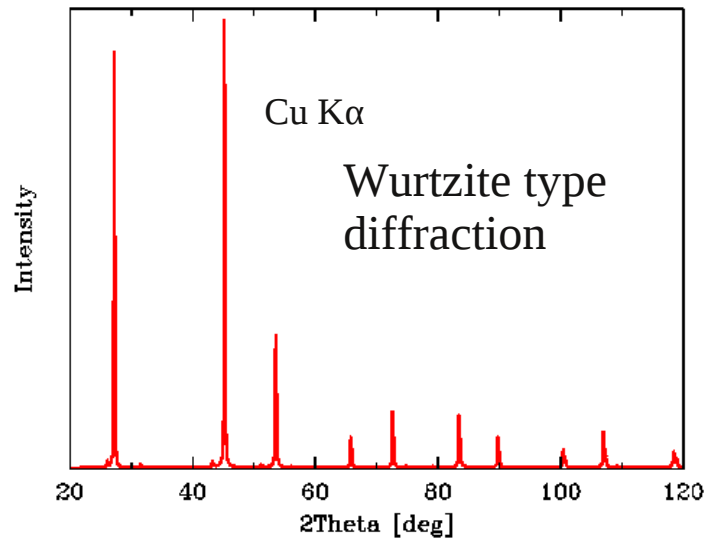


ZnSe Nanoparticles

pure crystalline ZnSe

Laboratory X-ray diffraction data

nano crystalline ZnSe



width of X-ray diffraction peaks

(rough) particle diameter, Scherrer Equation
actually diameter of structurally coherent part

Free particle ? Embedded in matrix?

instrumental effects

anisotropic shape

defects within structure

peak overlap

3.3 nm particles

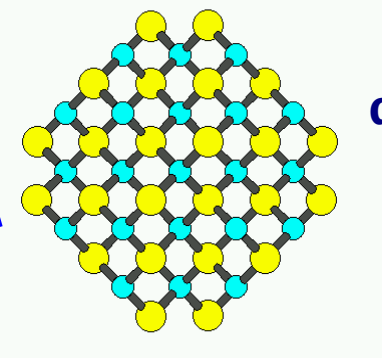
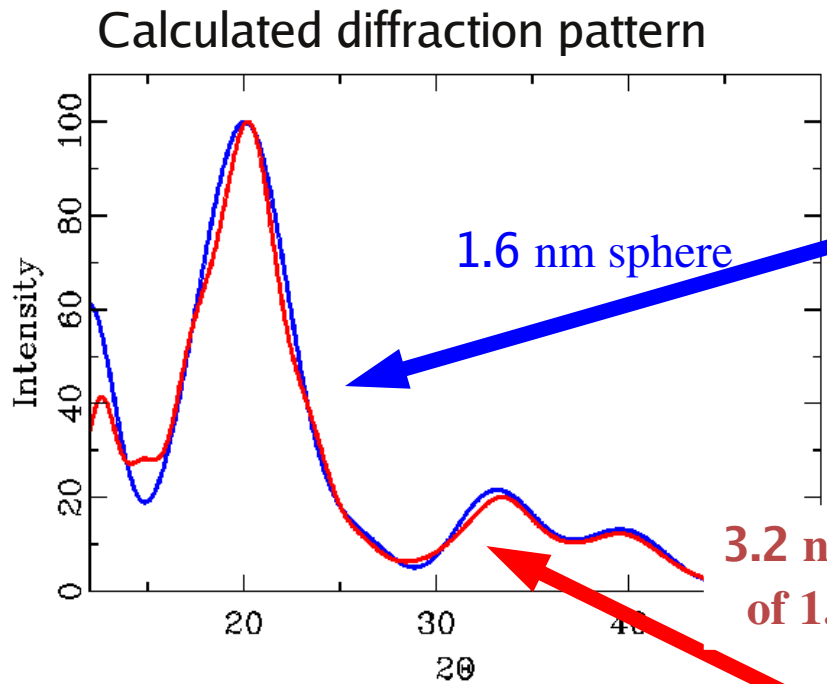
few, broad reflections

high background

well ordered nanoparticle ??

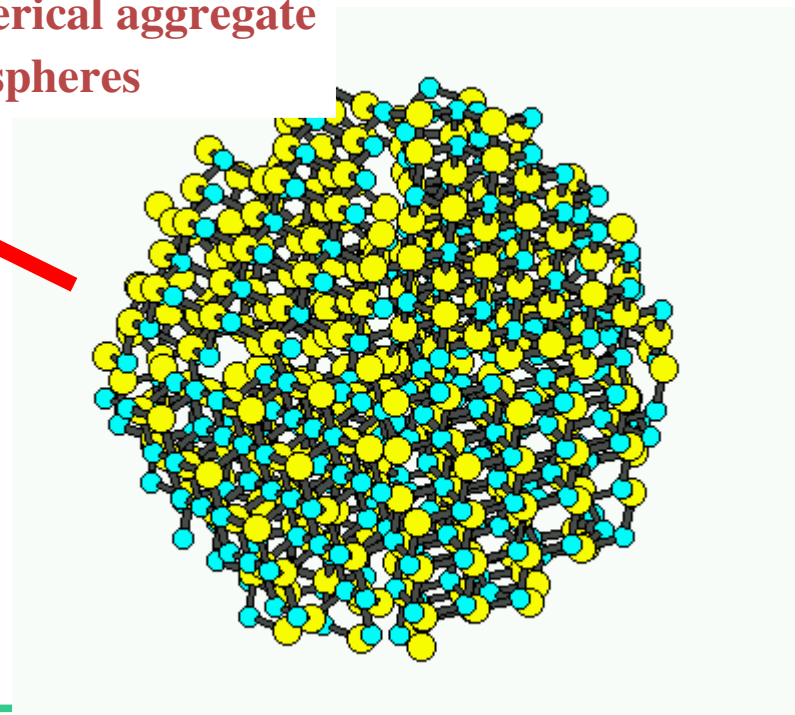
limited information on atomic order

Size from diffraction ?



diffraction size

Microscopy size
Small angle size
Spectroscopy (?)

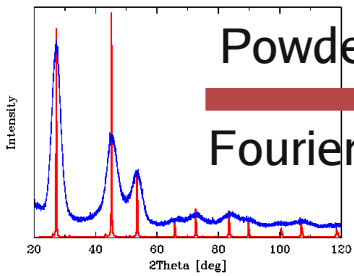


Specify technique from which a property was derived

mean values ?
distribution ?

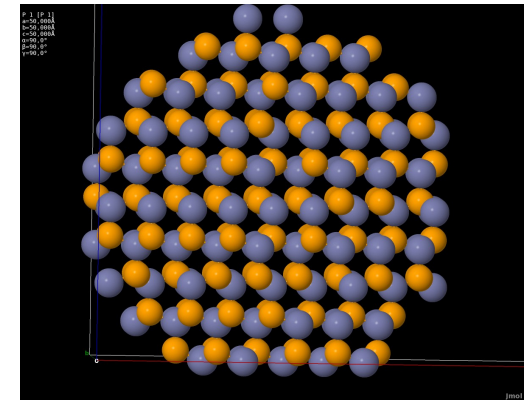
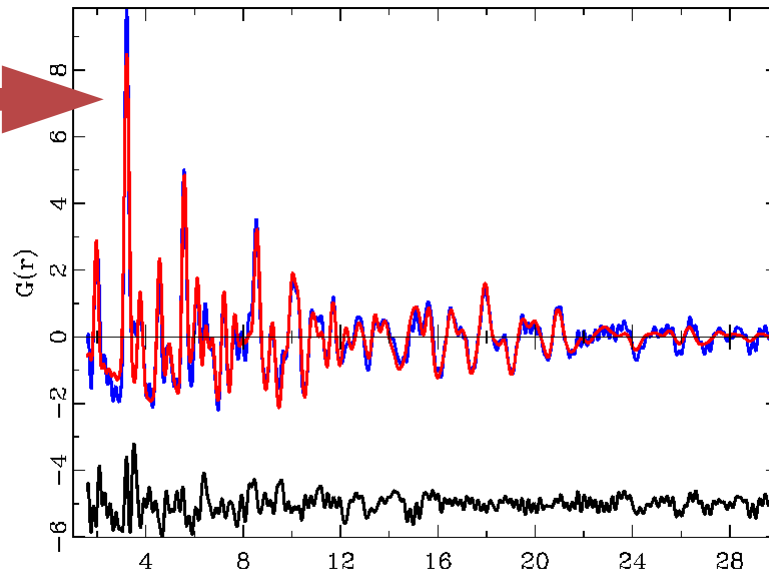


3.5 nm ZnO nanoparticles, Pair Distribution Function (PDF)



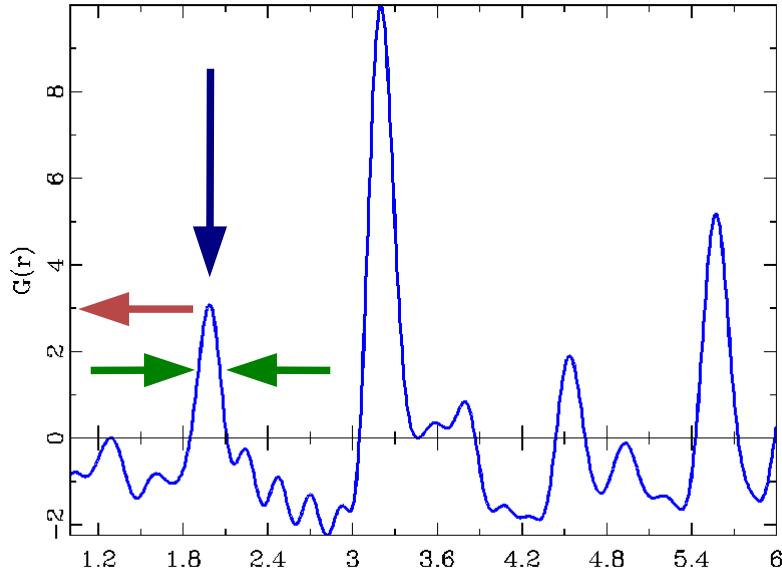
Powder pattern
Fourier transform

PDF is direct measure of
bond length
number of neighbors
bond length distribution

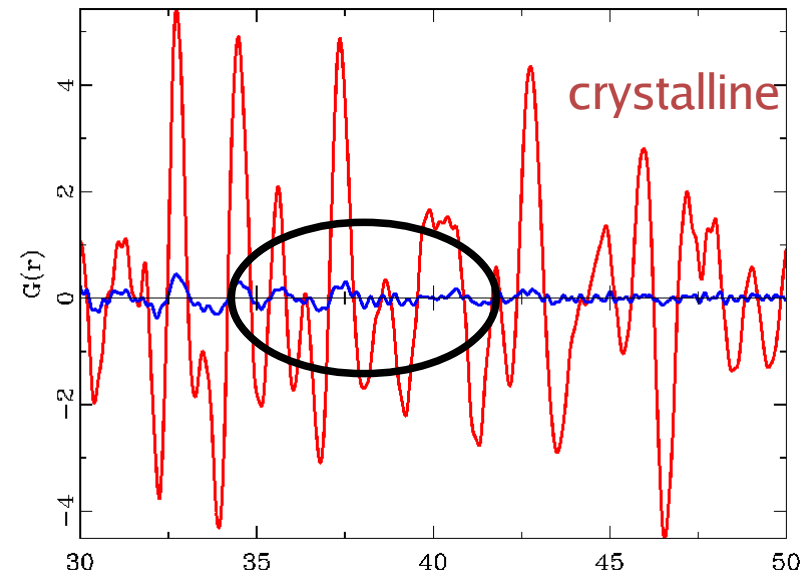


particle diameter
defects

distance



distance

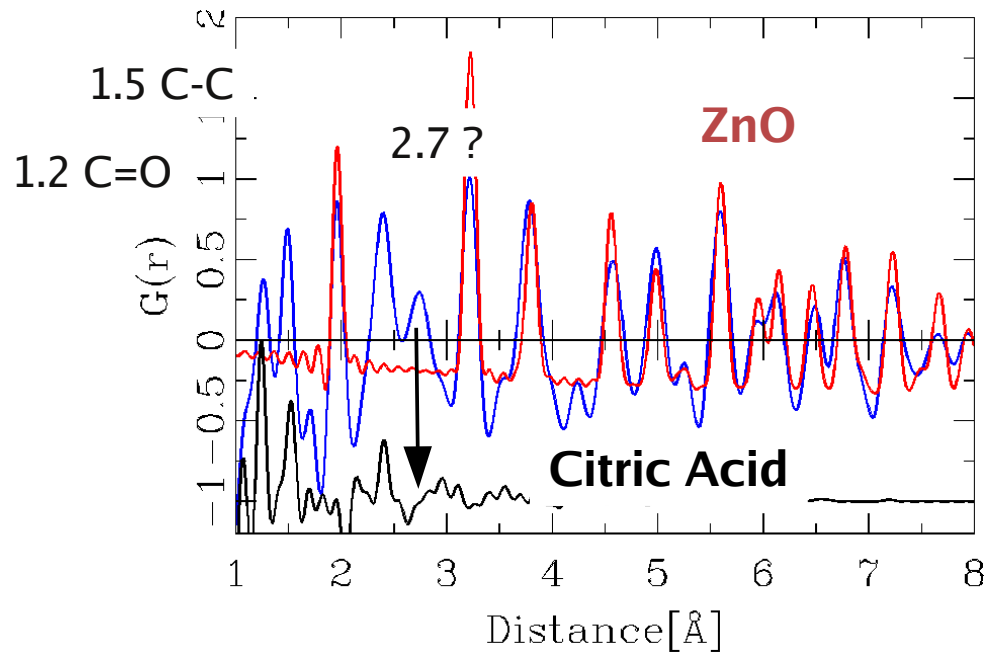


distance

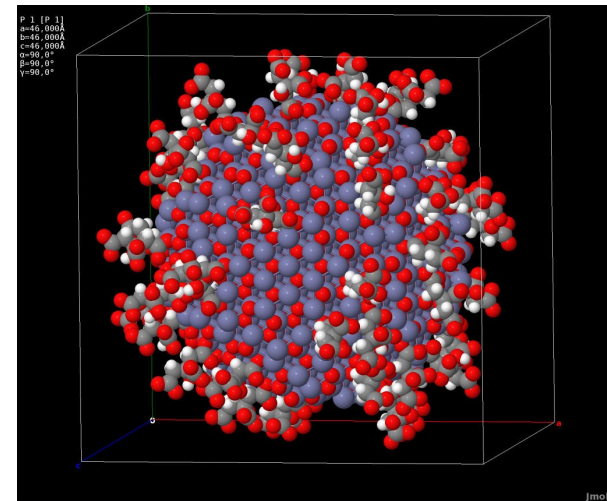
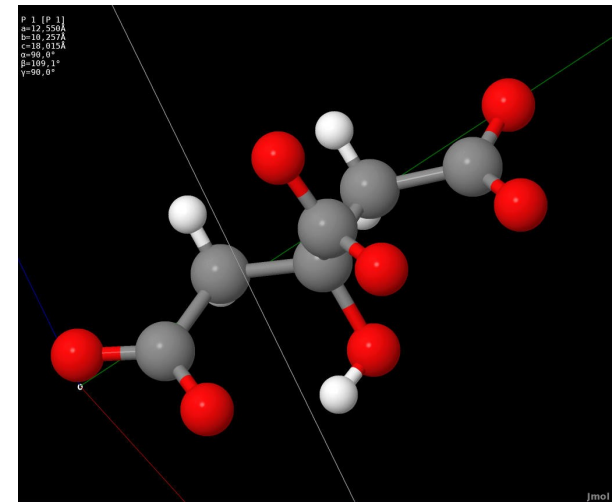


ZnO nanoparticles

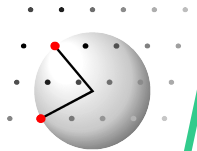
Neutron Pair Distribution Function NPDF, Los Alamos



Neutron data yield interaction
core \rightleftharpoons ligands



ZnO
with organic ligand



Which technique(s) were used ?

Size is a matter of technique

Diffraction

Small Angle scattering

Electron microscopy

Light scattering

What was derived about:
size; structure; defects
core; ligand
chemical composition

Fe - oxide NP as contrast in med. X-ray

Pure oxide is fine

Fe - hydroxide lethal !

What is known about
Physical
Chemical Properties
Biological

Are properties a function of size?

Different from bulk?

