50 years of the Institute of High Pressure Physics Polish Academy of Sciences

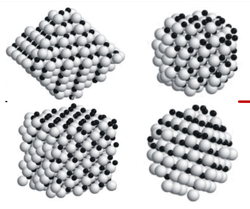
Highlights in III-V semiconductors, THz physics and nanomaterials

Anniversary Symposium „Unipress 50”

Real structure of nanocrystals revealed by diffraction and computer simulations

S. Stelmakh, B. Palosz, K.Skrobas, S.Gierlotka

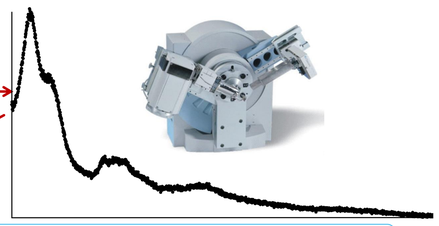
Pair Distibution Function (PDF) crystal structure analysis



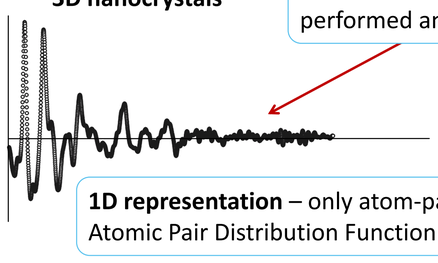
3D nanocrystals

Fourier transform performed by diffraction experiment

Reverse Fourier transform performed analytically



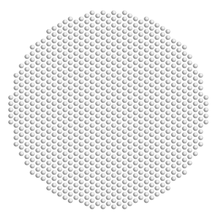
Experimental powder diffraction data



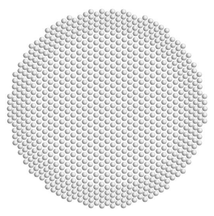
1D representation – only atom-pair distances
Atomic Pair Distribution Function - PDF

Diffraction peaks of nanocrystals are very broad and standard crystallographic tools are not suited for analysis of such data.

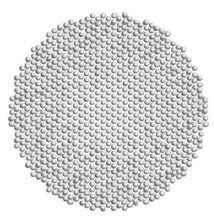
Real atomic architecture of a nanoparticle



A nanocrystal is not just a small perfect crystal !

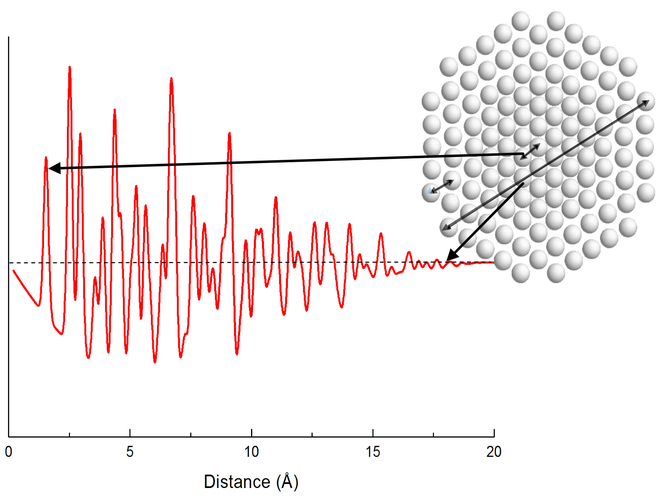


Core and shell model is too simplistic !

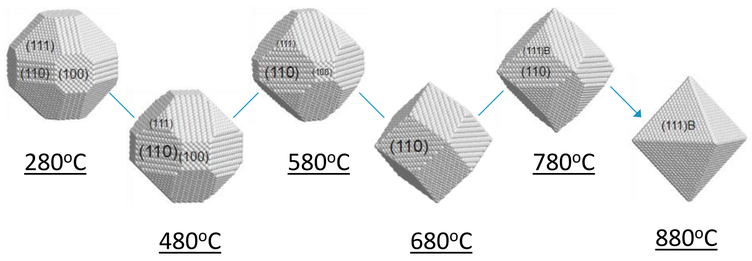


Nanocrystals have complex internal structure !

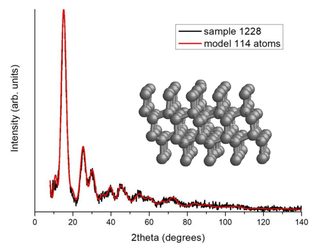
Peaks in Pair Distribution Function corespond to atomic pair distances. Measuring and comparing the short and the long distances one can tell the real structure of a nanocrystal. Relative abundance (peak hights) of various distances gives information on nanoparticle shape.



Diamond nanoparticles [3,4]



Evolution of shape of diamond nanoparticles upon annealig

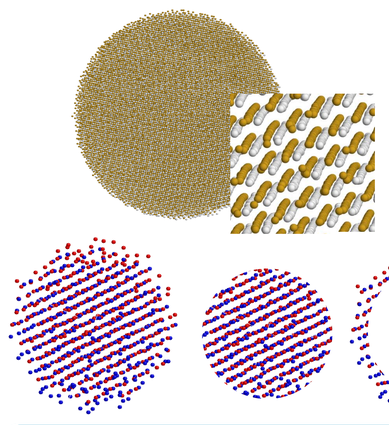


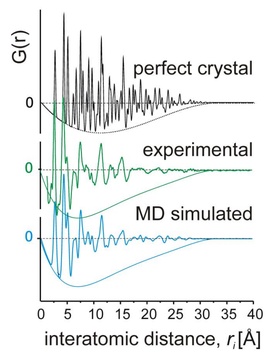
Ultrasmall diamond nanoparticles

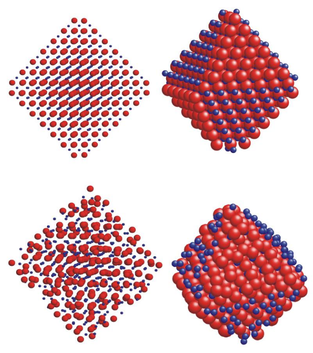
References

1. *S. Stelmakh, K. Skrobas, S. Gierlotka, B. Palosz, Application of PDF analysis assisted by MD simulations for determination of the atomic structure and crystal habit of CdSe nanocrystals, Journal of Physics: Condensed Matter 30, (2018), 345901. https://doi.org/10.1088/1361-648x/aad439*
2. *S. Stelmakh, K. Skrobas, S. Gierlotka, B. Palosz. Effect of the surface on the internal structure of CdSe crystal lattice based on molecular dynamics simulations. Journal of Nanoparticle Research 19,(2017),170.https://doi.org/10.1007/s11051-017-3852-4*
3. *S. Stelmakh, K. Skrobas, S. Gierlotka, B. Palosz, Atomic structure of nanodiamond and its evolution upon annealing up to 1200 °C: Real space neutron diffraction analysis supported by MD simulations, Diamond and Related Materials 93, (2019), 139-149. https://doi.org/10.1016/j.diamond.2019.02.004*
4. *E.A. Ekimov, M.V. Kondrin, S.G. Lyapin, Yu.V. Grigoriev, A.A. Razgulov, V.S. Krivobok, S. Gierlotka, S. Stelmakh, High-pressure synthesis and optical properties of nanodiamonds obtained from halogenated adamantanes, Diamond and Related Materials, 103, (2020), 107718. https://doi.org/10.1016/j.diamond.2020.107718*
5. *S. Stelmakh, K. Skrobas, K. Stefanska-Skrobas, S. Gierlotka, B. Palosz, Distortion of SiC lattice induced by carbon-coating on (100) and (111) surfaces - ab-initio and molecular dynamics study, in press*

Molecular dynamics (MD) simulations [1]





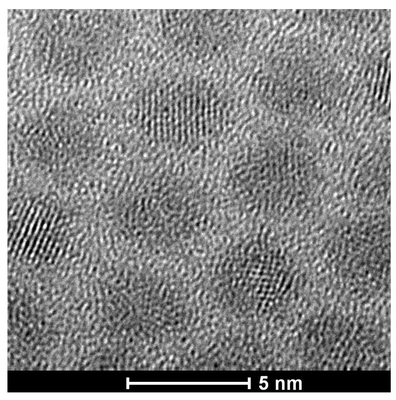


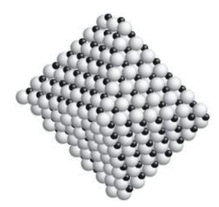
Molecular dynamics allows to propose a realistic model of a nanocrystal.

The surface of the model is altered with respect to the perfect lattice and the change propagates into the bulk.

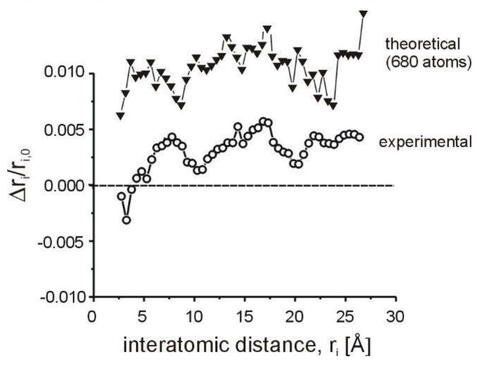
PDF functions calculated for MD models show excelent agreement with experimental data.

CdSe nanoparticles - quantum dots [2]



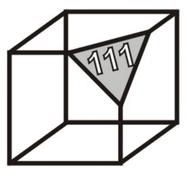


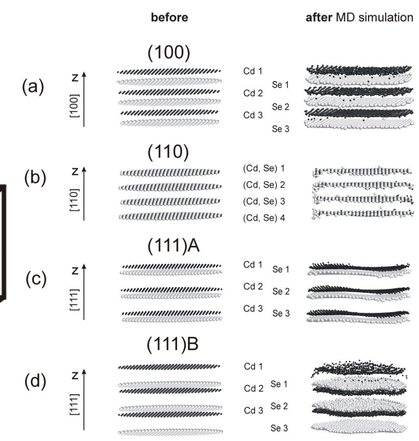
Differential interatomic distance function



PDF analysis suported by MD simulations show that CdSe quantum dots have octahedral shapes, which is not apparent from TEM images.

Molecular dynamics indicates various degrees of ordering depending on the orientation of the surface terminating the nanocrystal.

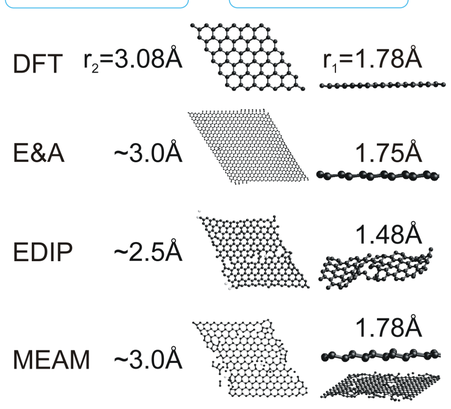




SiC nanoparticles [5]

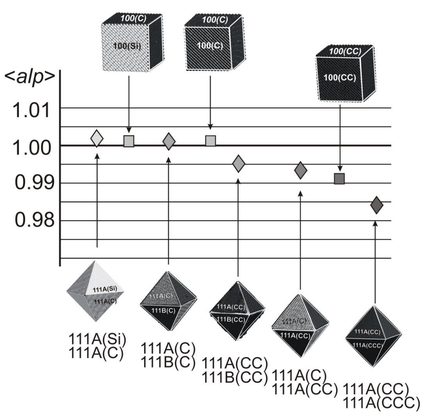
MD potential

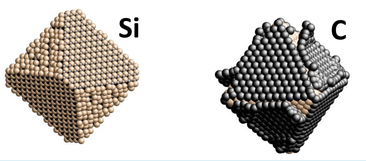
Surface layers



Extra carbon atoms on silicon carbide surface arrange into graphene-like sheets.

Apparent lattice parameter





Carbon coverage compresses SiC nanocrystals – average lattice parameter decreases.

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