NanoPDF - computer program to simulate and analyse the Pair Distribution Function of nanocrystals

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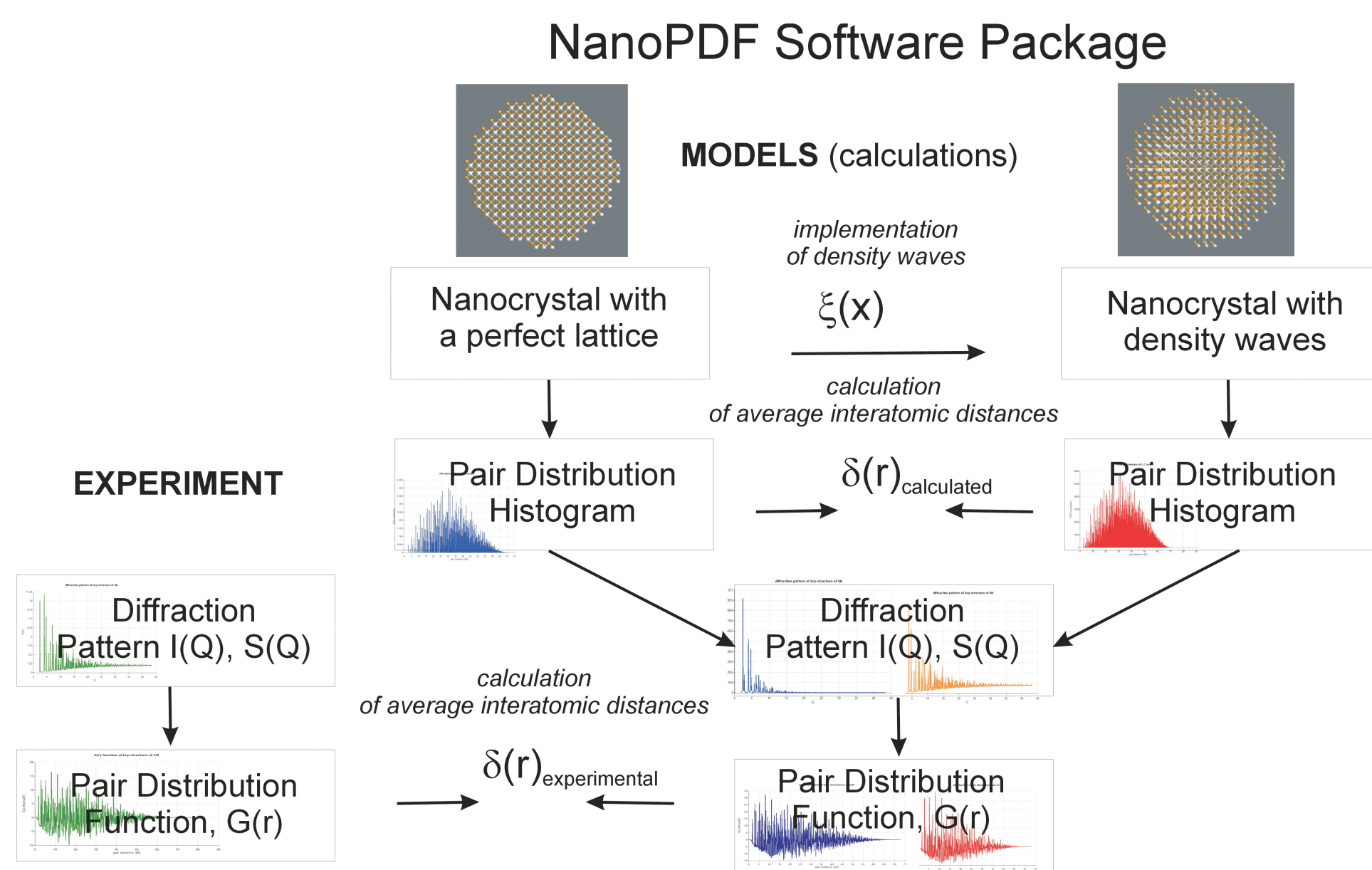*http://www.unipress.waw.pl/soft/crystallography/nanopdf/ e-mail: kskrobas@unipress.waw.pl*

Fig.1 Flow diagram of NanoPDF functionality

Fig.2 NanoPDF main window and models of nanocrystals

Fig.3 Experimental pattern of ZnO nanocrystals and calculated pattern of 8x2.4nm ZnO platelet

NanoPDF basic modelling functionality:
- Create atomistic model of a nanocrystal: sphere, rod or plate
- Call an external program (RasMol or RasTop) to display the model built
- Count and sort atomic pairs and calculate a Pair Distribution Histogram - PDH
- Using Debye formula calculate powder diffraction pattern **I** and a structure function **S**
- Display PDH(r), I(2Θ), I(Q), S(Q)
- Calculate the Pair Distribution Function G(r) by a Fourier transform of either self-calculated or user-supplied, e.g. experimental, S(Q)
- Model thermal motion either by random displacement of atoms from their equilibrium positions or by applying e^{-2M} factor during pattern calculation

Fig.4 Pair Distribution Histograms without and with thermal displacements of atoms - 8nm Si nanocrystal

NanoPDF advanced modelling functionality:
- Modify a model of a nanocrystal with a perfect lattice to introduce concentric shell-like sections with altered atomic density - a density wave
- Calculate the effect of the density wave on the postions of the peaks in the G(r) curve -the δ(r) function

Fig. 5 Diffraction patterns vs. 2Θ and Q and structure function S(Q) - 8nm Si nanocrystal

NanoPDF data analysis functionality:
- Define an analytical approximation of G(r) function of a nanocrystal of a given crystal structure, size and shape
- Fit an analytical form of G(r) to the user-supplied, experimental G(r).
- Fit experimental G(r) in small r-ranges to determine the deviation of the average interatomic distances from the case of perfectly periodic crystal lattice - the experimental δ(r) function

Fig. 6 Model modification panel - introducing thermal motion and density waves.

Fig. 7 Calculated diffraction data without and with random atom displacements

Structures available for modelling:
- Monoatomic: simple cubic, bcc, fcc, hcp, diamond-like e.g. metals, Si, diamond
- Biatomic: zinc blende, hcp perfect or including stacking faults e.g SiC, ZnS, GaN, CdSe, other II-VI and III-V semiconductors

Fig. 8 Models of nanocrystals: perfect, with a surface shell, with a density wave

Graphing capabilities:
- Built-in libraries for 2D plotting
- Display self-calculated and external x-y data
- Overlay multiple data sets in a single plot for comparison
- Scale incompatible data sets to common maximum intensity
- Linear or logarythmic y-scale
- Choice of lines, symbols and colors for data display
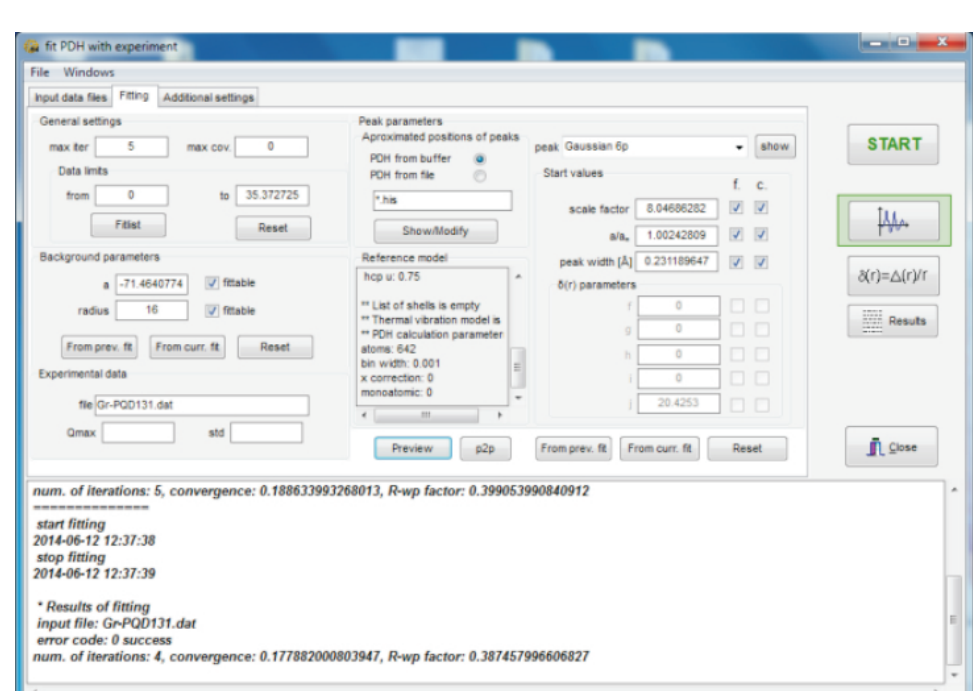- Zoom-in

Fig. 9 G(r) for a perfect nanocrystal and the one with a density wave. The curvie in the middle calculated in NanoPDF shows expected difference in the peak positions
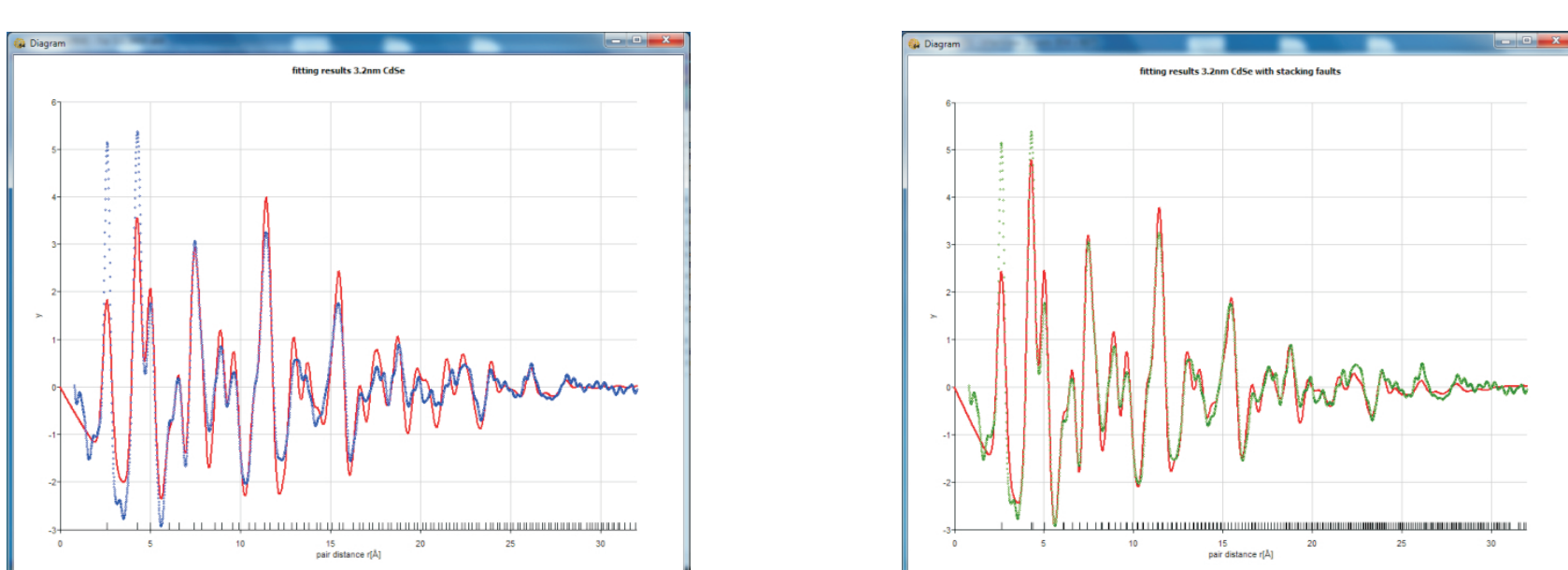

Fig. 10 Main window of the fitting section of NanoPDF

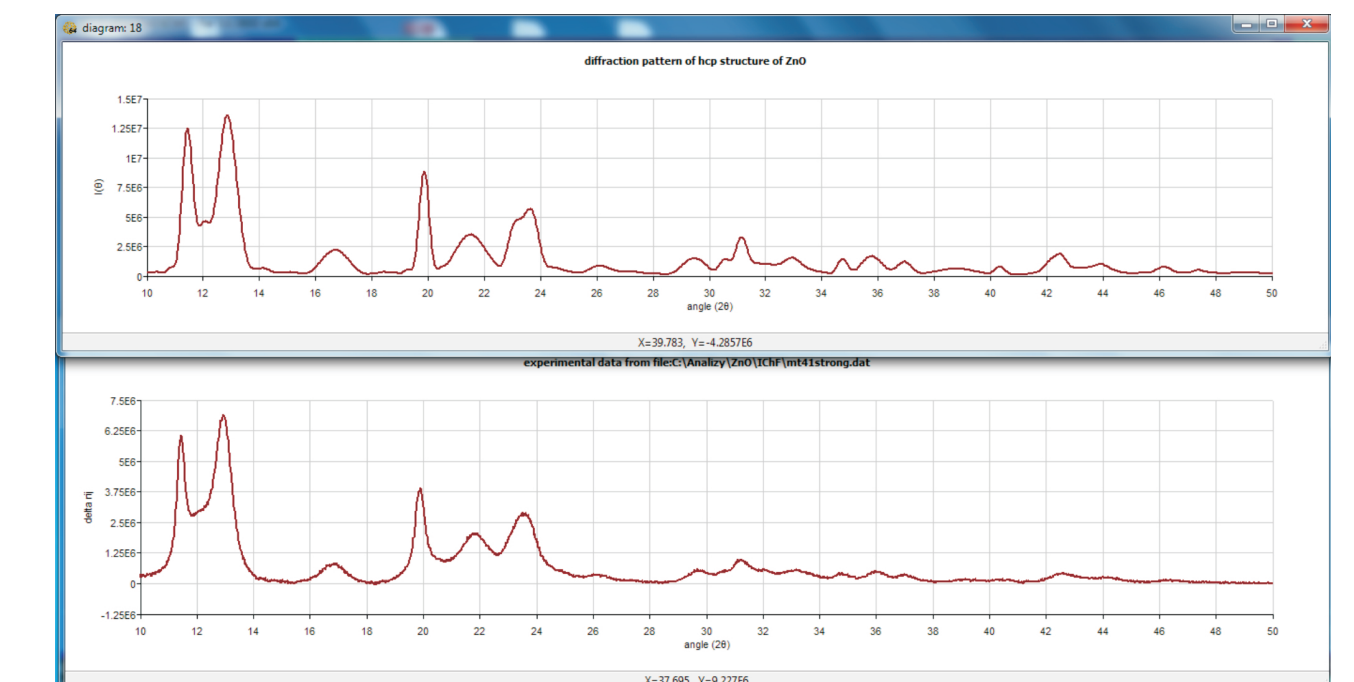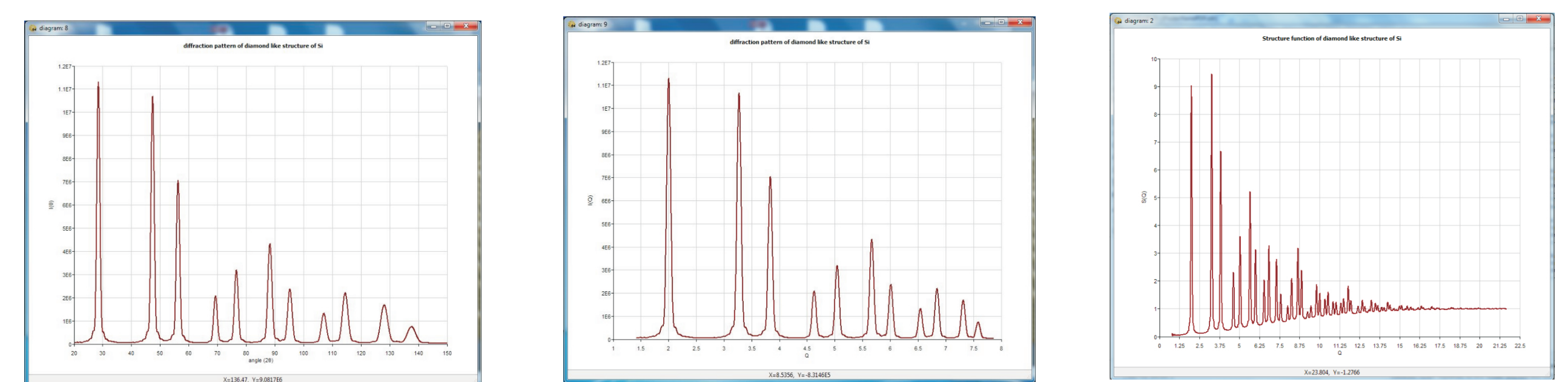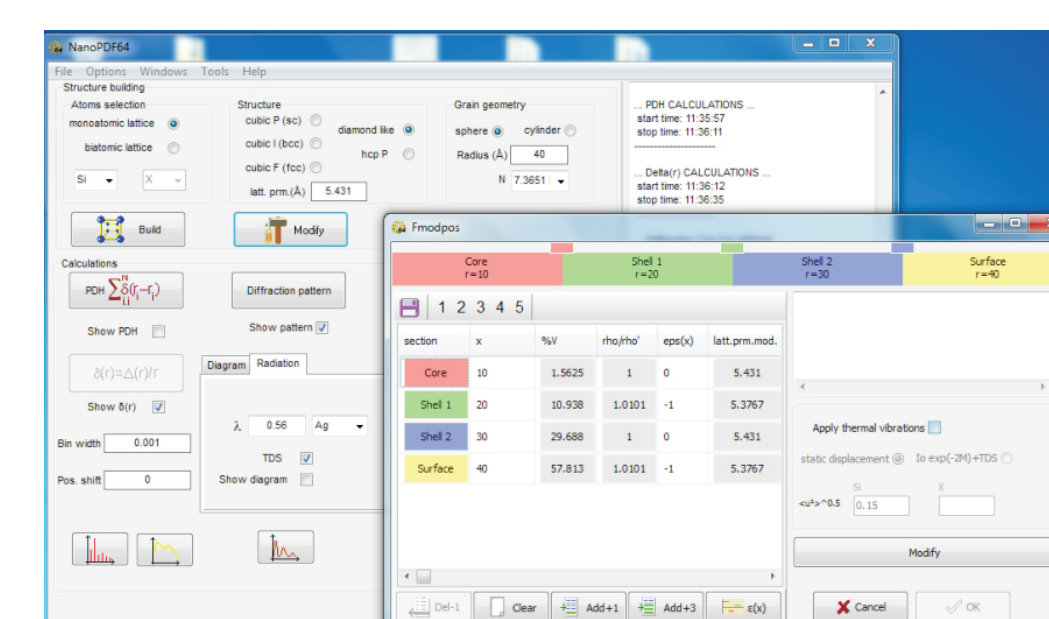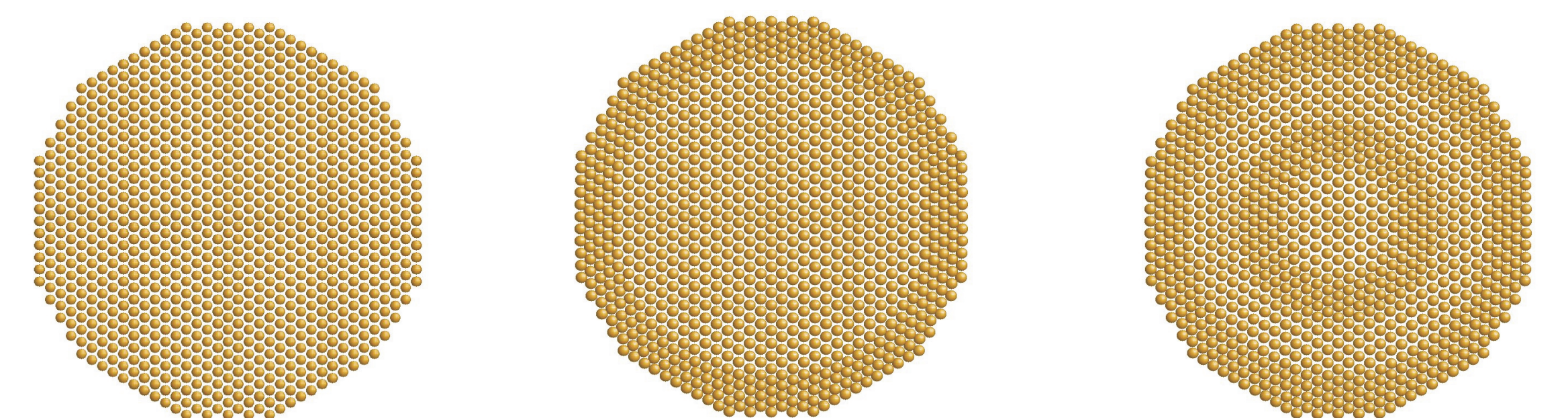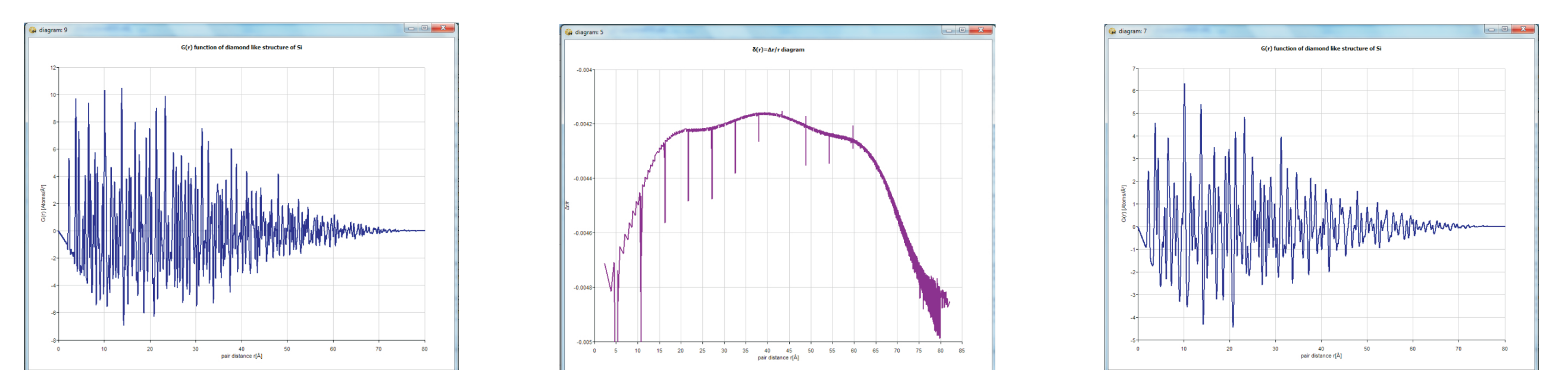Fig. 11 Experimental G(r) of CdSe quantum dots fitted with a model G(r) for a 3.2 nm nanocrystal with a perfect lattice and a model with 15% stacking faults