Figure 1. The XRD patterns: experimental (grey) and simulated (black) using structural models containing O layers (MgO) and OT ones (spinel) with OT concentration: a) 0, b) 0.1, c) 0.2 and additional SFs with probability: d) 0.15, e) 0.30. Squares and circles show first and second peaks of diffuse scattering.

Keywords: diffuse scattering, disorder

Analysis of short range phenomena in two novel materials using the PDF-method

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In the present contribution the results of our radial distribution (RDF) studies on partial crystalline or amorphous materials will be presented. Radial distribution functions give information on the occurrence of all atom-to-atom distances in the substance. Out of the intensity of their maxima one can read out details on the number of distances, out of their widths their distance variations.

In one case the modelling of the structural disorder in silicon-nano-particles with intended application as novel battery anode materials is covered. As these studies are performed on powders, simulations have to take into consideration all effects originating from the particle-ensemble like the distribution of particle size and shape. Together with the data of small angle scattering (SAXS) measurements, models of those materials are presented.

The second class of compounds are host-materials for organic-light-emitting-diodes (OLEDs). Host materials are applied as amorphous films and a comparison of the PDFs of crystalline and amorphous structure gives insight into the structural changes due to amorphisation. It is assumed that torsions induced by sterically demanding groups are correlated with electronic properties.

Keywords: short range analysis, models of disorder, partially amorphous materials, diffuse scattering