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MS39-O4

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

Philipp Hans[1], Reinhard B. Neder[2], Klaudia Hradil[1]

1 .X-ray center - TU Wien, Vienna, Austria
2. Crystallography and structural physics - Friedrich-Alexander Universität Erlangen-Nürnberg, Erlangen, Germany

email: philipp.hans@tuwien.ac.at

In the present contribution, we will show results and further progress in analysis of pair distribution function (PDF) studies on amorphous materials containing crystalline domains. The materials are of stoichiometry $(SiO_2)_x(TiO_2)_y$. - The synthesizers' ([1]) aim was to prepare a material that is similar to the zeolithe TS-1 (titanium silicalite), which exhibits catalytic properties (eg phenol hydroxylation) but is amorphous and thus mechanical more stable. - The focus of this work is not on catalytical activity but on structural features.

A big research question concerns the coordination number of the Ti-atoms with respect to oxygen. Extensive studies (Rietveld analyses and neutron scattering using isotope substitution) have been done on TS-1 (see [2]). Literature states that 4-fold coordination is necessary for the material to exhibit catalytic properties and that incorporation of Ti-atoms into the bulk-SiO_2, thereby substituting Si, happens only at low Ti-contents ([3]). The origin of catalytic properties of TS-1 is still an open topic and no consesus has been reached in literature.

The experimental PDF could be modelled with a contribution by amorphous SiO_2 and small spherically shaped crystalline TiO_2-particles in the Rutile modification, i.e. Ti in six-fold coordination. A model based on a pure glass phase with Si partially substituted by Ti in four fold coodinatikon did not result in as good an agreement. The features in the difference PDF indicate interaction between the particles and the surrounding matrix. TEM and SAXS measurements indicate a structure of elongated pores, but due to electrostatic charging in the TEM no magnification sufficient for the detection of the small TiO_2 particles could be achieved.

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