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From an X-ray diffraction [1], the lattice constant of diluted magnetic semiconductor $Zn_{1-x}Mn_xTe$ linearly changes with varying x (Vegard's law), while an XAFS results [2] showed almost unchanged Mn-Te and Zn-Te bond lengths (Pauling's rule). This discrepancy led to a question of how the large the large $MnTe_4$ tetrahedra can be squeezed into the small $ZnTe_4$ lattice.

X-ray fluorescence holography (XFH) is a new technique that allows one to investigate a three-dimensional local image around a specific element. The sample was irradiated by intense X-rays of certain energies beyond the Mn K absorption edge at BL37XU/SPring-8 in order to obtain the Mn K_α fluorescence hologram [3]. A three-dimensional atomic image around the Mn central atoms was derived from the hologram using Barton's algorithm. The nearest- and third-nearest-neighbour Te atoms were clearly visualized. However, the second-nearest-neighbour Zn or Mn atoms are barely visible in this image due probably to a highly distorted cation Zn(Mn) sub-lattice.

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Keywords: three-dimensional image reconstruction, X-ray fluorescence spectroscopy, magnetic semiconductors

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Investigation of $LaMn_{2-x}Fe_xSi_2$ ($0 \le x \le 1.2$) by Magnetic Measurements and Neutron Diffraction

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The various magnetic structures and phase transitions in the $LaMn_{2-x}Fe_xSi_2$ system have been thoroughly studied by X-ray powder diffraction, magnetic measurements and powder neutron diffraction. The substitution of Fe for Mn leads to a decrease in the lattice parameters and the magnetic interactions in the Mn sublattice cross over from a ferromagnetic character to an antiferromagnetic one. The magnetic structures of the $LaMn_{2-x}Fe_xSi_2$ compounds with x = 0.2, 0.475, 0.5, 0.7 and 1.0 have been determined between 2 and 450 K by neutron diffraction. A typical $SmMn_2Ge_2$-like magnetic behavior is observed for the x = 0.475 sample. The magnetic phase transition from ferromagnetism to antiferromagnetism for this sample occurs at the *intra*layer Mn-Mn distance $d_{Mn\text{-}Mn}$ = 2.89 Å. This value exceeds the well known corresponding threshold value $d_{Mn\text{-}Mn}$ = 2.87 Å in the pure Mn RMn_2X_2 compounds [1-2]. The results are summarized in the $LaMn_{2-x}Fe_xSi_2$ magnetic phase diagram [3].

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Keywords: rare-earth manganese silicides, layered structure, neutron diffraction

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Structural Reasons for the Giant Oxygen Isotope Effect in $Re_{0.5}Sr_{0.5}MnO_3$ Perovskites

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The giant oxygen isotope effect (a metal-insulator transition induced by ^{16}O for ^{18}O substitution) has been recently discovered in $Sm_{1-x}Sr_xMnO_3$ compound for x close to 0.5 [1]. We performed a neutron diffraction study for elucidating structural reasons of this transition. Both crystal and magnetic structures have been determined for several compositions with Re=Sm and ($Nd_{1-y}Tb_y$), y=0.228 and 0.456. These particular (Nd/Tb) ratios were chosen to model the average ionic radii of Sm and ($Sm_{0.5}Nd_{0.5}$) compositions respectively. In all studied samples the coexistence of ferromagnetic-metallic (FMM) and antiferromagnetic-insulating (AFMI) phases has been found at low temperature. From structural point of view both phases have the same *Pnma*-type structure but with strong difference in lattice parameters. The $d(x^2\text{-}y^2)$ orbital ordering in A-type AFMI phase leads to the huge shortening of Mn-O1 distances (≈1.2%) (as well as of b lattice parameter) and stimulates strong intragranular strains, which stabilize phase separated state. The same situation, though with different type of magnetic and orbital ordering in AFMI phase, has been found in LPCM-y type manganites, which also exhibit the giant oxygen isotope effect [2].

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Keywords: manganites, neutron diffraction, isotope effect

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X-ray Study of the Native Solid Hydrocarbons Transformation

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The subject of our investigation the native hydrocarbons (bitumens), which we defines as organic compounds with a primarily hydrocarbon basis. In the structural relation bitumens are characterized by the supermolecular organization with the sizes of elements from tens nanometers up to micron. The X-ray method opens new possible in the diagnostics of complex systems, using as numerical index a graphitization degree (Sg), which allows to diagnose as well as follow the dynamics and transformation mechanism of bitumens in the carbonization series: asphalt – asphaltite – kerite – anthraxolite – graphite.

The purpose of the research work is to study X-ray transformation of bitumens on the supermolecular level. The X-ray spectrum of bitumens of different transformation stages consist of two basic reflection 0.48 and 0.38 nm corresponding to the hydrocarbon polynaphtenic phase (N_f) and an amorphous graphite-like phase (G_f). The concentration of the latter increase with the growth of the catagenetic transformations degree. That is a final transformation product of natural bitumen is graphite. This testify to the single ransformation mechanism of natural bitumens. Thus, the X-ray methods allow to determine the genetic type of native organic substances and establish the catagenetic transformation level of the organic substances.

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Keywords: X-ray diffraction and structure, hydrocarbons, nanostructures

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The Influence of Synthesis Conditions on the Packing of the Spherical Particles of Silica in a Supramolecular Structure

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As a result of the conducted experiments on the synthesis and precipitation of monodisperse spherical silica particles (100-800 nm) in different conditions we have determined a direct relationship between the packing type of particles and pH, water concentration,