

ABSORPTION IN A SELF-CONSISTENT MODEL OF X-RAY SCATTERING

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Absorption is approached as a local and statistical event, taking place in contrast with a background of global and strictly determined pattern of X-ray scattering. While a detailed physical mechanism of the absorption phenomenon is considered irrelevant here, the main attention is given to the overall effects of absorption on the proposed earlier self-consistent model of X-ray scattering. In this model, we substitute a single dipole used in the original Ewald's papers by the plane of continuously distributed planes of dipoles, but we maintain his self-consistency principle as the main factor determining the entire scattering process. New aspects, diverging present approach from the commonly used, are following. Absorption takes place exclusively at the electron sites arranged in a set of dipole planes. The flux of photons incident on each dipole plane is divided into two branches. The first one, which suffers unknown frequency changes, is considered here redundant. It is defined by an introduced probability factor, separately given for each dipole plane. It can be proportional to the first or second power of the local EM intensity and defines the number of photons lost for diffraction event. The second branch is that of the unchanged wavelength. It is scattered under an exact satisfaction of Ewald's self-consistency principle and produces the same overall scattering as for non-absorbing crystals. It preserves conservation of energy for the not-absorbed portion of photons. Absorption and refraction in this model of scattering are distinct phenomena.

Keywords: DYNAMIC THEORY, SELF-CONSISTENCY, ABSORPTION**X-RAY AND NEUTRON DIFFRACTION STUDIES OF THE DINOSAUR AND MODERN ANIMAL BONES FROM THE GOBI DESERT, MONGOLIA**Sangaa Deleg¹ Balagurov Anatoly² Batdemberel Ganbat¹ Chultem Darjaa¹ Fuess Harmut³ Toebbens Daniel⁴

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The crystal structure of the dinosaur and modern bones were studied by X-ray diffraction and neutron diffraction. The dinosaur's bones were found in the Gobi desert, Mongolia. Fossil bones and modern bones mainly consisted of hydroxylapatite as the primary phases and of calcium oxide as the secondary phase. X-ray, high resolution and TOF neutron powder diffraction data were used to compare the crystallographic changes of fossil and modern bones. Neutron diffraction data analysis allows to determine hydroxyl anion contents in the phase. Crystal phases in those bones have been showed identical structure (in homology). The results of the investigations could be important for natural sciences, such as, evolution in biology and geology. In this work, however, we associate the notion of homology with identical crystal structure of different objects. The neutron and X-ray diffraction method has been used in study of bones for identifying crystal structure and evolution of mineral materials. With use of X-ray diffraction and neutron methods, it was shown that a dinosaur bone has a multiphase system, which in general consists of hydroxylapatite and different modifications of carbonate calcium: calcite, aragonite and vaterite. Our research aimed to clarify the matter of existence or absence of homology in a bone crystal structure of dinosaur and different animals, since possibility for comparative study of differences in molecular structure of dinosaur's and animal's organisms are very limited.

Keywords: X-RAY AND NEUTRON DIFFRACTION, CRYSTAL STRUCTURE, ANIMAL BONES**DETERMINATION OF THE β -QUARTZ CELL PARAMETERS USING NMD AZIMUTHAL ANGULAR DIFFERENCES**L. C. Campos¹ C. B. Ramos Parente² V. L. Mazzocchi² O. Helene³

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In a previous work, the absolute azimuthal angular positions (ϕ -positions) of some selected peaks of an experimental 00.1 Umweg neutron multiple diffraction (NMD) pattern, measured at 1003 K, were used for the determination of the β -quartz cell parameters. In this work it is a set of azimuthal angular distances between peaks that is used for the same purpose. Clearly, each selected peak can be combined with the (n-1) other selected peaks. For a better precision in the results it was preferred to combine peaks with opposite behaviors. That is to say, for a variation of the parameter being determined, a peak that has changed its ϕ -position towards a certain direction in the pattern is combined with another peak that moved along the opposite direction. A selection of pairs was done taking into account both behavior and sensitivity of the peaks to the parameter variation. The selection resulted in 36 and 71 pairs for the determination of c and a, respectively. An iterative method, similar to that used in the previous work, has been used in order to attain a better accuracy in the results. After 6 cycles of iteration, the process converged to a = 4.99643 (\pm 0.00057) Å and c = 5.46116 (\pm 0.00044) Å. Comparing these results with those of the previous work, namely a = 4.9957 (\pm 0.0014) Å and c = 5.46184 (\pm 0.00035) Å, one can observe that at least there was an improvement in the accuracy of a the error becoming of same magnitude as that of c.

Keywords: NEUTRON MULTIPLE DIFFRACTION CELL PARAMETERS β QUARTZ**NEUTRON POWDER DIFFRACTION STUDY OF THE MIXED-VALENCE MANGANITES**

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Complete structural determination of the $\text{Pr}_{1-x}\text{Na}_x\text{MnO}_3$ ($x = 0.025, 0.05, 0.075$ and 0.20) have been investigated by the powder neutron diffraction. The diffraction patterns were taken at $\lambda = 0.1362$ nm over a range of $2\theta = 5.5 - 67^\circ$ in steps of 0.1 at the room temperature and 7 K. In order to achieve more significant lattice parameters in the course of the charge ordering transition in the $x = 0.2$ sample, an additional X-ray diffraction measurement has been performed in low temperatures down to 80 K. Similarly to related systems with divalent alkali earths, the increasing monovalent sodium substitution in $\text{Pr}_{1-x}\text{Na}_x\text{MnO}_3$ decreases the Jahn-Teller deformation of the MnO_6 octahedra, lowers the resistivity and changes gradually the magnetic ordering from the layered type antiferromagnetism ($x = 0$) through canted arrangements ($x = 0.05$) to the pure ferromagnetism ($x = 0.10-0.15$) with $T(c) = 125$ K. The samples with the ferromagnetic ground state are not metallic below $T(c)$ but show appreciable magnetoresistive effects in a broad temperature region. The electronic localization at low temperatures is further enhanced in sample with the maximum sodium content $x = 0.2$ (actually 36% Mn^{4+}). The electron and neutron diffraction evidences that $\text{Pr}_{0.8}\text{Na}_{0.2}\text{MnO}_3$ exhibits a commensurate charge and orbital ordering of the $\text{Mn}^{3+}/\text{Mn}^{4+}(1:1)$ kind below $T(c) = 215$ K, followed with a transition to the antiferromagnetic arrangement of pseudo-CE type at $T(N) = 175$ K, analogous to that of previously studied $\text{Pr}_{0.65}\text{Na}_{0.35}\text{MnO}_3$. In addition, the present compound $\text{Pr}_{0.8}\text{Na}_{0.2}\text{MnO}_3$ undergoes below 50 K a spin reorientation and, simultaneously, ferromagnetic clusters in the charge ordered matrix are formed.

Keywords: NEUTRON DIFFRACTION, PEROVSKITES, STRUCTURAL REFINEMENT