before.

In this report the results of structural studies of phase transitions in $KNbO_3$ powder specimens are presented. For preparation of $KNbO_3$ samples with different sizes of ideal crystal structure (crystallites or blocks) different synthesis conditions is used. The study of $KNbO_3$ phase transitions using X-ray difractometer DRON-3M (CuK_α radiation) and special temperature cell at $20 \leq T \leq 960°C$ is made.

It is found that the decrease of coherent scattering areas below critical size (50 nm) lead to reduce of phase transition temperatures. It is established that there are strong changes of atomic positions and thermal parameters at these temperatures.

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Keywords: perovskites, phase transitions, nanocrystals

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Substitution of Manganese by Iron or Gallium in Electron-doped Manganites

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We investigate the temperature-dependant evolution of the magnetic moments in electron-doped manganites ($Y_{0.1}Ca_{0.9}MnO_3$, $Y_{0.15}Ca_{0.85}MnO_3$) $Y_{0.1}Ca_{0.9}MnO_3$ shows mainly G-type antiferromagnetic ordering with a Néel temperature of 110K and a minority ferromagnetic phase with an identical ordering temperature. For higher Yttrium concentrations as in $Y_{0.125}Ca_{0.875}MnO_3$ and $Y_{0.15}Ca_{0.85}MnO_3$ an additional phase develops with monoclinic nuclear space group $P2_1/m$ and C-type magnetic ordering, leading to a phase separated state below a magnetic phase transition temperature of approximately 160K.

The substitution of Manganese by other trivalent ions influences the temperature-dependant behaviour of this phases. For $Y_{0.1}Ca_{0.9}MnO_3$, Ga reduces the phase transition temperatures, while Fe reduces the Ferromagnetic intensities. Fe retains this behavoir for higher concentrations of Yttrium while Ga changes additionally the phase fractions of the G- and C-type phases.

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Keywords: magnetic perovskite materials, magnetic phase transitions, magnetic structures

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Dynamic Phase Transition of the Charge-density Wave Lattice

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The dynamic behaviour of the periodic media with lattice imperfections is ubiquitous and long-standing problem in many condensed material systems, because of the correlation to the unusual physical phenomena, for instance, the charge-density waves/spin-density waves to the nonlinear conductivity, the charge/spin stripes to the CMR and the high-T_C superconductivity, and the vortex lattice to superconductivity. In static systems, the imperfections in a medium result in a disordered ground state which prevents the system from forming a long-range order at low temperatures, therefore giving rise to unusual physical properties. In dynamic systems under a driving force, the disordered medium produces a more fascinating phase diagram. Analogous to the vortex lattice, the inhomogeneous distribution of charge densities also forms a periodic lattice below the transition temperature, namely charge-density waves (CDWs). Combining x-ray scattering and multiple diffraction, we demonstrate that the CDW lattice can be driven by a driving force to move and undergo a dynamic phase transition, i.e. from the disordered pinning state → ordered moving solid state → disordered moving liquid, and the nonlinear conductivity occurs through a phase jump of 2π.

Keywords: charge-density wave, phase transition, X-ray scattering

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Phase Transitions in Tetrachlorobenzene Studied by Neutron Powder Diffraction

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Polymorphism and phase transitions are a major issue in the understanding of the organic solid state. The 'Control and Prediction of the Solid State' (CPOSS) project[1] aims to increase our understanding of the polymorphic state using detailed screening to discover 'all' polymorphic forms and solid state phases combined with cutting edge experimental studies and computational studies.

Two polymorphs of tetrachlorobenzene have been reported[2-4]; the room-temperature β form ($P2_1/n$), and a low-temperature α form (P-1), with the phase change occurring at approximately 170K.

The nature of the phase transition, as well as the structure of the two polymorphic forms, has been investigated using the complimentary crystallographic techniques of single-crystal X-ray diffraction and neutron powder diffraction. In particular, the effect of temperature on the lattice parameters is considered, providing insights into the nature and mechanism of the phase transition.

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Keywords: neutron powder diffraction, polymorphism, phase transitions

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Polyhedral Compressibilities Drive Structural Phase Transitions in Perovskites

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Recent advances in laboratory based single-crystal techniques for measuring the intensities of diffraction from crystals held at high pressures in the diamond-anvil cell have been used to determine the role of polyhedral compression in the response of the ABO_3 perovskite structure type to high pressures. All perovskites studied exhibit compression of the BO_6 octahedra. We have been able to show that when the BO_6 octahedra are less compressible than the AO_{12} sites the octahedra become more tilted with increasing pressure [1]. In such perovskites there are no structural phase transitions to high-symmetry structures.

When the BO_6 octahedra are more compressible than the AO_{12} sites the structure becomes less tilted and evolves towards a higher-symmetry configuration [2]. Thus $LaGaO_3$ undergoes a Pbnm to R-3c transition with first-order character at approximately 2.5 GPa at room temperature. The structural evolution of $LaAlO_3$ has been followed in the R-3c phase before its transition to Pm3m at about 14GPa [3].

We have also developed a new model, based on the bond valence concept, that successfully predicts the relative compressibilities of the cation sites in most oxide perovskites [4] and hence their response, including phase transitions, to pressure.

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