

MS01.07.03 DYNAMICAL AND STRUCTURAL STUDIES OF FERROELECTRIC SALTS. A.V. Belushkin, Frank Laboratory of Neutron Physics, JINR, 141980 Dubna, Russia

In many ferroelectrics, structural transformations at phase transitions are accompanied by significant changes in lattice dynamics. Often the microscopic mechanism of phase transitions can be understood only on the basis of a simultaneous analysis of both structural and dynamical data. Recent results obtained by neutron diffraction, as well as inelastic and quasielastic neutron scattering will be reviewed.

1. KH_2PO_4 (KDP) is an extensively studied crystal which undergoes a ferroelectric phase transition at 122K ($I42d \rightarrow Fdd2$). Pressure reduces the transition temperature and above 17 kbar, KDP remains paraelectric down to 0K. The inelastic neutron scattering spectra measured from KDP at 20K at ambient pressure and at 20 kbar reveal dramatic changes in the lattice dynamics. These changes will be discussed together with the published structural data obtained at different pressures.

2. When KDP is mixed with $\text{NH}_4\text{H}_2\text{PO}_4$ (ADP), which undergoes an antiferroelectric phase transition at 148K, the ferroelectric transition temperature rapidly decreases. In the concentration range $0.2 \leq x \leq 0.8$, the $\text{K}_{1-x}(\text{NH}_4)_x\text{H}_2\text{PO}_4$ mixed crystals and their deuterated analogues show neither a ferro- nor antiferroelectric transition. At low temperatures, they reveal properties characteristic of a proton dipolar glass. Using neutron diffraction on a deuterated mixed powder ($x \approx 0.6$), structural changes were studied in the temperature range from 290K to 5K. At 5K, profile refinement was performed and revealed very unusual structural features. Structural anomalies observed in the temperature dependence will be discussed, together with the quasielastic neutron scattering data.

3. Structural and dynamical studies of $(\text{CH}_3)_2\text{NH}_2\text{Al}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ which undergoes a ferroelectric phase transition at 152K, will also be discussed.

MS01.07.04 NEUTRON SCATTERING INVESTIGATIONS OF THE DYNAMICS OF THIN FILMS ADSORBED ON SOLID SURFACES. J. Z. Larese, Chemistry Dept., Brookhaven National Laboratory, Upton, NY 11973, USA

High-resolution inelastic and quasielastic neutron scattering (INS) techniques are ideal probes of the dynamical properties of films adsorbed on solid surfaces. When these dynamical measurements are combined with data from structural, thermodynamic and computer simulation studies it is often possible to develop a rather complete picture of the microscopic properties of an adsorbed film system. In order to illustrate the power of INS techniques we will discuss several prototypical examples. In particular, the continuous melting of monolayer ethylene and the layer-by-layer melting of multilayer argon films on the basal plane of graphite and the rotational tunneling of methane films on the (100) surface of MgO. Some indication of how these studies might be used in the investigation of surface mediated chemical reactions will also be provided. This research was performed under the auspices of the U.S. Dept. of Energy, Material Science Division, under Contract # DE-AC02-76CH00016.

MS01.07.05 THE NATURE OF METHANE/RARE GAS MATRICES. B. Asmussen, Institut fuer Experimentalphysik der Universitaet Kiel, Olshausenstrasse 40, D-24098 Kiel, Germany

Methane molecules as substitutional impurities in rare gas crystals have become model systems for the investigation of rotational excitations of quantum rotors in cubic orientational potentials close to the limit of free rotation. The variation of the rare gas host matrix (neon, argon, krypton, xenon) allows for a variation of the strength of the potential. Inelastic neutron scattering (INS) is a powerful tool to obtain informations about this class of systems because the rotational spectra are a sensitive probe of the local symmetry of the rotor and the scattered intensities as function of momentum transfer Q provide a direct access to the wave function of the scatterer. Due to complete miscibility, the CH_4 /krypton system enables a systematic study of the concentration dependence of the INS spectra, whereas the CH_4 /neon system is an example for strong mismatch of host and guest. Additional information may be obtained by isotopic substitution. Rotational excitations are very sensitive to the scaled potential V/B (B being the rotational constant) and the tunnel splittings may change over several orders of magnitude on deuteration. A systematic study of the isotope effect with the partially deuterated methanes $\text{CH}_n\text{D}_{(1-n)}$ in argon and a description of the INS measurements by a model based on completely free rotation will be presented.

MS01.07.06 HIGH RESOLUTION NEUTRON SPECTROSCOPY OF BIOLOGICAL MATERIALS A. Deriu - Dipartimento di Fisica, and Unità INFN, Università di Parma, 43100 Parma, Italy

Biological materials at a molecular level are heterogeneous systems: they are made up from a heteropolymeric skeleton (polynucleotides, polypeptides, polysaccharides) or from complex multilayered sheets (lipid membranes) in interaction with an aqueous buffer. Water plays a major role in stabilising the large scale arrangement (ternary and quaternary structures) of biomolecular assemblies and controls the activation of most biological processes. It is precisely this 'composite' nature combining the high degree of mechanical stability of the solid biopolymer scaffolding with the liquid-like behaviour of the buffer, which accounts for the enormous structural and functional diversity of biomolecules.

Not only structure but also motion is of great importance at the molecular level of biology. The marked temperature dependence of the activity of biomolecules reflects their thermal mobility. A characterization at a microscopic scale of processes and interactions responsible for molecular flexibility and dynamics is a necessary starting point for a deeper understanding of the mechanisms which control the highly specific functions of most biological materials. Dynamical events in biomolecular systems occur on a very large time-scale ranging from femtoseconds to almost seconds. Within this interval, motions occurring in the picosecond to nanosecond time-scale are of particular interest and relevance since they cover the transition region from 'discrete' local excitations of small molecular subunits to slower processes involving co-operative motions of massive parts of the macromolecular assembly. This time window is well covered by inelastic and quasielastic neutron scattering, these techniques can therefore play a relevant role in improving the understanding of molecular motions which affect the functionality of biomolecules.

Neutron high resolution spectroscopic studies of biomolecular dynamics have been pursued actively in the past fifteen years. As a result of instrumental advances and progresses in molecular dynamics simulations it is nowadays possible to describe quantitatively the complex low frequency motions exhibited by biologically active systems. Some selected examples referring to different biopolymers and membrane model systems will be illustrated.