kind of molecular properties of water: one is to disturb crystallization, while other is to promote crystallization. The competition between them can generate a pure amorphous state. Furthermore, lattice relaxation occurs around the boundary between crystal domains and the amorphous solid, since sharp Bragg peaks are observed at any phases.

Keywords: ionic materials, DSC/XRD, phase transitions and structure

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Debye-Waller factors and quantum phase transition in KH_2PO_4

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KDP (KH_2PO_4) is a typical ferroelectrics, in which the proton distribution changes through the phase transition. We measured scattering intensity from the single crystal by using neutron 4-circle diffractometer (FONDER) installed at JRR3M in JARERI, Tokai. The crystal structures at different temperatures between 10 and 300K are refined. The Debye-Waller factors are determined carefully. Though the transition temperature, the factors for K, P and O change without noticeable anomaly and approach the zero temperature values. However, the proton's factor along the double-well axis shows discontinuous behavior indicating the modification of the hydrogen bonding. The figure shows U_{11} vs. temperature; U_{11} of the split atom H changes continuously. The temperature dependence is compared with a quantum model of the structural phase transition. The phase transition mechanism seems to be not a typical order-disorder or displacive type but a quantum type transition

Keywords: neutron structure determination, Debye-Waller factor, quantum wells

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Lattice instability of FeNi and Fe_3Pt Invar alloys

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Elastic diffuse scattering of neutrons was found around various Bragg peak positions for typical Invar alloys, $Fe_{1-x}Ni_x$ ($0.35<x<0.6$), ordered $Fe_{72}Pt_{28}$ and disordered $Fe_{72}Pt_{28}$ alloys. Diffuse scattering intensities depend on temperature and Ni concentrations and increase with decreasing temperature and decrease with increasing Ni concentrations. The pattern of diffuse scattering intensity changes from peak to peak. The reasonable agreement with observed diffuse peak patterns was obtained for the analysis using Huang diffuse scattering for the nucleus of an anisotropic defect. Since all of these Invar alloys are located close to the phase boundary of fcc-bcc martensitic transformation, Huang diffuse scattering is considered to be due to the formation of premartensitic embryos. From the comparison of calculated diffuse scattering intensities in reciprocal lattice space with those for a simplified model, actual lattice deformation of embryos in real space was determined. The lattice deformation is described as a shear wave propagating along the [1 1 0] direction and with the [1 -1 0] polarization vector. From these data, the early stage of fcc-bcc martensitic transformation in Fe and Fe alloys is discussed. Since the regions of temperatures and Fe concentrations for which diffuse scattering are observed coincide with those for which the Invar anomalies are observable, the formation of premartensitic embryos seems to be strongly related to the Invar effects for these alloys.

Keywords: invar alloys, Huang diffuse scattering, premartensitic phase

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Photoinduced disorder-to-incommensurate order phase transition in an Fe(II) spin crossover complex

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Molecular multistability has attracted an increasing interest in the context of functional molecular materials. The possibility of switching between different stable states under external perturbation like temperature, pressure or light excitation allows to tune and control the macroscopic properties (magnetic, electronic, optic) of the system. In the solid state, the coupling between purely molecular aspects and intermolecular interactions may lead to collective phenomena, i.e. photo-induced phase transitions [1]. Spin crossover (SCO) materials are typical examples of such photo-switchable molecular systems [2]. We investigate the light-induced switching process in the SCO complex $\{Fe(abpt)_2[N(CN)_2]_2\}$, through time and temperature dependent photo-crystallographic measurements. Upon laser light excitation, an unprecedented collective long range ordering of the dicyanamide $[N(CN)_2]$ groups develops, resulting in a displacive modulation of the crystal structure with wavevector $q = 0.331(2)a^*+0.658(2)b^*-0.000(3)c^*$, incommensurate with the underlying reciprocal crystal lattice. The corresponding structural analysis of the metastable HS phase is performed under the superspace group approach, using JANA [3]. A lattice structural instability is evidenced as the basis for the disorder-to-incommensurate order phase transition. A Frenkel-Kontorova-like model of competing interactions within two layer subsystems is proposed to elucidate the origin of the incommensurability.

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Keywords: solid-state phase transformations, incommensurate ordering, photochemistry