

13.2-3 LATTICE DYNAMICS OF THE FORCE

CONSTANT DISORDER CRYSTAL $\text{Pd}_{0.90}\text{Ru}_{0.10}$.

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The peculiar electronic and magnetic properties of Pd make the alloys of Pd with its neighbouring elements appropriate systems for a study of the contribution of the electronic structure to the lattice dynamics of transition metals. $\text{Pd}_{1-x}\text{Ru}_x$ system belongs to a class of force constant disorder crystals whose components have nearly equal masses but different binding characteristics. This system forms a solid solution up to the concentration of Ru somewhat higher than 10% at. The influence of Ru on the magnetic and electronic properties of Pd matrix is different from that of Rh /E. Maliszewski, S. Bednarski and J. Sosnowski, Zeit. Physik B36, 127 /1979/; E. Maliszewski, Report INR 1856/II/PS/A, /1980//. As Ru is added to Pd, the high susceptibility, the enhancement factor, the electronic specific heat coefficient of Pd are all progressively reduced. The mechanical strength of Pd is increasing with Ru concentration in Pd and is three times larger at 8% at. Ru. The present measurements of the phonon dispersion curves have been carried out along the directions [100], [110] and [111] in the $\text{Pd}_{0.90}\text{Ru}_{0.10}$ crystal by using neutron inelastic scattering. From these results and phonon data for Pd, the phonon frequency shifts $\Delta\omega(\vec{q})$ and the self-energy functions $\Sigma_j(\vec{q}, \omega_j(\vec{q}))$ have been determined for all phonon branches in this crystal. The Born-von Karman analysis, using the seven-neighbour model, has been carried out and the force constants and elastic constants calculated. The frequency shifts exhibit the large dependence on wave vector and on polarization, which is characteristic for the force-defect crystals. This dependence is even more evident on the plot of self-energy functions. The pronounced softening of all SEF branches observed at the definite wave vectors is a manifestation that another phase is appearing. This sharp decrease of SEF for the definite wave vectors and frequencies /normal modes/ is an interesting result because SEF act like additional force constants in the disordered crystal.

13.2-4 LATTICE DYNAMICS OF DISORDERED KLiSO_4 AND CsLiSO_4 . By G. Eckold, Th. Hahn and B.O. Hildmann,

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KLiSO_4 and CsLiSO_4 exhibit tridymite- and Iemm-framework structures, resp., with alternating SO_4^- and LiO_4^- coordination tetrahedra. As a common feature of both substances the almost rigid SO_4^- -groups are tilted with respect to the high-symmetry orientation of the ideal structures. In KLiSO_4 there are three different orientations of the tetrahedra with respect to the threefold axis, in CsLiSO_4 two orientations with respect to the mirror plane; all these 'split-positions' occur with equal probability. As a first step to the understanding of the dynamics of crystals with this type of disorder we present the phonon dispersion for KLiSO_4 as well as for CsLiSO_4 .

Inelastic neutron scattering experiments have been performed on the triple axis spectrometer UNIDAS at the FRJ-2 reactor in Jülich. The most exciting feature of the phonon dispersions is the appearance of an optical phonon branch with strong longitudinal character and with frequencies approaching zero in the vicinity of the Γ -point. Within the accessible q-range, i.e. $|q| = 0.04 \text{ \AA}^{-1}$, this lattice mode is nearly temperature independent. In KLiSO_4 it is observed both in the room temperature phase and in the low temperature monoclinic phase, i.e. it is not affected by the phase transition at about 190 K. This mode is neither a spurious excitation due to resolution effects of the spectrometer nor an unweg-excitation due to the Renninger-effect. It cannot be explained within the hexagonal structure model of KLiSO_4 . However, the split-model describing the disorder of SO_4^- -tetrahedra implies that in local regions the structure is monoclinic. Since the orientations of SO_4^- -groups change with time a hexagonal average-structure is obtained. Assuming that the characteristic frequencies for transitions between different split-positions are far below the lattice-mode frequencies (THz) the phonon dispersion is governed by monoclinic symmetry. Therefore, in the lattice dynamics there is no principle difference between the disordered room temperature phase and the ordered monoclinic phase as long as the phonon wavelengths are not too large. In the monoclinic structure the low-frequency lattice mode corresponds to a tilting motion of the SO_4^- -tetrahedra. Rigid-ion model calculations are in progress. At the Γ -point, this mode might drive the phase transition to the macroscopically ordered monoclinic phase. This would be consistent with the observed diffuse-elastic scattering just above the transition temperature.