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Phonon softening in alpha-u metal at low temperature

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Alpha-U has been observed to undergo the following sequence of transformations at $T_0 < 43K$ (lower limit of stability of the structure) a transition involving modes for which $\mathbf{q_{CDW}}$ = < q_x, q_y, q_z>; ortho.: Cmcm $T_0 = 43K_>$ mono.: C2/m11 (q_x, q_y, q_z) $T_1 = 37K_>$ mono.: P211 (1/2, q_y, q_z). The phonon dispersion was measured by neutron inelastic scattering in the range (200, 43K) of existence of the high-temperature orthorhombic phase and in the range of the phase transformations at 43, 37 and 22K. Soft branches were associated with the normal-to-incommensurate transitions in Brillouin zone: (201). The main component of the displacement pattern is consistent with the symmetry for a Σ_4 phonon mode. The static displacements associated with the displacive transition are produced by low-frequency and damped phonons at positions $\mathbf{q_s}$ [(q_x, q_y, q_z)] which on approaching the second-order phase transition (T_0) soften more than those with $\mathbf{q_c}$ = [1/2, 0, 0], but not totally. Increasing the energy resolution by using cold neutrons on the three axis spectrometer IN14 near (101), we have seen in the range T-T_0 = 7K a small deviation from the linear law of Curie. The experimental phonon softening [1] which is accompanied by large changes in cell parameters at T_0, is dependent on q_y (T), q_z (T) contrary to predictions of the Yamada theory. At T_0 = 43 K the modulation wave vector of the incommensurate low-temperature condensing soft mode is $\mathbf{q_{min}}$ = [0.497 (1), 0.13 (1), 0.21 (1)] ($\mathbf{q_{CDW}}$. The electronic instability which causes Kohn anomaly also triggers the displacive (Peierls) transition.

[1] Marmeggi J.-Cl., & al. J. Phys. Soc. Jpn, 2001, A70, 22.

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Chemically-induced renormalization phenomena in relaxor-ferroelectric $PbSc_{0.5}Ta_{0.5}O_3$

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Relaxors are special class of ferroelectrics that exhibit a broad, diffuse phase transition over a temperature range and a strong frequency dependence of the dielectric constant as a function of temperature. Near room temperature they exhibit very high dielectric permittivity, electrostrictive and electrooptical coefficients, which determine relaxors as multi-functional materials, with a wide range of technological applications, including non-volatile memory devices. The global, average structure of relaxors, detectable by diffraction methods, remains pseudo-cubic even at liquid helium temperatures, whereas their nanoscale structure is rather complex. Near the Curie range and under zero-field conditions the ferroic clusters are sized only a few unit-cell parameters and they create and annihilate within 10^{-5}-10^{-6} s. Thus, because of its length- and time-scale sensitivity, inelastic light scattering is vital for gaining structural information. The mechanism of paraelectric-to-relaxor ferroelectric phase transition is still not clarified. To better understand the local structural phenomena occurring in relaxors we have applied Raman scattering and X-ray diffraction on single crystals of stoichiometric $PbSc_{0.5}Ta_{0.5}O_3$ (PST), solid solutions of type $PbSc_{0.5}Ta_{.5}O_3$-$PbSc_{0.5}Nb_{.5}O_3$ and $PbSc_{0.5}Ta_{.5}O_3$-$PbSnO_3$, A-site mixed $(Pb_{1-x}A''_x)Sc_{0.5}Ta_{0.5}O_3$ (A'' = Ba,), as well as Ru-doped $PbSc_{0.5}Ta_{0.5}O_3$. The analysis of the temperature evolution of phonon anomalies shows that the variations in the chemical compositions favour different types of structural distortion near the temperature of the dielectric permittivity maximum, which reflect on the shape and size of the polar domains developing on cooling.