05.1-33   THE MODULATED STRUCTURE OF QUARTZ INTERMEDIATE PHASE BETWEEN α AND β PHASES. By <u>K. Gouhara</u> and N. Kato, Department of electronics, Nagoya University and Department of Physics, Meijo University, Nagoya, Japan.

Recently, it has been revealed that quartz has an incommensurate phase (IP) between α (D_3^4) and β (D_6^4) phases (K. Gouhara, Y. H. Li and N. Kato; J. Phys. Soc. Jpn. <u>52</u> (1983) 3821, G. Dolino, J. P. Bachheimer and C. M. E. Zeyen; Solid State Commun. <u>45</u> (1983) 295). The structural change occurs on four levels of spatial scale from Å to cm (N. Kato and K. Gouhara; Jpn. J. Appl. Phys. <u>24</u> (1985) 157). The purpose of this article is to elucidate the modulated structure of IP based on our data obtained by the fine-beam Laue method. Group theoretical considerations tell us that so-called Σ_2-mode of the thermal vibration is frozen. Many authors, recalling the transition between D_3^4 and D_6^4 in the present case, consider that B_1-mode is predominant. However, our observed intensities of satellites fit primarily to an accoustic transversal vibration (E_1-mode) as pointed out previously (J. Phys. Soc. Jpn. <u>52</u> (1983) 3647). Questions, therefore, are whether alternatively B_1-mode can explain the observed intensity or what extent of B_1-mode is involved. The satellite intensity $I(q_1)$ having the modulation vector q_1 must be proportional to the square of the structure factor given by

$$F_s(q_1) = 2\pi i \cdot (g \cdot U(q_1)) \qquad (1)$$

where $\quad U(q_1) = \sum_k f_k u_k(q_1) \exp(2\pi i g \cdot r_k) \qquad (2)$

(K. Gouhara and N. Kato; J. Phys. Soc. Jpn. <u>54</u> (1985) 1868). q_1: Modulation vector ($l=1, 2$ and 3). g: The reflection vector. f_k: The atomic structure factor ($k=1, 2, 3$ for Si, $k=4\sim9$ for O). u_k: The displacement amplitude. r_k: The time averaged position of k-th atom.

Three models are examined. E is a purely transversal accoustic vibration with a single parameter u (amplitude). Three modes having $q_1 // \pm b_1$ (approximation) exist in real space. B is a purely optical vibration of B_1 symmetry. For reducing parameters, Grimm's model (H. Grimm and B. Dorner; J. Phys. Chem. Solids, <u>36</u> (1975) 407) is adopted. Then all atomic displacements can be described by a single parameter v (that of Si atom). M is a linear combination of E and B with a weight parameter $w=v/u$. For satellites near 22 Laue spots, the calculated intensity is compared with our results.

In several reflections, the mixture of B_1 mode with $w>0.1$ is certainly harmful. However, model M with $w=0.1$ seems most plausible in the case of $(\bar{1}, \bar{3}, 2)$ reflection (see Table). In conclusion, the mixing weight is 0.15 at most.

	Model	parameter	$I(q_1)$	$I(q_2)$	$I(q_3)$
C A L	E	$u=1.8\times10^{-3}$ Å	0.189	0.021	0.335
	B	$v=1.8\times10^{-3}$ Å	0.527	0.527	0.527
	M	$v=0.1 \cdot u$	0.256	0.006	0.258
		$v=0.2 \cdot u$	0.333	0.009	0.192
EXP. (ratio)			1	~0	~1

05.1-34   HIGH-PRESSURE STRUCTURAL STUDIES OF THE PHASE TRANSITIONS IN $PbTiO_3$ AND $H_2C_4O_4$. By <u>R.J. Nelmes</u>, R. Ramirez, R. Restori and Z. Tun, Department of Physics, University of Edinburgh, Scotland.

The phase transitions in $PbTiO_3$ and $H_2C_4O_4$ (squaric acid, or H_2SQ) both exhibit strong pressure dependence, with dT_c/dP of the order of -100 K GPa^{-1}.
$PbTiO_3$ has a first-order ferroelectric phase transition on cooling through $T_c = 763$ K at atmospheric pressure. In neutron-diffraction studies of the structural changes through T_c we have found evidence that the transition involves order/disorder behaviour in the Pb atoms. This is surprising: $PbTiO_3$ has long been regarded as an example of a material with a purely displacive transition. However, multi-site disordering of the Pb atoms above T_c, ordering onto one of these sites below T_c, could account for the large P-dependence of T_c. We have now made X-ray diffraction studies of $PbTiO_3$ under pressure, using a diamond-anvil pressure cell (DAC), and have determined the crystal structure at a number of pressures up to 4.5 GPa. We find evidence of an anomalous P-dependence for the structural displacements in the ferroelectric phase.
H_2SQ has an antiferroelectric phase transition on cooling through $T_c = 373$ K. The transition involves ordering of the H atoms which, above T_c, are 50:50 disordered over two off-centre sites, δ apart, in the O--H--O bonds linking the C_4O_4 groups. As for $PbTiO_3$, we have studied the nature of the transition in H_2SQ at atmospheric pressure by high-resolution neutron diffraction and have used X-ray diffraction, with a DAC, to explore the structural changes with pressure. In addition, we have now collected neutron-diffraction data at high pressures (up to 2 GPa) at room temperature and also ~10 K above the pressure-reduced T_c. The results show the relationship between the P-dependence of T_c and the changes in the H-bond dimensions with pressure, especially the H-site separation δ.

05.1-35   MARTENSITIC PHASE TRANSFORMATION OF SINGLE CRYSTAL LITHIUM FROM bcc TO A 9R-RELATED STRUCTURE. H. G. Smith, Solid State Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831.

A neutron elastic and inelastic scattering study of single crystal bcc lithium was performed above and below the martensitic phase transformation in the vicinity of 75 K. The transformation is abrupt and the bcc lattice partially transforms to a 9R-related (Sm-type) structure, which is uniformly embedded throughout the sample. Several variants were observed and one was oriented with the (H0L) zone in the scattering plane of the spectrometer. The 9R c* and a* axes of this variant are nearly along the [110] and [1$\bar{1}$0] bcc directions, respectively. The (10L)9R and (20L)9R reflections were broadened and shifted from their ideal positions compared to the (00L)9R reflections, indicative of numerous stacking faults. On warming above 100 K, the sample reverts back to a single crystal with the same bcc orientation. No pronounced soft mode behavior was observed.