21-Crystallography at Non-Ambient Temperatures and/or Pressures; Phase Transitions

MS-21.01.04 STRUCTURAL EVOLUTION OF α-QUARTZ UNDER HIGH PRESSURES AND TEMPERATURES : A MOLECULAR DYNAMICS STUDY. By Surinder M Sharma, M S Somayazulu, S K Sikka, S L Chaplot and R Chidambaram, Bhabha Atomic Research Centre, Bombay 400 085, INDIA.

Pressure induced amorphization in α-quartz has been studied by molecular dynamics. Anisotropic amorphization occurs at about 20 GPa at 300 K. The structure is observed to contain two dimensional amorphous layers along the original ab plane, with different layers sheared along the c axis. This shearing is found to reduce with increase in the initial temperatures and completely vanishes for temperatures in excess of 750 K. The α-quartz structure close to the amorphization contains oxygens that are almost in a close packed configuration as suggested by Hazen et al (Sol. St. Comm. 72, 502, 1989). However, the oxygen sublattice is still far away from an ideal b.c.c. packing arrangement postulated by Bingelli and Chelikowski (Nature, 353, 344, 1991). Simulations carried out up to 80 GPa at 300 K reveal that the coordination number of Si saturates at a value of 6 beyond 60 GPa. The retrieved phase is observed to be permanently densified and continues to be anisotropic, with a coordination number of 4.3. On increasing the temperature of this phase beyond 1100 K, the coordination number of Si returns to a value of 4 and the resultant amorphous phase is found to be isotropic, accompanied by the formation of six membered ring structure which is different from that of the crystalline phase of α-quartz.

MS-21.01.05 HIGH PRESSURE DIFFRACTION STUDIES AT BSRL. By Y.C.Zhao, Beijing Synchrotron Radiation Lab., China

PS-21.01.06 CRYSTAL-STRUCTURE STUDIES OF II-VI, III-V AND GROUP IV SEMICONDUCTORS AT HIGH-PRESSURE USING ANGLE-DISPERSIVE POWDER-DIFFRACTION TECHNIQUES. By R.J. Nelmes, M.I. McMahon*, N.G. Wright and D.R. Allan, Department of Physics, University of Edinburgh, U.K.

Angle-dispersive powder-diffraction techniques, coupled with an image-plate area detector, have been developed at SRS Daresbury for crystal-structure studies at high pressure. The combination of high sensitivity and high resolution obtainable with these techniques has revealed new phases and unsuspected structural relationships in II-VI, III-V and group IV semiconductors. For example, silicon has been found to have an intermediate phase between the well-known β-tin and primitive hexagonal phases, reminiscent of the structural sequence found in InSb, while CdTe has been found to have a cinnabar phase between the well-known zincblende and NaCl phases, as previously found only in HgTe and HgSe. Details of this work, along with other recent results from InSb, InP, Ge and HgTe will be presented.

PS-21.01.07 HIGH-PRESSURE STRUCTURAL STUDIES USING SINGLE-CRYSTAL X-RAY DIFFRACTION TECHNIQUES. By D.R. Allan*, J.S. Loveday and R.J. Nelmes, Department of Physics, The University of Edinburgh, U.K.

We are applying single-crystal x-ray diffraction techniques to studies of the relationship between crystal structure and physical properties as they vary under pressure. For example, the superconducting transition temperature (T_c) in copper-oxide superconductors is believed to be strongly linked to a particular Cu-O bondlength. We are making a detailed comparison of $YBa_2Cu_4O_8$ and $La_{1.85}Sr_{0.15}CuO_4$, which both show a large rate of change of T_c with pressure. But initial results reveal quite different behaviour for the crucial Cu-O bondlength in the two materials. This is important, as it suggests that there is not a single, common mechanism for T_c variation. We are now extending this work to higher pressures where the difference may be expected to become even more definite and significant.

We are also studying the icosahedral boron-rich materials α-boron and B_4C in relation to recent work on their electrical conductivity. Models have been developed which are based on bipolaron hopping, and require the icosahedral units to be more compressible than the structural unit-cell to account for the anomalous P-dependence of the conductivity. We have started work to test whether these models are well founded.

The recent results from both of these programmes will be presented.

PS-21.01.08 CRYSTAL-STRUCTURE STUDIES TO 10 GPa USING NEUTRON POWDER DIFFRACTION TECHNIQUES. By R.J.Nelmes*, J.S.Loveday and R.M.Wilson, Department of Physics, The University of Edinburgh, UK; J.M.Besson, S.Klotz and G.Hamel, Physique des Milieux Condensés (CNRS), Université Paris VI, France; and S.Hull, ISIS Facility, Rutherford Appleton Laboratory, UK.

We have been developing an opposed-anvil pressure cell, able to compress samples of sufficient size for accurate crystal-structure studies to above 10 GPa. This cell is in use at the UK pulsed-neutron source, ISIS. After completing improvements to the signal-to-background and to attenuation corrections, we have been able to carry out successful structural studies in which good data to d-spacings of ~0.5 Å have been obtained. Rietveld profile refinement of these data yield interatomic distances with a precision of ~0.003 Å or better at all pressures.

Completed studies to date include the P-dependence of the O-D distance in D_2O ice VIII up to 10 GPa, which shows that the O-D distance varies significantly less than has been widely supposed on the basis of spectroscopic studies and assumptions about the interatomic potential; the compressibility of the icosahedra relative to the unit-cell volume in boron carbides B_4C and B_9C, which is a crucial variable in models of the transport properties of these materials; the H(D)-ordering transition in deuterated squaric acid ($D_2C_4O_4$) at 3.5 GPa, in relation to

