340 12-Amorphous, Imperfectly Ordered and Quasi-periodic Materials

PS-12.01.20 STRUCTURE OF THE INCOMMENSURATE PHASE OF 4,4′-DICHLORODIPHENYL SULPHONE AT 90 K. *By F. J. Zúñiga, J. M. Pérez-Mato* and T. Breczewski. Departamento de Fisica de la Materia Condensada, Facultad de Ciencias, Universidad del Pais Vasco, Apdo. 644, Bilbao, Spain*

The structure of the incommensurate phase of 4,4′-dichlorobyphenyl sulfone[1,2], $C_{12}H_8Cl_2O_2S$, has been determined at 90 K using the superspace formalism. The refinement of the atomic modulation of displacive type, wavevector $\mathbf{q}=0.780(2)\mathbf{b}^*$, has been performed in the superspace group P(I2/a):(s,-1), using main and first order satellite reflections. A model of the distortion including zero, first and second order harmonics has been considered in the modulation. The final agreement factors are R = 0.042, R_o=0.039 and R_I=0.043 for all, main and satellite reflections respectively. Second order harmonics are critical in the refinement as they decrease the R_I factor from 0.12 down to 0.043. The primary distortion is described by a mode of Λ_2 symmetry involving intermolecular motions and an important intramolecular twist of the phenyl groups. Crystal data of the average structure : T=90K, M_r=287.2, orthorhombic, I2/a, a=20.20(2), b=4.910(2), c=12.054(9)Å, β=90.02(4)°, V=1195(2) Å^3, Z=4, D_x=1.597 Mgm^{-3}, λ(Mokα)=0.7107 Å, μ=0.67 mm^{-1}, F(000)=584.

References

1- Pusiol, D. J., Wolfenson, A. E. and Brunetti, A. H. (1989). Phys. Rev. B40, 2523.
2- Kasano, H., Koshiba, T., Kasatani, H. and Terauchi, H. (1990). J. Phys. Soc. Jpn. Lett. 59, No. 2, 408.

PS-12.01.21 CHANGE OF STRUCTURE OF Co-ÅKERMANITE AT ELEVATED TEMPERATURES. By K. Hagiya, N. Haga, M. Ohmasa*, K. Ohsumi[1] and K. Iishi[2]
Department of Life Science, Himeji Institute of Technology, Japan
1: Photon Factory, National Lab. for High Energy Physics, Japan
2: Dept. Mineralogical Sci. and Geology, Yamaguchi University, Japan

Hemingway *et al.* (Canadian Mineral., 1986, 24, 425-434) and Seifert *et al.* (Phys. Chem. Minerals, 1987, 14, 26-35) found that each Bragg reflection in X-ray and electron diffraction patterns of synthetic åkermanite ($Ca_2MgSi_2O_7$) taken at room temperature is accompanied by a set of satellite reflections. These satellites indicate that the modulation in the material is incommensurate. They also reported that the satellite reflections decrease in intensity at elevated temperature and disappear at higher temperature. Similar phenomena were also found in electron diffraction patterns of synthetic Co-åkermanite, $Ca_2CoSi_2O_7$ (Iishi *et al.*, N. Jb. Miner. Mh., 1989, 1989, 219-226). The incommensurate modulation in the cobalt analogue was determined by five-dimensional refinement of the structure (Hagiya *et al.*, Acta Cryst., 1993, B49, in press). The results revealed that the modulation is caused by the shifts of the constituent atoms.

Temperature dependence of intensities of the satellites was examined *in situ* to determine the transition temperature between the incommensurate and normal phases and also to observe change of modulation of the structure. Synchrotron radiation was employed as an X-ray source, because the intensities of the satellites are weak and diminishment of them must be detected. A fragment of the sample was mounted in a small gas blow system with an electric heater attached on the Weissenberg camera at BL-4B in the Photon Factory, National Laboratory for High Energy Physics, Tsukuba, Japan, and diffraction patterns were recorded on the imaging plate (Fuji Co.Ltd., Miyahara et al., Nucl. Instrum. Methods, 1986, A246, 572-578) at selected temperatures. The radius of the cylindrical camera is 100mm. The incident X-ray was monochromatized by 111 of Si crystal and the wave length 1.029Å was determined by calibration with diffraction of a GaP crystal. The temperature of the sample was varied from room temperature to 300°C at arbitrary intervals and was estimated from that measured by a thermocouple to regulate the furnace with a calibration curve determined before the experiments.

The observation of the satellites by synchrotron radiation revealed that their intensity decreases linearly from room temperature to 200°C and weakens to background level at about 216°C. Thus the transition temperature between the incommensurate phase to normal one was determined to be 216°C. The transition was ascertained to be reversible. The intensity of the satellites decreases linearly from room temperature according as the temperature raises, and becomes half at about 150°C. The reduction of the intensity is ascribed to the decrease of the amplitude of the modulation wave.

PS-12.01.22 CRYSTAL STRUCTURE OF NANOPARTICLES OF ZnS Binny Thomas and M Abdulkhadar*, School of Pure & Applied Physics, Mahatma Gandhi University, Ettumanoor, Kerala - 686 631 INDIA

Finding the crystal structure of nanoparticles, microcrystals or microclusters is a crucial and challenging problem in the study of their properties. The physical properties of microclusters have been reported to be critically dependent on their size and crystal structure. It is important to understand how the structural properties change as atoms, molecules and even small clusters of these come together to form progressively larger clusters and finally acquire the bulk structure. In microclustures, the surface atoms represent a large fraction of the volume of the material and the resultant excess free energy is expected to cause a contraction of the lattice without drastic changes in the crystal structure. The problem of determination of vital characteristics of small particles such as the morphology, structure and the lattice parameters becomes increasingly difficult as the size of the particles becomes smaller.The crystal structure and lattice parameters of these systems of particles is often ambiguous since the lattice will be generally disordered and the crystal structure will be anomalous.

Changes of lattice parameter of small metal particles with respect to the bulk values have been reported in many cases. The study of small particles of semiconductor materials are considered important since the electronic properties of small clusters of these materials may be different from the bulk electronic properties. Small particles of semiconductor materials such as CdS have been extensively studied by many researchers and it has been reported that for particles of size between 15 to 40 A , a unique structure does not exist. The authors report here the crystal structure of

small particles of ZnS of size about 40 A prepared chemically using zinc sulphate and sodium sulphide at room temperature. The size of the particels has been determined using TEM and from Xray diffraction pattern using the Scherrer formula. Xray diffraction and electron diffraction results have been used for the study of the structure of the particles. As expected, the xray diffraction lines are broadened. The electron diffraction rings show a strong broadening and are diffused indicating a high degree of disorder in the particle lattice. The d values calculated from the electron diffraction pattern are found to be close to (but slightly less than) those of the JCPDS data corresponding to wurtzite structure (8H). The diffraction ring also points to the presence of the 10H polytype. The slightly lesser d values indicate that the lattice has undergone a small contraction. The electron diffraction pattern does not contrain enough rings for an unequivocal determination of the lattice parameters `a' and `c'. The lattice parameter `a' calculated using the JCPDS value for the parameter `c' is found to be slightly less than the standard value. The decrease in the interplanar spacing and the lattice parameter points to a lattice contraction of about 2%.

PS-12.01.23 **A CLIFFORD ALGEBRA APPROACH TO N-DIMENSIONAL CRYSTALLOGRAPHY.** By A. Gómez*, J.L. Aragón, F. Dávila† and H. Terrones , Instituto de Fisica, UNAM, Apartado Postal 20-364, 01000 México, D.F. †Departamento de Matematicas, ESFM-IPN, U.P. Adolfo López Mateos, Edif. 9, 07300 México, D.F.

The discovery of materials such as incommensurate structures and quasicrystals makes necessary to extend crystallography to more than three dimensions. Problems arise since some identities (such as cross products and normals to planes) and concepts are no longer valid in higher dimensions. In this work n-dimensional lattices are described with the language of Clifford algebra. This point of view allows to reformulate the crystallography in a concise language valid in any dimension. A system of definitions and algebraic identities has been developed to be used as an efficient and versatile computational tool.

PS-12.01.24 STUDY OF EDGE DISLOCATIONS IN $Al_{62}Cu_{20}Co_{15}Si_3$ DECAGONAL QUASICRYSTALS BY MEANS OF HIGH RESOLUTION-ELECTRON MICROSCOPY. By H. Zhang and Z. Zhang, Beijing Laboratory of Electron Microscopy, Chinese Academy of Sciences, P.O. Box 2724, Beijing 100080, China.

High resolution electron microscopy (HREM) studies indicate that the edge-type dislocations in small angle boundaries in $Al_{62}Cu_{20}Co_{15}Si_3$ decagonal quasicrystals dissociate into two partial dislocations. By performing Burgers circuit around these partial dislocations, the projected Burgers vectors of these partial dislocations on the plane normal to the twofold A2D axis can be determined as $\mathbf{b}_1=[a_1/2, a_2, 0, 0, 0, 0]$ and $\mathbf{b}_2=[a_1/2, -a_2, 0, 0, 0, 0]$, respectively. The total Burgers vector is $\mathbf{b}=\mathbf{b}_1+\mathbf{b}_2=[a_1, 0, 0, 0, 0, 0]$ which has a modula of about 0.4 nm equal to the periodicity along the tenfold axis of the decagonal quasicrystal. As reported previously, the dislocations at a small-angle boundary in decagonal quasicrystals are out of contrast when any reflection parallel to twofold axis is used to form electron diffraction-contrast images under two-beam conditions. This implies that the Burgers vector of these dislocations is parallel to the tenfold axis. However the HREM images show that the dislocations observed in conventional contrast images actually consist of two close partial dislocations separated by about 3 nm from each other. The Burgers vector of each partial is not parallel to the A10 axis but makes an angle of 30° with it. Since these two partials are very close to each other and the Burgers vector components along the twofold axis are equal but of opposite sign, the distortions of the quasilattice between the two partials compensate. Therefore, the net lattice distortion determining the diffraction contrast is along the tenfold direction. Consequently, only the effect of the total Burgers vector is usually observed in conventional electron diffraction contrast images.

PS-12.01.25 TRANSMISSION ELECTRON MICROSCOPE STUDIES OF DEFECTS IN DECAGONAL QUASICRYSTAL. BY Y.F.Yan* and R.Wang, Department of Physics, Wuhan University, 430072 Wuhan, China and Beijing Laboratory of Electron Microscopy, Chinese Academy of Sciences, P.O. Box 2724, 100080 Beijing, China

Studies of defects in quasicrystals have attracted extensive attention because of their importance not only for structure studies, but also for understanding of many of their physical and mechanical properties. Defects such as dislocations, dislocation pairs, dislocation multipairs, dislocation dipoles, rectangular dislocation networks and stacking faults in $Al_{70}Co_{15}Ni_{15}$ decagonal quasicrystalline were studied by means of transmission eletron microscope. The Burgers vector of which the dislocation pairs and multipairs and dislocation dipoles consist are parallel to the ten-fold axis. The rectangular dislocation networks consist of two dislocation sets whose Burgers vectors are parallel to the ten-fold axis and a two-fold axis A2P or A2D. The fault planes of the stacking faults are perpendicular to the ten-fold axis and the displacement vectors are lying in the fault planes and parallel to a two-fold axis A2D.

PS-12.01.26 TRANSMISSION ELECTRON MICROSCOPIC OBSERVATION OF PHONONS COUPLED WITH PHASONS IN IMFERFECT DECAGONAL QUASICRYSTALS, By W. Geng and Z. Zhang, Bejing Laboratory of Electron Microscopy, P. O. Box 2724, 100080 Beijing, P. R. China.

We report, for the first time, on transmission electron microscopic (TEM) observation of phonons coupled with phasons in imperfect decagonal quasicrystals of $Al_{63}Cu_{17.5}Co_{17.5}Si_2$.

Phasons and phonons are topological defects which dominate the elastic property of quasicrystals, therefore are of general interest. Phonons exist both in ordinary crystals and quasicrystals but for the phason there is no analogue in normal crystals. Since the phonon distortion will relax with speed of sound while the phason distortion relaxes with diffusion, only phasons can frequently be observed by high resolution electron microscopic (HREM) images.

In study of imperfect decagonal quasicrystals of $Al_{63}Cu_{17.5}Co_{17.5}Si_2$, we observed a serie short lines with dark contrast in the electron diffraction contrast-images under two-beam conditions. The contrast of these lines is not produced by Moire fringes, precipitates, and misfit dislocations between the decagonal phase and its crystalline surface structures. HREM images and Fourier-filtered HREM images reveal that these short lines with dark contrast result from the obvious bending or distortion of quasilattices. There are lattice "jags" corresponding phasons densely distributed at the area centered by the short lines, implying that the phonons represented by the lattice distortion are coupled with phasons. Above TEM results show that phonons coupled with phasons do exist in imperfect decagonal quasicrystals.