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PS-10.01.31 DISORDERED INTERSTRATIFIED STRUCTURES OF SINGLE CRYSTAL HIGH-TEMPERATURE SUPERCONDUCTORS Bi-2212. By V.A.Drits*, O.V.Frank-Kamenetskaya, T.I.Ivanova, A.S.Bookin, I.V.Rozdestvenskaya, S.V.Moshkin, M.Yu.Vlasov and Yu.L.Kretser, Department of Crystallography of St.-Petersburg University, Moscow Geological Institute, Russia

Two different types of disordered two-compound interstratified structures in Bi-2212 single crystals were discovered by analysis of X-ray basal reflection profiles based on the theory of X-ray diffraction by microdivided systems with a layered structure (G.Tchoubar, V.Drits, X-Ray Diffraction by Disordered Lamellar Structures, Berlin, 1990).

Profiles of 001 ($l=8,10,12$) single crystal basal reflections (scanning along c^*) were received in four-circle autodiffractometer Syntex P2 (Mo-radiation, graphite-monochromator). Three single crystals of Bi-2212 obtained in various growth and oxygen annealing conditions were investigated. The single crystal electron probe microanalysis shows the existence of admixture layers of structure related Bi superconductive phases and various Bi/Sr- and Bi/Cu-ratio in Bi-2212 layers. The structures of first type are described by disordered alternation of Bi-2212 layers with layers of newly discovered (A.Bush, SPbChT, 1992, 5, 9, 364 (russ)) Bi-4413 phase. Probability of occurrence of Bi-4413 layers is 5%. The second type structures are characterised by alternation of Bi-2212 layers with different Bi/Sr- and Bi/Sr-ratio and different c -constant respectively. The probability of occurrence of admixture layers is 30-40%. Tendency to segregation of each kind of layers is distinct feature of these structures.

PS-10.01.32 EFFECT OF THE OXYGEN PRESSURE DURING ANNEALING ON CRYSTAL STRUCTURE AND PROPERTIES OF SINGLE CRYSTALS OF Bi-SUPERCONDUCTOR. By M.Yu.Vlasov*, T.N.Kaminskaya, O.V.Frank-Kamenetskaya, S.V.Moshkin, Yu.L.Kretser and V.V.Krivosoy, Department of Crystallography of St.-Petersburg University, Russia.

The cupola-like dependence between T_c and the density of holes in structures of Bi-2212 and Bi-2223 phases (W.A.Groen et al, Physica C, 1990, 165, 1, 55; H.Hattory et al, Jpn.J.of Appl.Phys, 1990, 29, 1, L26) permits to expect the existence of nonmonotonous dependences between oxygen content, T_c and c lattice parameter of these phases. There are some data published for single crystals of Bi phases which do not contradict this proposition. The present study has been undertaken to investigate the dependence of the c lattice parameter of Bi-2212 and Bi-2201 phases on the oxygen content which had been altered by annealing of these crystals at different oxygen partial pressure. Single crystals of Bi-2212 and Bi-2201 phases have been prepared by the method of spontaneous crystallization from solution. Fourteen of them sized $1 \times 1 \times 0.1$ mm have been annealed under oxygen pressure from 0.0001 to 150 atm and temperature 350 - 5500; the exposition time has been 40-80 hours. Electron microprobe analysis data (Camscan-4DV) have revealed the cation

homogeneity of all single crystals studied. The temperature of transition to superconducting state has been determined by the dependence of magnetic susceptibility on temperature, the tension of alternating magnetic field has been $\sim 1e$. The c lattice parameter has been determined from the position of basal reflections (0036 and 0038 for Bi-2212; 0016, 0022 and 0024 for Bi-2201). All reflections have been measured with DRON X-ray diffractometer.

As the result the nonmonotonous dependences of the c parameter on the oxygen pressure during annealing have been revealed for both Bi-2212 and Bi-2201 phases. This permits us to propose the existence of phase transition normal metal-superconductor-normal metal in studied single crystals. The antipate correlation between T_c - pc^2 and c - pc^2 dependences (minimum of c -parameter corresponds to maximum of T_c value) has been stated for Bi-2212 single crystals. The position and intensity of extremum depend on the Sr/Ca cation ratio. The increase in T_c value with the increase in oxygen partial pressure in Bi-2212 occurs, as well as in perovskite-like phases in La-Sr-Cu-O and Y(TR)-Ba-Cu-O systems, until it leads to the structure compression along Z axis. Opposite directed changes of the c lattice parameter with increase in oxygen content may be explained by analogy with 1-2-3 phase by localization of additional oxygen atoms in various crystallographic structure positions. The influence of oxygen atoms redistribution, connected with order-disorder transition, on the c -parameter cannot be excluded.

PS-10.01.33 STRUCTURAL DESIGN OF ORGANIC CONDUCTORS AND SUPERCONDUCTORS WITH MERCURY-CONTAINING ANIONS. By O.A.Dyachenko*, S.V.Konovallikhin, V.V.Gritsenko, R.N.Lyubovskaya and Lyubovskii R.B. Institute of Chemical Physics in Chernogolovka, Russian Academy of Sciences, Russia.

The study of organic conductors based on bis-(ethylenedithio)tetrathiafulvalene (ET) with mercury-containing anions is a promising direction of investigation in the field of synthetic organic metals and superconductors. The X-ray crystallographic structure determinations have been carried out of the electroconducting compounds: $(ET)_4[Hg_{2.78}Cl_8]$ (1), $T_c = 1.8$ K, $P = 12$ kbar (Dyachenko, O.A., Takhirov, T.G., Atovmyan, L.O., Zhilyaeva, E.I. & Lyubovskaya, R.N. Inter. Conf. Advanced Methods in X-ray and Neutron Structure Analysis of Materials, Karlovy Vary, Czechoslovakia, 1987, 59.), $(ET)_4[Hg_{2.89}Br_8]$ (2), $T_c = 4.3$ K (Lyubovskaya, R.N., Zhilyaeva, E.I., Pesotskii, S.I., Lyubovskii, R.B., Atovmyan, L.O., Dyachenko, O.A. & Takhirov, T.G. JETP Lett., 1987, 46, 188-191), $(ET)_2[Hg_{1.41}Br_4]$ (3), $T_c = 2.0$ K (Dyachenko, O.A. & Lyubovskaya, R.N. Inter. Conf. on Science and Technology of Synthetic Metals (ICSM'90), Tubingen, Germany, 1990, 254), $(d_8-ET)_4[HgBr_2.Hg_2.Br_6]$ (4), T_c (onset) = 3.0 K at 0.3 kbar, $(ET)_8[Hg_4Cl_{12}(PhCl)_2]$ (5), which is metallic to 1.3

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K (Dyachenko, O.A., Gritsenko, V.V., Mkyan, Sh.G., Shilov, G.V., & Atovmyan, L.O. *Izv. AN SSSR. Ser. Khim.*, 1991, 2062-2070), $(\text{ET})_8[\text{Hg}_4\text{Cl}_{12}(\text{PhBr})_2]$ (6) which is metallic to 10 K, $(\text{ET})_8[\text{Hg}_4\text{Br}_{12}(\text{PhCl})_2]$ (7) with $T_{\text{MI}} = 90$ K, $(\text{ET})_8[\text{Hg}_4\text{Br}_{12}(\text{PhBr})_2]$ (8) with $T_{\text{MI}} = 125$ K (Gritsenko V.V., Dyachenko, O.A., Shilov, G.V., Lyubovskaya, R.N., Afanasyeva, T.V., Lyubovskii, R.B. & Makova, M.K. *Izv. AN. Ser. Khim.*, 1992, 894-902), $(\text{ET})_8[\text{Hg}_4\text{Br}_{12}(\text{MePhCl})_2]$ (9), $(\text{ET})_4[\text{Hg}_3\text{I}_8]$ (10) (Takhirov, T.G., Krasochka, O.N., Dyachenko, O.A., Atovmyan, L.O., Aldoshina, M.Z., Goldenberg, L.M., Lyubovskaya, R.N., Merzhanov, V.A. & Lyubovskii, R.B. *Mol. Cryst. Liq. Cryst.*, 1990, 185, 215-226), $(\text{ET})_4[\text{Hg}_2\text{I}_6]$ (11), $(\text{ET})_2[\text{Hg}(\text{SCN})_2\text{Cl}]$ (12) with $T_{\text{MI}} = 50$ K (Konvalikhin, S.V., Shilov, G.V., Dyachenko, O.A., Lyubovskaya, R.N., Aldoshina, M.Z. & Lyubovskii, R.B. *Izv. AN. Ser. Khim.*, 1992, 903-909), $(\text{ET})_2[\text{Hg}(\text{SCN})_2\text{Br}]$ (13) with $T_{\text{MI}} = 140$ K, $(\text{ET})_2[\text{Hg}(\text{SCN})\text{Cl}_2]$ (14) with $T_{\text{MI}} = 35$ K (Konvalikhin, S.V., Shilov, G.V., Dyachenko, O.A., Aldoshina, M.Z., Lyubovskaya, R.N. & Lyubovskii, R.B. *Izv. AN. Ser. Khim.*, 1992, 2323-2331), $(\text{ET})_2[\text{Hg}(\text{SCN})_2\text{Br}_{0.66}\text{Cl}_{0.33}]$ (15) with $T_{\text{MI}} = 70$ K and $(\text{d}_8\text{-ET})_4[\text{Hg}_2(\text{SCN})_4\text{Cl}_2]$ (16) with $T_{\text{MI}} = 86$ K. The named compounds are characterized by a variety of electroconducting properties including superconductors (1-4), metals (5-8, 12-16) and semiconductors (9-11). As a result of a comparative study of the crystal structures of the compounds (1-16) and organic conductors related to them, a variety of the types of ET packing in the conducting layers and the anion structures have been shown. The factors affecting the structural design and electroconducting properties of the organic conductors and superconductors are discussed.

10.02 - Fullerenes

MS-10.02.01 SYNCHROTRON X-RAY STUDY OF THE ORIENTATIONAL ORDERING IN SINGLE CRYSTAL C_{60} . By P. Wochner, P. C. Chow, G. Reiter, S. C. Moss, University of Houston, Houston, TX 77204-5506 USA; J. D. Axe, J. C. Hanson, R. K. McMullan, Brookhaven National Laboratory, Upton, NY 11973 USA; P. Zschack, Oak Ridge National Laboratory, Oak Ridge, TN 37831 USA; M. C. Nelson, University of Illinois, Urbana, IL 61801 USA.

The determination of both the single molecule and intermolecular interaction potentials provides a key to the understanding of the orientational ordering transition at 260K. These potentials can be extracted, respectively, from Bragg (P. C. Chow et al., *Phys. Rev. Lett.*, 1992, 69, 2943-2946) and diffuse X-ray scattering experiments which probe the orientational pair correlations between C_{60} molecules as a function of their separation (J. R. D. Copley and K. H. Michel (preprint)). We will show that even in the orientationally disordered state, with continuously re-orienting C_{60} molecules, a given molecule will show preferential orientation resulting in deviations from a spherical distribution. These deviations allow us to evaluate the probability of orientation

$P(\tilde{\omega})$ and the effective single molecule potential energy $V(\tilde{\omega})$, where $\tilde{\omega}$ is the set of Euler angles.

In a large single crystal, grown by J. Z. Liu and colleagues at UC Davis, we have observed anisotropic zone boundary diffuse scattering, extending well above the first-order transition temperature T_c , which is strongly dependent on the scattering wave vector, \tilde{Q} . This scattering is associated with the form factor variation for a single molecule in the crystal field, which is then modulated by the scattering from coherent orientational correlations. We will present current progress in our determination of the interaction potential.

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MS-10.02.02 CRYSTAL STRUCTURES OF C_{60} AND OF $(\text{HYDROQUINONE})_3\text{C}_{60}$. By H.-B. Bürgi and M. Foertsch, Laboratory of Crystallography, University of Bern, Switzerland; R. Restori and D. Schwarzenbach*, Institute of Crystallography, University of Lausanne, Switzerland; O. Ermer, Institute of Organic Chemistry, University of Köln, Germany.

Pure C_{60} undergoes a phase transition at 250K. The low-temperature structure (cubic $\text{Pa}\bar{3}$) shows a twofold orientational disorder; the corresponding populations are in thermal equilibrium (Bürgi, H.-B. et al., *Angew. Chem. Int. Ed.*, 1992, 31, 640-643). We now report the high-temperature structure (cubic $\text{Fm}\bar{3}\text{m}$) determined from published synchrotron X-ray data (Chow, P. C. et al., *Phys. Rev. Lett.* 1992, 69, 2943-2946). The room-temperature scattering density distribution has been parametrized in terms of a combination of oriented symmetry-related molecules, and of a freely spinning molecule. Corresponding populations are 61% and 39%. The oriented part of the model is obtained, in good approximation, by imposing symmetry $\text{m}\bar{3}\text{m}$ on the energetically more favourable major orientation in the low-temperature structure of C_{60} . The orientational probability density distribution has been calculated from the molecular libration tensors. It shows maxima for C_{60} orientations possessing $\bar{3}\text{m}$ crystallographic site symmetry. It is also relatively large for the C_{60} orientations with cubic site symmetry $\text{m}\bar{3}$. The smallest energy barrier for reorientation between different $\bar{3}\text{m}$ orientations *via* a $\text{m}\bar{3}$ orientation appears to be less than 2 kJ mol^{-1} . On average, 75% of the intermolecular contacts of the oriented molecules are longer than those observed in the low-temperature structure, the other