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defect structures are only metastable which is important for the long time use of these materials.

In spite of a lower concentration of vacancies (tetragonal) Y-TZP ($Zr_{1-2x}Y_{2x}O_{2-x}$ with $x \approx 0.03$) shows superior conductivity at temperatures below 1000 K, roughly. This is related to a more random distribution of the defects. In addition, the diffusion pathways as determined from pdf-maps differ appreciably in both materials being slightly more favourable in TZP (where they are restricted to certain double layers) mainly due to the more favourable arrangement of the atoms in the tetragonal structure. The conductivity can be further enhanced by alloying with Ti or Ce which may again be related to an increasing "tetragonality" (c/a ratio, z(O) parameter).

Although similarities with zirconia are present in ceria ($Ce_{1-2x}Y_{2x}O_{2+x}$, $0 \leq x \leq 0.1$) the disorder is more complex as evidenced by additional weak superlattice peaks which may be assigned to certain substoichiometric phases CeO_{2-y} . Moreover, the disorder depends on preparation conditions and changes with temperature.

In $LiNbO_3$ (and isotypic $LiTaO_3$) deviations from stoichiometry occur without alloying with other atom species. New structure refinements disagree with previously reported disorder models: no vacancies on the Nb lattice, excess Nb on Li sites with corresponding Li vacancies. At high temperatures Li becomes mobile leading to an order-disorder phase transition at 1480 K. Diffuse planes perpendicular to (-221) are assigned to uncorrelated Nb-O-Nb chains as identified from a static contribution to the corresponding temperature factors. Intensity concentrations at low temperatures (25 K) indicate the onset of short range order correlations.

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DS-12.02.05 Diffuse Scattering from the Organic Conductor $C_1TET - TTF.(AuI_2)_{2/3}$.

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The sample is electrochemically prepared with a constant current of $25 \mu A$ at $25^\circ C$ in a 1,1,1-trichloroethane/ acetonitrile solution of $C_1TET - TTF$ (Bis(methylthio)ethylenedithio-TTF, a hybrid molecule between $BEDT - TTF$ and $TTC_1 - TTF$) and tetrabutylammoniumdiiodoaurate. The crystals are very brittle little black bars.

X-ray diffraction intensity data of a single crystal of $C_1TET - TTF.(AuI_2)_{2/3}$ were collected with graphite monochromatized radiation on an Enraf Nonius CAD4F diffractometer, all reflections with h odd being weak. The spacegroup is $P2_1/c$ with $a = 7.54 \text{ \AA}$, $b = 22.45 \text{ \AA}$, $c = 11.67 \text{ \AA}$, $\beta = 100.14^\circ$, $V = 1945.2 \text{ \AA}^3$ and $Z = 4$, one unit being $C_{10}H_{10}S_8(AuI_2)_{2/3}$. The structure was solved and refined with DIRDIF and Xtal 3.0 software packages. Final conventional refinement gives $R = 0.065$, $wR = 0.055$ and $S = 2.988$.

The structure consists of ordered organic residuals forming zigzag layers parallel (100), leaving channels along [100] and disordered gold-iodine chains within these channels. In the average structure the disorder shows up as very large temperature factor parameters of gold and iodine in the chain direction, fractional occupation numbers and unphysical distances between peak positions ($\approx 1 \text{ \AA}$). Rotation photographs on a Weissenberg camera show diffuse planes perpendicular to the a-axis with h-indices 0.8, 1.6, 2.4 and 3.2. The planes consist of diffuse peaks superimposed on slowly varying greyness. The diffuse scattering can be explained by a tentative model with independent chains of four (AuI_2^-) -ions per five times the a-axis length. More results will be presented in detail.

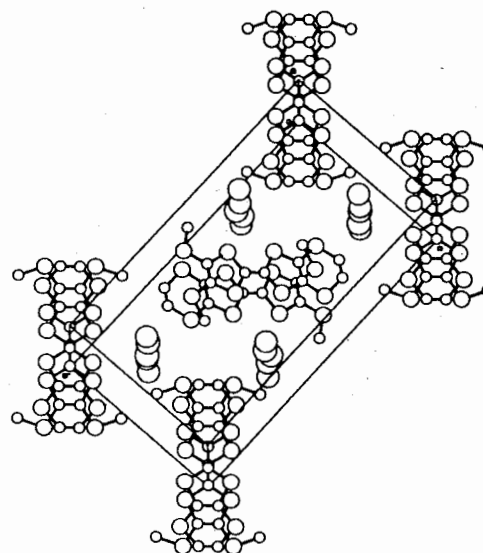


Fig. 1. The structure of $C_1TET - TTF.(AuI_2)_{2/3}$.

DS-12.02.06 X-RAY DIFFUSE SCATTERING STUDY OF DISORDERS IN ORGANIC CONDUCTORS AND SUPERCONDUCTORS by J.P. Pouget*, Laboratoire de Physique des Solides (CNRS UA2), Université de Paris Sud, 91405 ORSAY, France

Electronic and structural properties as well as instabilities exhibited by quasi one dimensional (1D) conductors are very sensitive to disorders such as those created by irradiation or substitution. Disorder in particular induces electronic localization, suppresses the superconductivity and pins the $2k_F$ spin and charge density wave (SDW and CDW respectively) modulations (k_F is the Fermi wave vector of the 1D electron gas). In spite of these dramatic effects there is only very few detailed studies of the structural modifications induced by the disorders in the different families of low dimensional organic conductors and superconductors.

Substitutional and orientational disorders present in the family of quasi-1D organic superconductors $(TMTSF)_2X$ based on the tetramethyltetraselenafulvalene molecule and where X is monovalent anion like PF_6 , ReO_4 have been characterized by simulations of their X-ray diffuse scattering

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pattern. It is found that in most of the cases the disorder is random but accompanied by molecular displacements (size effect). Its consequences on the various instabilities by these salts will be discussed. In particular those involving the ordering of non centrosymmetrical anions X will be interpreted in term of random interactions or random fields due to the disorder. Incommensurate $2k_F$ SDW and $2k_F$ CDW modulations observed in many quasi 1D conductors can collectively slide under the action of an external electric field when its intensity overcomes a threshold value due to the pinning of the waves to defects. The microscopic basis of this pinning mechanism is up to now poorly documented. Very recently we have succeeded to observe, in the TTF-TCNQ family of charge transfer salts disordered by irradiation or substitution, asymmetric X-ray diffuse scattering effects allowing to determine the phase of the CDW as well as its spatial variation in the vicinity of the defects. This work has been done in collaboration with V.ILAKOVAC, Q.LIU and S.RAVY. It has been partly supported by the CEC ESPRIT - Basic Research Action MOLCOM 3121.

DS-12.02.07 SMALL AND LARGE ANGLE SCATTERING OF ALLOYS CONTAINING COHERENT PRECIPITATES. By G. Kostorz, Inst. of Applied Physics, Swiss Federal Institute of Technology (ETH) Zürich, Switzerland.

A recent study of the small angle x-ray scattering of Al-rich Al-Ag single crystals (Ph.A. Dubey, B. Schönfeld and G. Kostorz, *Acta Met. Mater.*, 1991, **39**, 1161-1170), resulted in a model for the internal structure of Ag-rich Guinier Preston zones (ϵ) forming after an appropriate heat treatment. For the proposed Ag-enriched outer layer of the precipitates, additional confirmation was sought by a diffuse x-ray scattering experiment. The results and the reliability of the information obtained will be discussed for this alloy and other related binary systems. In Ni-rich Ni-Al-Mo alloys, Mo serves to modify the mismatch δ of lattice parameters of the f.c.c. matrix and the coherent, ordered γ precipitates forming during decomposition at intermediate temperatures. Single crystals were grown and small angle neutron scattering was used to study the growth rate, size, shape and arrangement of the precipitates as a function of δ in considerable detail. Dependable data for δ were obtained from high-resolution x-ray diffraction and subsequent analysis of broadened Bragg peaks. The value of δ has a dramatic influence on the decomposition kinetics and the morphology of these two-phase systems.

PS-12.02.08 FULLERENES AND THE STRUCTURE OF CARBONS

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The discovery of the cage-like molecular allotropic forms of carbon, the fullerenes, in particular C_{60} ("buckminsterfullerene"), has been extensively documented (H. W. Kroto, *Angew. Chem. Int. Ed. Engl.*, 1992, **31**, 111-129). In C_{60} it was postulated that a carbon atom is located at each vertex of a truncated

icosahedron. This structure was subsequently confirmed in single crystal and powder preparations variously using spectroscopy and diffraction (W. Krätschmer et al., *Nature*, 1990, **347**, 354-358; W. L. F. David et al., *Nature*, 1991, **353**, 147-149).

The possible role of the fullerenes in the constitution of semi- and non-graphitic carbons is considered in the context of (a) several recent studies, (b) the conclusions drawn in earlier investigations on carbons, including the anticipation of cage-like structures by J. Gibson, M. Holohan, and H. L. Riley (*J. Chem. Soc. Lond.*, 1946, Part I, 456-461), and (c) the way in which we may now interpret some of Rosalind Franklin's very detailed analyses of carbons (*Acta Cryst.*, 1950, **3**, 107-117).

PS-12.02.09 STRUCTURAL STUDY OF AMMINE GROUP IN $Ni(NH_3)_6Cl_2$ BY X-RAY DIFFRACTION. By M.Shiono*, Y.Yada, N.Achiwa, Department of Physics, Kyushu University, Higashi-ku, Fukuoka, Japan and N.Koyano, Research Reactor Institute, Kyoto University, Kumatori, Osaka, Japan.

Crystals of Hexa-ammine Metal complexes are commonly known to have disordered structures due to the rotational motions of the ammonia molecules. We have analysed the electron density distributions of hydrogen atoms in $Ni(NH_3)_6Cl_2$ single crystal (space group $Fm\bar{3}m$, $a = 10.080(1)\text{\AA}$) by X-ray diffraction. Difference Fourier synthesis is used in order to clarify the density of hydrogens.

Data were collected with 4-circle diffractometer, Rigaku AFC-5R. Monochromatized Mo $K\alpha$ radiation was used. The total number of reflexions measured was 3699 ($(\sin\theta_{max}/\lambda) = 1.09\text{\AA}^{-1}$). Averaging procedure gave 328 independent reflexions. Least-squares refinement and D-synthesis were performed with 145 reflexions ($F \geq 3\sigma(F)$).

The D-Fourier map of the hydrogen density is shown in Fig.1. The square figure with a peak at the each corner is comparable with the neutron diffraction result of $Ni(ND_3)_6Br_2$ (Hoser, A., Prandl, W., Schiebel, P. and Heger, G. (1989). *Physica B*. **156-157**, 85-87.). The map in (001) plane is shown in Fig.2. Cross sections of the hydrogen density are clearly seen. In addition, density of lone pairs of nitrogens appears across the triangular craters from the hydrogen density.

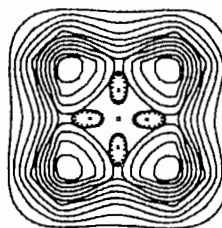


Fig.1

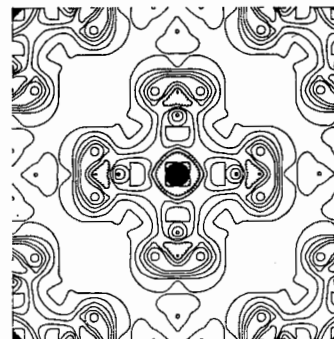


Fig.2