

ML-10.02 CRYSTAL STRUCTURE AND SUPERCONDUCTING TRANSITION OF HIGH T_c MATERIALS

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High-temperature superconducting crystals (HTSC) are a unique class of compounds for structural studies. They are remarkable not only because of their superconducting properties, which is important as such, but also because they exhibit diverse structural effects. Microtwinning, statistical occupancy of the atomic sites, probable inconsistency between the local and macro symmetry, incommensurate modulation of the structure - that is but a short list of structural specific features of HTSC. Besides, their composition is variable, their structure and properties are to a large extent dependent on the preparation conditions and thermal treatment of samples, therefore, there are hardly any other objects to be found in which all the above mentioned specific features are encountered.

In some cases the structural effects can result in difficulties in the determination of the true symmetry of HTSC crystals. The most vivid example is (La,Sr)₂CuO₄ crystals, whose orthorhombic phases are twins⁴ by pseudomerohedry over the (110) planes. Due to a small difference in a and b parameters the reflections from different twin patterns almost fully overlap. Special techniques are required for a reliable detection of the twinning effect. If they are taken into account correctly, the determination of the space group is no problem, as a rule. Another specific feature of (La,Sr)₂CuO₄ crystals is a statistical Sr atom distribution over La sites. Depending on the quantity of the added Sr, the distribution is either odd or ordered. We have shown that Sr ordering influences drastically the superconducting transition temperature.

An ordered O atom distribution in the structure of the orthorhombic phase of YBa₂Cu₃O_{7-d} plays an important role as well. The incorporation of Al or Pt impurity atoms into the Cu₁ site, as well as vacancies at this site can give rise to tetragonal macrosymmetry. We suppose that in this case the orthorhombic microsymmetry is retained. Therefore, a macrotetragonal crystal can be regarded as a micro (nano?) twin made of blocks with orthorhombic symmetry. Such interpretation is in good agreement with crystal-chemical rules which regulate oxygen coordination of copper atoms.

The superconducting phase transition is inevitably accompanied by qualitative changes of the electronic structure of the substance. The question is whether the crystal structure undergoes significant changes in this case. The data on the superconducting phase of YBa₂Cu₃O₇ are controversial. The study of Tl-containing 2212 single crystals reveals a slight effect due to redistribution of valency interaction of Cu in the CuO₅ pyramid layer. Admittedly, it is these layers that are the structural elements responsible for superconductivity. Apparently, further studies of compounds with other types of "superconducting" layers (eg. CuO₆ octahedra in Tl-2201) will give an answer to the above question.

ML-11.01 NEUTRON AND X-RAY REFLECTOMETRY OF SURFACES AND INTERFACES by R.K.Thomas, Physical Chemistry Laboratory, Oxford University, South Parks Road, Oxford, OX1 3QZ UK

Neutron and x-ray specular reflection at grazing incidence give information about structure normal to an interface on a length scale appropriate for many molecules adsorbed at interfaces. Although such measurements have recently become relatively routine there is a need for more systematic interpretation. This can be done by using partial structure factors in conjunction with either isotopic labelling (in neutron reflection) or a combination of x-ray and neutron data. The method is particularly powerful because simple relations may often be derived between the partial structure factors.

The determination of the structure of amphiphilic layers at the surface of aqueous solutions, using the above methods, will be described in detail. The partial structure method allows the separation of the contributions of each part of the amphiphile to the structure of the surface. Furthermore the effects of roughness of the surface are easily distinguished from true structural features.

ML-12.01 DECAGONAL QUASICRYSTAL AND CRYSTAL-LINE APPROXIMANTS, By K.H.Kuo, Laboratory of Electron Microscopy, Chinese Academy of Sciences, P. O. Box 2724, 100080 Beijing, China

1. *Decagonal quasicrystal (DQC)* is a 2D QC with a periodic tenfold rotational axis. Its high-resolution electron microscopic (HREM) image shows a quasiperiodic array of decagons. This aperiodic array is lifted to 5D space and projected onto a 2D external space. The majority of projected points fall inside a decagon. This supports the Penrose tiling model with long range position order. 2. *Crystalline approximant (CA)* has a composition and local structure similar to a QC. Its electron diffraction pattern shows a tenfold array of strong diffraction spots analogous to that of a DQC. By substituting a rational ratio of two consecutive Fibonacci numbers for the irrational golden number $\tau=(1+\sqrt{5})/2$ along two quasiperiodic directions in the plane normal to the tenfold axis in a DQC, various CAs will result. The larger the Fibonacci numbers, the larger the lattice parameters. A dozen of hexagonal, orthorhombic and monoclinic Al-rich Al-TM (transitional metal) CAs with lattice parameters in τ inflations and as large as 9.8 nm have been found. 3. *Crystal structures of CAs*, such as the orthorhombic Al₃Mn and the monoclinic τ^2 -Al₃Co, have been derived from their kindred CAs with the aid of HREM images. This was further proven by X-ray diffraction analysis. The subunits in these structures are slightly deformed pentagons, decagons, stars, 36° or 72° rhombus, and they form a periodic network displaying various crystalline symmetries. 4. *DQC structural models* have been derived from an aperiodic arrangement of the structural subunits of CAs and they compare favourably with those determined by X-ray diffraction methods.