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Keywords: implantation, X-ray diffraction, amorphous scattering

MS82.29.3

Acta Cryst. (2005). A**61**, C104

Direct Observation of a H_2 Molecule Swallowed by Open-mouthed C_{60}

Hiroshi Sawa[a], Yasujiro Murata[b], Michihisa Murata[b], Koichi Komatsu[b], [a]*Photon Factory, High Energy Accelerator Research Organization (KEK).* [b]*ICR, Kyoto University, Japan.* E-mail: hiroshi.sawa@kek.jp

Various types of endohedral fullerene complexes are known to date. However the metallofullerenes are generally produced by arc-discharge method, but the use of such extremely drastic conditions is apparently not suitable for encapsulation of unstable molecules or gases. We recently succeeded in incorporation of a H_2 molecule in 100% into a derivative of an open-cage C60 [1]. In order to observe the endohedral H_2 molecule directly, the X-ray diffraction analysis using synchrotron radiation were carried out. We observed a single H_2 molecule encapsulated in fullerene cage using structure analysis and maximum entropy method [2]. This H_2 molecule is floating inside of the hollow cavity and considered to be completely isolated from the outside (Fig.1).

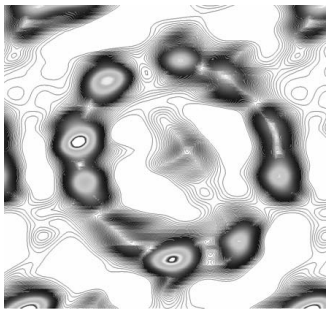

Fig.1. The MEM electronic density distributions of H2 endohedral open-cage C60.

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Keywords: fullerenes, synchrotron X-ray diffraction, single-crystal structure analysis

MS82.29.4

Acta Cryst. (2005). A**61**, C104

Anomalous X-ray Scattering Methods for Structure Investigations of Semiconductor Nanostructures

Václav Holý[a], Julian Stangl[b], Günther Bauer[b], Tobias Schülli[c], Till Hartmut Metzger[c], [a]*Charles University Prague, Czech Republic*. [b]*J. Kepler University Linz, Austria*, [c]*ESRF Grenoble, France*. E-mail: holy@karlov.mff.cuni.cz

X-ray study of the structure of semiconductor nanostructures (quantum dots and wires) is a challenging task. Several methods have been developed for the determination of shape and local chemical composition of quantum dots and wires (see [1] for a review); the methods are based on a surface-sensitive scattering geometry, where the penetration depth of the incoming x-ray beam is limited by a very small incidence angle. Usually, a direct determination of the structure from the measured data is not possible; instead, the experimental data are fitted to a suitable structure model.

An anomalous x-ray scattering experiment uses two different x-ray energies close to and far away from the absorption edge of a selected element [2]. By comparing the data obtained at these energies one can determine the local chemical composition in the nanostructures without using any model *a-priori*. Moreover, measuring the energy dependence of the diffracted intensity close to the absorption edge (diffraction anomalous fine structure – DAFS) one can determine the local atomic ordering in the nanostrucures [3].

Several examples of anomalous scattering and DAFS experiments will be presented and the limits of these methods will be discussed.

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Keywords: nanostructures, surface X-ray scattering, anomalous scattering

MS82.29.5

Acta Cryst. (2005). A**61**, C104

Magnetic Imaging of Biquadratic Coupling in Ferromagnetic Bilayers*

George Srajer[a], D. Haskel[a], J. C. Lang[a], C. K. Stevenson[a], Y. Choi[a], J. S. Jiang[b], S.D. Bader[b], [a]*Advanced Photon Source, Argonne National Laboratory.* [b]*Materials Science Division, Argonne National Laboratory.* E-mail: srajerg@aps.anl.gov

Physical properties of thin magnetic nanostructures are dominated by exchange interactions between the layers. These interactions in most cases induce collinear coupling of spins. The much smaller noncollinear coupling of spins is also allowed through the biquadratic term in the exchange Hamiltonian. Recently, Vlasko-Vlasov et al. [1] observed unusual coupling of two ferromagnetic layers in contact. They studied junctions of SmCo and Fe layers and deduced noncollinear magnetic configurations based on magneto-optical imaging of the top Fe layer. To simultaneously probe the magnetization in the surface Fe layer and in the buried SmCo layer, we used circularly polarized synchrotron radiation. Element-specific hysteresis loops were performed by tuning the energy of the synchrotron radiation to the absorption edges of Fe (7.110 keV) and Sm (6.710 keV). In addition, fluorescence imaging of magnetic domains was performed by using focused circularly polarized x-rays (1 μm by 1 μm). Hysteresis and imaging data unequivocally demonstrated that the Sm and Fe magnetizations were perpendicularly coupled. *This work is supported by the U.S. DOE, Office of Science under Contract No. W-31-109-ENG-38.

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Keywords: magnetic structures, synchrotron X-rays, X-ray imaging

MS83 COMPUTATIONAL PROBLEMS AND SOLUTIONS FOR APERIODIC CRYSTALS

Chairpersons: Christer Svensson, Vincent Favre-Nicolin

MS83.29.1

Acta Cryst. (2005). A**61**, C104-C105

Towards the Routine Application of Computing System Jana2000

Michal Dušek, Václav Petříček, *Institute of Physics, Praha, Czech Republic.* E-mail: dusek@fzu.cz

The program Jana2000 [1] was originally written as a special refinement tool for modulated structures. During almost 20 years of development it integrated many crystallographic methods that gave the program exceptional flexibility. On the other hand, it has been always difficult keeping all the possibilities accessible not only for specialists, but for everybody interested in solution of a modulated structure. With progress in the experimental methods the number of modulated structures grows amazingly. Many of them can be solved relatively easily using just the basic knowledge about aperiodic crystals.

We anticipate this trend by creating set of wizards for guiding the user to solution of simple structures, keeping - of course - all possibilities opened to complicated cases. This development is far from completion but important steps have been already done. First of all - unified tools are available for standard and modulated structures and also for powder and single crystal data that allow solving the basic and modulated structure using the same program. The phase problem (in three dimensions) can be resolved by rendering the data to SIR or EXPO and reading back the results. Automatic symmetry determination is possible for space as well as super space groups. Adding of hydrogen atoms (and generally defining geometry constraints for standard and modulated structures) has been automated to the extent usual in routine crystallography. In the lecture we shall present the outlined methods and envisaged features of Jana2005.