Microsymposia

This purpose will be illustrated by two examples. The disorder previously evidenced either by the splitting of atoms over different sites in tunnels of Sr$_2$(AlO$_2$)$_3$Bi$_2$O$_3$ [1] or the large ADP of oxygen atoms of CsMPO$_2$ [2] (Fig. 1) can be elucidate just by observing satellite reflections (Fig. 2) and then solving the modulated structure [3] using superspace formalism.


Keywords: aperiodicity, disorder

MS.88.5


Relationship of the aperiodic structure to the nanostructure

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This paper aims to evidence that some typical aperiodic crystal materials, such as the composite and the modulated ones, show a nanostructured material and just this nanostructure conditions the unique properties of the aperiodic material. The fragments, as the “basic units”, that make up the material are nanoscaled and aperiodically arranged with respect to each other. To the preparation of such nanostructure, the consolidated and fashioned fragments (as the nanoparticles or nanolayers) can be composite or modulated in a bulk material. This process is widespread in biology with the variety of self-assembly [1].

The key problem is, the nanoworld is of quantum nature that creates the peculiar dynamics of the odd electrons (i.e. the active electrons, they show the unpaired spins) in the nanostructured material [2, 3]. And just this peculiar electron dynamics breeds the prominent features of the aperiodic material. For studying these effects, Electron Spin Resonance (ESR) can offer an especially efficacious help means.

From the experimental and theoretical results with ESR in combination with other methods, some peculiarities of dynamics of electrons in the real aperiodic materials can be summarized as follows:

1) The active electrons in the aperiodic structure can be considered as the Quasi-Free Electrons (QFEs) moving in a Nano Resonant Cavity (NRC) with nanoparticles or in a Nano Wave Guide (NWG) with nanowires and nanolayers of the nanoscaled Short-Range Order.

2) The QFEs must obey a “Compressed Distribution” as a normal Gauss form of the state density. This very outstanding peculiarity follows:

- The interaction of the QFEs with the surroundings (Jahn-Teller effect) can generate a strong local crystal field of low symmetry in the aperiodic structure, especially in the aperiodic structure of the living body.

- When the scale of the fragments (particles, wires or layers) extend out of the nanorange, the material becomes polycrystalline and its above mentioned peculiarities will disappear.

- As illustrative examples, the results on Composite Fivefold Aperiodic Structure of Dental Enamels [4] and Superconducting Nanomechanism in YBCO Compounds [5] are briefly analysed.


Keywords: aperiodic, nanostructured aperiodic, aperiodic structure and nanostructure

MS.89.1


Twenty years of the crystallographic information framework

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The Crystallographic Information File (CIF) format was adopted by the International Union of Crystallography (IUCr) as the standard for exchanging and archiving crystallographic information in 1991 [1] and has continued to be developed actively during the past two decades.

The initial specification used the Self-Defining Text Archive and Retrieval (STAR) format developed as a universal exchange mechanism [2] and subsequently used in a number of other scientific fields including botany, chemistry and NMR structure determination. Later developments including machine-readable dictionaries of data identifiers with associated attributes helped to separate the semantic content of CIF from its syntactic structure, allowing easy interchange with XML or other widespread formats. Work has continued to extend the dictionary definition language to include information about the permitted data content in a manner that computers can process directly. Latest work focuses on specifying algorithmic relationships between individual data items.

The result has been an information system that includes its own recipes for computational validation of related data items. This has allowed CIF to be used in electronic publishing and in database applications, where validation, integrity checking and format transformations can be performed automatically and with no or little information loss. Consequently, CIF underpins the entire publishing workflow of IUCr journal articles reporting crystal structures [3], and is an important intermediary in the management of the curated structural databases such as Protein Data Bank [4] and Cambridge Structural Database.

CIF separates semantics from syntax to a large degree, and has a rich granularity in its item descriptions. It adopts a uniform approach that treats experimental data and associated descriptive information (often called ‘metadata’) in the same way. It has come to be accepted as a standard across the entire field of crystallography that can handle raw image data, information about structure solution and refinement, the positional and displacement parameters of a derived structural model, and all aspects of an associated publication. In all these ways, it serves as a model for effective information flow – a model that is increasingly being used for case studies by other disciplines seeking to improve their data management strategies [5]. Predating the Web and XML, CIF remains at the leading edge of scientific information management systems.

MS.89.2

Data management for photon and neutron sources

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Photon and Neutron sources, such as the UK’s Diamond Light Source and ISIS Spallation Neutron Source are large-scale facilities providing high resolution data for crystallography and other materials analysis techniques. Traditionally, the raw data generated from such facilities has been managed by the instrument and user scientists themselves. However, the current generations of such facilities can undertake a large number of experiments, and generate hugely increased volumes of data. As a consequence, the traditional approach has become unsustainable and a more automated approach to data management has had to be developed.

In this talk, I shall outline the data management infrastructure developed within STFC to manage raw data. This infrastructure takes an integrated approach to aggregate, store and catalogue data generated at ISIS and Diamond. In particular, I shall describe ICAT, a suite of tools which catalogues data as it is generated by beam lines, and provides access to that raw data to its user community, allowing them to search and retrieve their data, within the facilities themselves or within their home institution. This is provided using a service application programming interface so that a variety of different search and analysis tools can be interfaced to search and access the data, and also register and catalogue derived data.

The management of raw data is part of a wider scientific process, starting from proposals for research through to the publication of results. We shall further discuss how the ICAT and similar tools can be extended to support this wider process by allowing data to be federated across a number of different data sources and also linking the raw data to analysed and published data so that the provenance of data can be tracked; this is being considered in the project Integrated Infrastructure in Structural Sciences (I2S2). This allows data to be formally cited and reused, and results to be validated. We relate this work to the publication process being developed by the International Union of Crystallography, tracing the relationship between raw data generated from beam lines, and the CIF files lodged during the publication process.

This integrated data infrastructure is being taken forward by the European Photon and Neutron Data Infrastructure initiative (PaNData), a consortium of European photon and neutron sources serving an expanding user community of tens of thousands of scientists across Europe. The experiments in these facilities are of increasing complexity, they are increasingly done by international research groups and many of them will be done in more than one laboratory. The resulting data needs to be accessible over the Internet and remain on-line until the results are published and in many cases much longer to allow re-processing and to allow for the preservation of knowledge. PaNData is developing common data formats, data and software catalogues within the framework of a common data policy.

Keywords: data management, information management, large-scale facilities

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