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From the Braggs to José Alfredo: Exploring the *Rare Synchrotron Worlds*

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Abstract

The auditorium is invited to a trip around the world of synchrotron crystallography. As a motivational resource we appeal to a parallel with the *rare worlds* of Mexican composer José Alfredo Jiménez.

The journey begins with a quick sampling of newly created materials with extraordinary properties. We discover shape-memory alloys, levitating superconductors, super-hydrophobic materials, artificial neurons, super thermal insulators, auxetic systems and invisible metamaterials.

Physical properties have their origin in the materials' structures. The central station of our tour is a visit to the incredible world of the facilities to investigate in detail the materials' structures, in particular crystal structures. The operation and performance of electron microscopes, research reactors and synchrotrons are observed. We visit Chihuahua, the Lady of the Desert. There, at ***CIMAV***, the ***SEM, TEM*** and ***STEM*** microscopes show us from the components of the muscular micro-anatomy to the individual atoms of a superconducting ceramic. We fly over the Golden Gate of San Francisco and at the ***Stanford Synchrotron*** we explore the perfection of Naica's giant

crystals with diffraction and x-ray absorption techniques. We cross North America and fly over the Atlantic ocean, heading for the United Kingdom. From the plane, if we're lucky, we identify the Stonehenge ring. We land at the ***Diamond Light Source***. Luis Jr. shows Diamond diffractometers, which have X-ray beams so intense that they evaporate the biological samples in fractions of a second. From instantaneous diffraction experiments, researchers at Diamond are able to decipher biological structures of high complexity. We go to continental Europe, to the South of France. We fly over Mont Blanc and land in Grenoble. There we visit our friend Juan at the ***Institute Laue-Langevin (ILL)***, a research reactor with neutron beams intense enough to decipher (among other things) magnetic structures and the locations of light atoms. Neighboring the ILL we find the great ***European Synchrotron Radiation Facility (ESRF)***. The energy spectrum of ESRF photons is as broad as that of the investigations carried out there. Fortunately Mexico has Hiram, our microabsorption research facilitator there. From Grenoble to the South. We strolled through Venice on our way to the ***Elettra Synchrotron***. We study spectra, diffractograms, magnets, ceramics, materials subjected to high temperatures and under electric fields. In short, we carry out state-of-the-art research on the synchrotrons within our reach.

Our next stage is a world of abstraction or fantasy: the mathematics of crystallography.

The crystallographers move in an inverted world, something akin to the *camera obscura* images of Vera Lutter. The ***reciprocal and diffraction spaces*** lead us to decipher the direct structures of the crystals. The abstract world of ***mathematical groups*** provides us with indispensable tools, from the systematic characterization of the structural symmetry of any object to the selection rules for infrared and Raman spectroscopy. The classical and the magnetic crystallographic groups allow us to predict the existence or not, and the tensorial structure, of the physical properties. The Neumann Principle is evident in the anisotropy of crystal properties, as described in the ***Material Properties Open Database*** (MPOD).

At the atomic level, the crystalline world is one of continuous competition between ***order and disorder***. With our synchrotron arsenal we work to decipher it. The sharp ***diffraction maxima*** provide us with the overall crystalline structure of the most diverse single- and polycrystalline materials, from simple inorganics to complicated drugs and biological objects. The ***diffuse scattering*** informs us about amorphous structures and local (thermal, elastic, electromagnetic) disorders.

X-ray absorption spectroscopy allows us to observe structures at a local level, with a different approach. XANES, EXAFS and other techniques shows us the ionic valence states, the pair distribution function, with elemental selectivity, and the identification of amorphous phases.

The synchrotron light illuminates for us the labyrinths of the Euler space, which is the space of crystalline orientations in a textured polycrystal. We measure orientation distribution functions and apply tools that model the influence of texture on the properties of polycrystals.

Results

The following is a representative example of our own work with synchrotron light: "X-ray study of maghemite-like spinel γ-$FeCrO_3$". High-resolution synchrotron radiation X-ray diffraction (XRD) patterns were obtained at the Stanford synchrotron, beamline 2-1 and processed by means of the Rietveld method. Investigated maghemites were studied by XAFS in both Fe and Cr K-edges to clarify the short-range structure. Theoretical modeling of X-ray absorption near edge structure transitions was performed. The extended X-ray absorption fine structure (EXAFS) spectra were fitted considering the facts that the central atom of Fe is able to occupy octahedral and tetrahedral sites, each with a weight adjustment, while Cr occupies only octahedral sites. Interatomic distances were determined, by fitting simultaneously both Fe and Cr K-edges average EXAFS spectra. The results showed that the cation vacancies tend to follow a regular pattern within the structure of the iron-chromium maghemite ($FeCrO_3$). All the figures bellow are representative of this study.

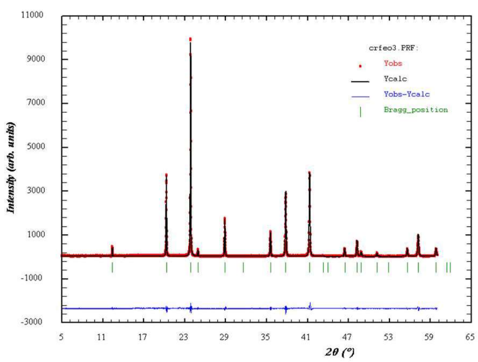

Figure 1: High resolution XRD

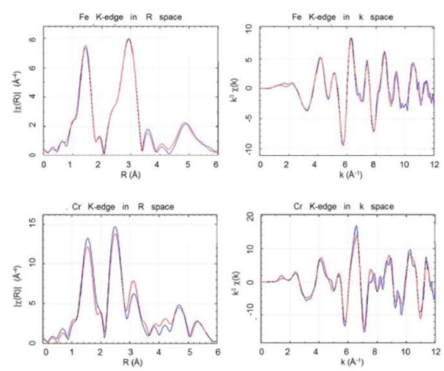

Figure 2: EXAFS

Future perspective

Human curiosity largely escapes the limits of planet Earth. Crystallography already has detailed reports on the structures of the Moon's and Mars' minerals. Work has been done with samples brought to Earth by the Apollo 11 expedition and is underway today by the Martian rover

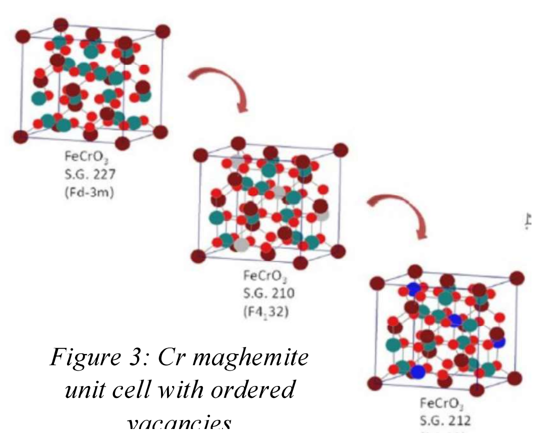

Figure 3: Cr maghemite unit cell with ordered vacancies

Curiosity. The detection of water in Martian clays from the 2D diffractograms obtained in situ by Curiosity and interpreted by the Rietveld method on Earth is explained. Recently (September 5, 2017) marks the 40th anniversary of the launch of the Voyager mission into interstellar space. This automatic station, powered by a thermoelectric generator of radioisotopes, has sent to the Earth abundant information about the outer planets of the Solar System (SS). It is already outside of the SS and carries a greeting of the humanity to possible extraterrestrial civilizations. The presentation concludes with humanist commentaries by the renowned Carl Sagan (1934-1996).

Acknowledgements

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