MS40 O1

Learning the basics of crystallography on the web.
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Many interesting websites are currently offering a large selection of crystallographic materials ranging from lecture notes and wikipedias to interactive simulations. The web being probably the primary source of information, the interested reader will quickly find the information he is looking for. However, the novice in the field of crystallography will certainly face some difficulties in learning the basics of crystallography from the web mainly because of the lack of structured information provided from different websites.

In order to help anyone wishing to acquire elementary notions of crystallography, we have recently published an interactive course presenting the basics of crystallography, which is freely accessible on the web [1]. The course is based on a series of applets, *i.e.* platform independent pieces of software, not only developed in the author's lab but also by other authors.

The course covers the basics of symmetry including point and space group, reciprocal space and X-ray diffraction, Fourier transform, structure solving techniques and some elements of crystalline architectures. It is also highly interactive, *i.e.* each concept is illustrated by interactive demonstrations. Solving exercises will facilitate understanding of the concepts. Therefore, the course contains approximately 50 exercises, which can better be solved by using the available applets.

The course can be used in many different ways. For example, the applets can be used interactively by a teacher in front of a classroom in order to illustrate some new concepts. Anyone wishing to understand the basics of crystallography can also use the course privately. Any other method, which is a combination of both examples, is also conceivable.

In order to provide some additional help, we have setup a web forum where anyone can ask questions specific to the course or make some suggestions. It is hoped that the community of users will provide many answers.

[1] G. Chapuis and N. Schoeni, eCrysgtallography course, http://escher.epfl.ch/eCrystallography

MS40 O2

Molecular architectures, nanometric voids and computer graphics
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Keywords: molecular graphics, nanovoids, structure

The revolution caused by the quantum mechanics in the early years of the last century, gave to the chemists the proper conceptual tools to understand, at atomic level, the structure of simple molecules and of complex enzymes.

The enormous development of the diffractometer techniques and of the visualization/simulation of the molecular world by powerful computers has allowed to study and understand how chemical forces are responsible of the formation of extraordinary molecular and crystalline structures whose features span from the coding for genetic information through the building up of nanometric channels to selectively drive ions in and out the living cells or to achieve controlled reactions in zeolitic materials. The interpretation and the study of molecular architectures is nowadays carried out by means of a virtual microscope, i.e. a computer and a sophisticated software which allows to virtualize nanometric details with an unprecedent level of control. In this contribution the control that chemical forces can exert at the nanometric level will be highlighted by analyzing the case of water ice, the aquaporine channel mechanism, the diffusion of molecules in the nanocavities of zeolites and in hybrid crystalline materials. The presentation will also stress how the comprehension of the above cases at the molecular level is made possible by the use of modern computer graphics software. Many of the aspects discussed here can be expanded by the students by accessing to the structural and bibliographic information through internet and proper computer graphics software.

MS40 O3

Imaging Fourier Transforms for Crystallography
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Keywords: Teaching physics and crystallography, Fourier Transform, Digital Images

Teaching crystallography implies the development of notions and tools such as Fourier Transforms, convolution, resolution etc. that are not necessarily evident for beginners. Whereas kinematic diffraction theory is widely spread with lot of books and teaching manuals, students are often left alone in front of the above typical notions and one may feel a need in tools allowing to experience these concepts with its own hands. In order to help students and beginners in the field, some interactive web sites have been created (*e.g.* reference [1]) and praticals using the Mathematica software were recently developed by Dumas *et al.* [2].

In this communication we will address an analogy between diffraction in crystallography and digital image manipulations (Fig. 1), using the free part of the electron microscopy Digital Micrograph friendly software from Gatan [3].
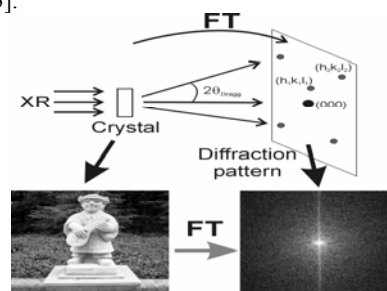

Fig. 1 Analogy diffraction / digital images