MS40 O1

Learning the basics of crystallography on the web.
Gervais Chapuis, *Laboratoire de cristallographie, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland.* E-mail: gervais.chapuis@epfl.ch

Keywords: crystallographic education, computer-aided crystallographic teaching, undergraduate education crystallography

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
Piero Ugliengo *Department of Chimica IFM, University of Torino, Italy.*
E-mail: piero.ugliengo@unito.it

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
Emmanuel Aubert, Claude Lecomte Laboratoire de Cristallographie et Modélisation des Matériaux Minéraux et Biologiques, UMR CNRS7036, Nancy-Université, Nancy, France. E-mail: emmanuel.aubert@lcm3b.uhp-nancy.fr

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].

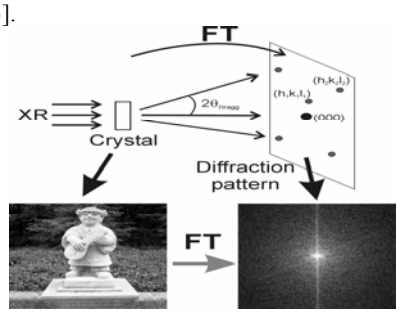

Fig. 1 Analogy diffraction / digital images

We will first describe how digital images are coded and introduce Fourier Transform. Then we will use the analogy with X-ray diffraction to address some points about resolution (Fig. 2), about the phase problem in crystallography and the relation between Direct & Reciprocal spaces.

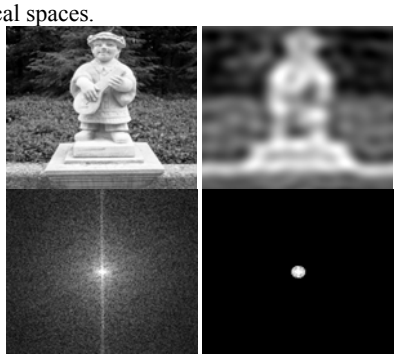

Fig. 2 Digital images and their Fourier Transforms

[1] Schoeni, N. and Chapuis, G. (2006) http://lcr.epfl.ch/page37304.html
[2] Dumas, P., Vanwinsberghe, J. and Cura, V. (2006) Crystallographic Teaching Commission of the IUCr Newsletter No.**1** 4-10.
[3] Gatan (2003). Gatan Inc., Pleasanton, CA, USA.

MS40 O4

Plane Symmetry in Traditional Javanese Batik Patterns Annegret Haake[a], Haryani Winotosastro[b], *[a]Jaminstr., 11 b, D-61476 Kronberg, Germany. [b]Tirtodipuran 54, 55143 Yogyakarta, Indonesia.*
E-mail: haake.xx-tex@t-online.de

Keywords: batik art, plane symmetry, teaching aid

Batik is a traditional method of resist cloth-dyeing in Java, Indonesia. Liquid wax is partly applied on the cotton before dyeing in cold solutions, so that the spots covered by wax remain uncoloured. In the past, only plant dyes were used. The cloths measured 1 m x 2,50 m and were worn as a skirt by both, men and women. At traditional occasions, the cloths are still worn in the same way. Most of the countless motifs are of pre-Islamic origin (before 15th century). It is remarkable that all these motifs follow the laws of plane symmetry in spite of they are drawn by hand; the patterns are carried out till the natural border of the cloth. The predominant symmetry groups are p2, p4mm and pm, but p1, cm, p4 and other groups with rotational symmetry 1, 2 or 4 can be realized in traditional batik patterns. In opposition to that, rotational 3- and 6-fold symmetries are rarely found in real traditional patterns. In a former publication [1], it was already stated that the symmetry elements in traditional Javanese batik patterns were symbolizing the Asian philosophy models "Dualism" and "Mandala" (or Javanese "Mancapat"). It was also said that the unlimited translational symmetry of a pattern symbolized infinity, and at the same time it had a meditational effect on the batik-artist who was concentrated on her work [2]. (The waxing is a domain of women). Besides the Indian compass model "Mandala" the most important Asian philosophy-model is "Dualism"="co-existence of opposites" (male/female, dark/light, +/-, heaven/earth, yin/yang, left/right, above/below etc.). There are many examples for "Dualism" in batik designs. Dark/light is produced by the dyeing, yin/yang is representing the rotation about 180°, and above/below is given by the symbols for "upper and lower world" in "Semen"-patterns. Left/right is found in Mancapat examples as well as in the central motifs of "Semen"-patterns. „Semen"-patterns describe the environment of the Javanese through symbolic pictures of Hinduistic origin, which are symmetrically ordered and repeated in two directions. That means, the motifs appear in fixed distances and surroundings. As well the motifs themselves, as their situation to each other had a symbolic meaning, which should be positive for the wearer. After a law of the 18th century, some patterns were dedicated to the ruler and his family, only. Those patterns were called „Larangan" (= forbidden patterns). Educated Javanese pay attention to that, until today. The cloth, which was exclusively made for the ECM24-congress, contains many ancient patterns with their names. The patchwork-look is based on real patchwork jackets, which were worn by animistic priests and later the Islamic ruler of Yogyakarta in Central Java.

[1] Haake, A., Comp. Math. Applic. Vol. 17, pp. 815-826, 1989.
[2] Hardjonegoro, K.R.T., Indonesian Textiles, Proc. 1979, pp. 229-242

MS40 O5

Olex2: Making Small-Molecule Crystallography Accessible To Everyone. Horst Puschmann, Oleg Dolomanov *Department of Chemistry, University of Durham, UK.* E-mail: horst.puschmann@durham.ac.uk

Keywords: molecular graphics, small molecule, model building

Olex2 is a new, powerful molecular graphics program that provides a whole host of fully customizable tools for small-molecule crystallography to suit the analytical chemist and practicing crystallographer alike.
What sets it apart from most other programs of its kind is the fact that Olex2 can interact seamlessly and intelligently with refinement programs such ShelXL. Moreover, Olex2 incorporates its very own refinement program (based on the cctbx), making new areas of small-molecule refinement accessible for the first time. Highly sophisticated refinement tools–those traditionally thought to be only usable by fully trained expert crystallographers–can be accessed and addressed intuitively, thus making building even complicated models very easy.
The User Interface to Olex2 has a high degree of redundancy: the entire program can be driven from the command line only (mostly using the syntax familiar from ShelXP), context menus (right-click) and a highly flexible and customizable GUI provide full flexibility while not compromising the underlying features.
Olex2 is available free of charge for academic use and can be downloaded from http://www.olex2.org.