Ομιλία, Αίθουσα σεμιναρίων 005, Τμήμα Βιολογίας Πανεπιστημίου Πατρών

7 Μαίου 2010 και ώρα 2 μ.μ.

Ομιλητής Dr. Stavros Nicolopoulos

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Electron crystallography commission

Την **Παρασκευή 7 Μαίου 2010** και ώρα 2.00 μ.μ. στην αίθουσα σεμιναρίων (005) του τμήματος Βιολογίας του Πανεπιστημίου Πατρών, θα ομιλήσει ο κ. Σταύρος Νικολόπουλος με θέμα: "**Combining precession electron diffraction-3D electron diffraction tomography and powder X-Ray diffraction to solve complex structures**"

Abstract

Precession electron diffraction (PED) is a new promissing technique for electron diffraction patterns collection very close to kinematical condition (like in x-ray diffraction) allowing this way to solve ab-initio crystal structures of nanocrystals. PED intensities are kinematical, (X-ray like), up to a thickness of 100 nm and they can be used to solve the structure of very small nanocrystals in a semi-automatic way. PED technique can be used in older or new TEM (100-400 kV) and is very effective tool to upgrade older instruments to modern electron diffractometry equipments.

X-Ray diffraction techniques (synchrotron or conventional sources) are currently used for standard ab-initio structure determination; however in many cases structure solution is not possible for several reasons like reflection overlap inherent to powder data , poor crystallization , peak broadening related to nm crystal size or existence of unknown polymorprhs.

Taking into account that X-Ray and electron scattering factors show similar trends with sin□□, strong and weak reflections in X-Rays are also observed as strong and weak quasi-kimematical PED reflections. Information coming from PED data (using TEM equipped with precession) is very useful for identifying weak X-Ray reflections, estimating accurate individual *hkl* intensity contributions in case of overlapping X-Ray intensities, and obtaining crystallographic phases of *hkl* reflections in ZA projections.
Information from PED can be combined with *hkl reflections from X-Ray* powder diffraction to accurately solve and refine *ab-initio* structures using either *charge-flipping* algorithms or direct methods.

On the other hand another exciting development in electron crystallography is the 3D diffraction tomography technique which consists in an automatic collection of a series

of randomly oriented PED patterns of the same crystal through the whole TEM angular range (usually from -45º to +45º) at 1º angular intervals.The resulting 3D electron diffraction set of reflections can be visualized as clear 3D picture of the reciprocal cell of the crystal ; exciting applications like direct cell determination, crystal defect (like twinning or streaking) or industrial applications like polymorph screening are possible now.