

The high accuracy to the angular change of a crystalline specimen was applied to the studies of strain in multilayers [3]. And then, many strain measurements at the interfaces of various multilayer materials have been successfully conducted. Recent years, strain analysis can be conducted using automatic analysis programs, which take account of dynamical diffraction effects [4].

In the present review, the large angle technique is explained, analyses of stacking faults and dislocations are demonstrated and examples of strain measurements of semiconductor layer materials are presented.

[1] Tanaka M. et al., *J. Electron Microsc.*, 1980, **29**, 408. [2] Wen J., Wang R., Lu G., *Acta Cryst.*, 1989, **A45**, 422. [3] Cherns D., Kiely C. J., Preston A. R., *Ultramicroscopy*, 1988, **24**, 355. [4] Kraemer S. et al., *Ultramicroscopy*, 2000, **81**, 245.

**Keywords:** LACBED, lattice defect identification, interface analysis

### KN33.30

*Acta Cryst.* (2005). A61, C8

#### Ultrafast Electron Crystallography

Ahmed Zewail, California Institute of Technology, Pasadena, CA, USA. E-mail: zewail@caltech.edu

In this talk, we will overview recent advances in crystallography bringing in the dimension of time in what we term ultrafast electron crystallography (UEC). The new approach make it possible to record frames of diffraction at different times and with resolution reaching the picosecond-femtosecond time scale. Examples will be given to recent studies of crystals, interfaces, and macromolecular structures. We will also compare with studies of isolated molecular systems. UEC promises to be a powerful advancement for many applications and we will conclude by highlighting some of the new directions.

**Keywords:** ultrafast crystallography, interfaces, macromolecules

### KN34.30

*Acta Cryst.* (2005). A61, C8

#### Structural Studies of Amyloid

David Eisenberg<sup>1</sup>, Rebecca Nelson<sup>1</sup>, Michael R. Sawaya<sup>1</sup>, Melinda Balbirnie<sup>1</sup>, Anders Ø. Madsen<sup>2,3</sup>, Christian Riek<sup>3</sup>, Shilpa Sambashivan<sup>1</sup>, Yanshun Liu<sup>1</sup>, Mari Gingery<sup>1</sup>, Robert Grothe<sup>1</sup>, <sup>1</sup>Howard Hughes Medical Institute, UCLA-DOE Institute for Genomics and Proteomics, Box 951570, UCLA, Los Angeles CA 90095-1570. <sup>2</sup>Centre for Crystallographic Studies, Department of Chemistry, University of Copenhagen, Universitetsparken 5, DK-2100 KBH, Denmark. <sup>3</sup>ESRF, B.P. 220F-38043 Grenoble Cedex, France. E-mail: david@mbi.ucla.edu

Numerous soluble proteins convert to insoluble amyloid fibrils having common properties. These fibrils are associated with neurodegenerative diseases, such as Alzheimer's and Parkinson's, and can also be formed in vitro. In the case of the yeast protein Sup35, conversion to amyloid fibrils is associated with a transmissible infection akin to that caused by mammalian prions. A seven-residue peptide segment from Sup35 forms both amyloid fibrils and closely related microcrystals, which reveal the atomic structure of an amyloid spine. It is a double  $\beta$ -sheet, with each sheet formed from parallel segments stacked in-register. Sidechains protruding from the two sheets form a dry, tightly self-complementing steric zipper, bonding the sheets. Within each sheet, every segment is bound to its two neighbouring segments via stacks of both backbone and sidechain H-bonds. The structure illuminates the stability of amyloids as well as their self-seeding characteristic.

Amyloid structure has also presented long-standing, fundamental puzzles of protein structure. These include whether amyloid-forming proteins have two stable states, native and amyloid, and whether all or only part of the native protein refolds as it converts to the amyloid state. We find that a designed amyloid of the well-characterized enzyme ribonuclease A contains native-like molecules capable of enzymatic activity. Also these functional molecular units are formed from a core ribonuclease A domain and a swapped complementary domain. These findings are consistent with the zipper-spine model for amyloid3 in which the fibrils are formed from 3D domain-swapped

functional units, retaining native-like structure.

**Keywords:** amyloid, protein structures, biological macromolecules

### KN35.30

*Acta Cryst.* (2005). A61, C8

#### The Surface Structure of Model Catalyst in Action Investigated by X-ray Diffraction

S. Ferrer<sup>(1)</sup>, Marcelo D. Ackenmann<sup>(2,3)</sup>, O. Robach<sup>(4)</sup>, B.L.M. Hendriksen<sup>(3)</sup>, I. Popa<sup>(2)</sup>, J. Frenken<sup>(3)</sup>, <sup>(1)</sup>ALBA Edifici Ciències. C-3 central. UAB. 08193 Bellaterra. Spain. <sup>(2)</sup>Kamerlingh Onnes Laboratory, Leiden University, PO Box 9504, 2300 RA Leiden. <sup>(3)</sup>ESRF, 6, rue Jules Horowitz, F-38043 Grenoble cedex, France. <sup>(4)</sup>CENG-CEA Avenue des Martyrs, F-38043 Grenoble cedex, France. E-mail: ferrer@cells.es

There are few techniques which allow to investigate surfaces at atmospheric pressures. One of them is surface x-ray diffraction which has detection limits of adsorbed gases below one atomic layer. The talk will describe experimental results on the adsorption of CO, H<sub>2</sub> and their reaction to form methane on a Ni (111) single crystal surface in a range of pressures from Ultra High Vacuum to 1 bar. The important role of surface carbide will be discussed. Also, results on the oxidation of CO to CO<sub>2</sub> on Pt(110) surfaces at atmospheric pressures will be reported. The experiments show that Pt oxides are better catalysts than pure Pt and that metastable oxides are formed under reaction conditions.

**Keywords:** synchrotron X-ray diffraction, heterogeneous catalysis, adsorption

### KN36.30

*Acta Cryst.* (2005). A61, C8

#### Strategies and Design Principles in Biomineralization

Lia Addadi, Steve Weiner, Department of Structural Biology, Weizmann Institute of Science, Rehovot, Israel. E-mail: lia.addadi@weizmann.ac.il

Organisms are able to produce mineralized skeletons with complex architectures, having unusual shapes and organization. This is the result of sophisticated strategies that control the design and construction of the materials at all hierarchical levels, from Angstroms to millimeters.

In order to understand the mechanisms used by organisms to build their skeletal materials, we study the various components of the mineralized tissues, the interfaces between them, their structures and relations of structure to function.

The minerals are deposited in a matrix composed of biological macromolecules. Common minerals used are the calcium carbonate polymorphs aragonite and calcite in the form of single crystals or polycrystalline ensembles. Organisms are able to override the crystal natural propensities, and can shape calcite and aragonite almost "at will". These features depend also on the involvement of transient amorphous precursor phases, which transform into single crystals in a slow controlled process [1]. All these properties stem from direct or indirect control of specialized macromolecules, whose sequences, structures and functions are only beginning to be understood [2].

[1] Politi Y., Arad T., Klein E., Weiner S., Addadi L., *Science*, 2004, **306**, 1161-64. [2] Gotliv B.A., Kessler N., Sumerel J. L., Morse D.E., Tuross N., Addadi L., Weiner S., *ChemBiochem*, 2005, **6**, 304-314.

**Keywords:** biomineralization, amorphous, calcium carbonate