analysis, metabolome analysis, gene disruption experiments, and other methods as necessary.

**Keywords: structural genomics, functional genomics, model organism**

**MS15.25.5**

*Acta Cryst*. (2005). A**61**, C26

**Structural Proteomics : a Rich Source of Purified Proteins for Functional Assays**

Aled Edwards, E. Kuznetsova, M. Proudfoot, S. A. Sanders, C. F. Gonzalez, O. V. Litvinova, A. V. Savchenko, C. H. Arrowsmith, A. F. Yakunin, *Banting and Best Department of Medical Research, University of Toronto, Toronto, Ontario, Canada M4G 1H1*. E-mail: aled.edwards@utoronto.ca

Structural proteomics efforts generate 2-3 times more purified proteins than structures. We have developed general enzymatic assays to screen individually purified proteins for enzymatic activity. The assays have relaxed substrate specificity and are intended to identify sub-subclasses of enzymes (phosphatase, phosphodiesterase, esterase, protease, dehydrogenase, and oxidase) to which the unknown protein belongs. Further biochemical characterization of proteins is facilitated by the application of secondary screens with natural substrates (substrate profiling). We demonstrated the feasibility and merits of this approach for hydrolases and oxidoreductases, two very broad and important classes of enzymes and identified over 40 new enzymes (phosphatases, phosphodiesterases, esterases). The screens were also applied to quickly characterize the large family of unknown proteins in *E. coli*, the haloacid dehalogenase (HAD)-like hydrolases.

**Keywords: structural proteomics, enzyme screens, phosphatases**

---

**MS16 HIGH RESOLUTION X-RAY INELASTIC SCATTERING**

***Chairpersons:*** Gian Carlo Ruocco, Alfred Baron

**MS16.25.1**

*Acta Cryst*. (2005). A**61**, C26

**Dynamics of Glassy Materials by High Resolution Inelastic X-ray Scattering**

Daniele Fioretto, *Dipartimento di Fisica, Università di Perugia. INFM - CRS Soft, Università di Roma La Sapienza.* E-mail: fioretto@fisica.unipg.it

The nature of short wavelength excitations in glassy materials is highly debated in the physics of disordered materials. What is the length scale beyond which the continuous homogeneous medium approximation breaks down in glasses? What is the microscopic origin of sound attenuation in strong and in fragile glasses? Is there any relationship between propagating acoustic modes and the boson peak?

The development of high resolution inelastic x-ray scattering technique allowed us to experimentally address these problems by measuring the dynamical structure factor $S(Q,E)$ of glassy materials in the mesoscopic region between 1 and some tens $nm^{-1}$, both varying the energy ($E$) at fixed exchanged wave vector ($Q$) and varying $Q$ at fixed $E$ [1]. A review is here reported, together with a comparison with results obtained by complementary techniques like Brillouin light scattering [2] and inelastic ultra-violet scattering [3].

[1] Sette F., Krisch M.H., Masciovecchio C., Ruocco G., Monaco G., *Science*, 1998, **280**, 1550. [2] Fioretto D., Mattarelli M., Masciovecchio C., Monaco G., Ruocco G., Sette F., *Phys. Rev. B*, 2002, **65**, 224205. [3] Masciovecchio C., Gessini A., Di Fonzo S., Comez L., Santucci S.C., Fioretto D., *Phys. Rev. Lett*.,2004, **92**, 247401.

**Keywords: glasses, X-ray scattering, light scattering**

**MS16.25.2**

*Acta Cryst*. (2005). A**61**, C26

**Collective Dynamics of Liquid Metals: from Simple to Extremely Non-Simple**

Shinya Hosokawa, *Faculty of Engineering, Hiroshima Institute of Technology, Japan.* E-mail: hosokawa@cc.it-hiroshima.ac.jp

Recent developments in high-resolution inelastic X-ray scattering using third-generation synchrotron radiation facilities allow one to investigate the collective dynamics of a wide variety of liquid metals. The IXS studies have started from simple liquid metals such as the first experiment of liquid Li [1], Na, and Mg, and encompassed to several non-simple metals such as liquid Ga, Ge, and Si [2]. The experimental results revealed characteristic common features in the collective dynamics: 1) A clear indication for propagating modes, and 2) a positive deviation of the collective excitations by about 20 % from the hydrodynamic value. In addition, an indication of a short time (sub-picosecond) retaining of the nearest-neighbour correlation is visualized from the quasielastic line of some non-simple liquid metals [2]. A generalized Langevin formalism with a memory function containing two viscoelastic decay channels [3] is commonly used for analyzing the above IXS data.

In this paper, we review the experimental technique of IXS for liquid metals, and then the common feature of the collective dynamics of liquid metals in detail. Some of them are discussed in connection with results of ab initio molecular dynamic simulations.

[1] Sinn H., et al., *Phys. Rev. Lett.*, 1997, **78**, 1715. [2] Scopigno T., et al.,*J. Phys.: Condens. Matter*, 2000, **12**, 8009. [3] Hosokawa S., *et al.*, *J. Phys.: Condens. Matter*, 2003, **15**, L623. [4] Levesque D., et al., *Phys. Rev. A*, 1973, **7**, 1690.

**Keywords: X-ray inelastic scattering, phonons, liquid metals**

**MS16.25.3**

*Acta Cryst*. (2005). A**61**, C26

**Vibrational Dynamics of Iron in Proteins**

J. Timothy Sage, *Department of Physics, Northeastern University.* E-mail: jtsage@neu.edu

High-resolution x-ray measurements near the nuclear resonance reveal the complete vibrational spectrum of a Mössbauer nucleus. I will illustrate novel opportunities that this site-selective method provides for characterizing the vibrational dynamics of $^{57}$Fe at the active sites of heme proteins, iron-sulfur proteins, and related model compounds. (1) Quantitative data on the frequency, the amplitude, and in some cases, the direction of all iron vibrations provide a uniquely detailed benchmark for modern quantum chemical vibrational predictions, with which they can be directly compared on an absolute scale. (2) Measurements on oriented single crystals of iron porphyrins reveal low-frequency out-of-plane vibrations that we identify with the long-sought heme “doming” mode, similar to the motion that takes place on oxygen binding to heme proteins. Moreover, the experimental data provide a direct experimental estimate of the force constant for Fe displacement normal to the heme plane and suggest that this Fe motion is an important element in protein control of biological reaction energetics. (3) Comparisons with calculations and with independent Raman isotope shift measurements probes the extent to which active site vibrations couple to global protein motions.

**Keywords: heme proteins, Mössbauer spectroscopy, vibrational spectroscopy**

**MS16.25.4**

*Acta Cryst*. (2005). A**61**, C26-C27

**High-Resolution Inelastic X-ray Scattering of Materials of Geophysical Interest**

Guillaume Fiquet, *IMPMC, UMR CNRS 7590. University Pierre et Marie Curie, Paris, France.* E-mail: fiquet@lmcp.jussieu.fr

Inelastic X-ray scattering (IXS) has progressively arisen as one of the major spectroscopic tools with the advent of bright X-ray sources of 3$^{rd}$ generation. It offers the unique opportunity to investigate the phonon or electronic properties *in situ*, at various conditions of pressure and temperatures, and is thus very well suited to the study of the composition and dynamics of the Earth and planetary interiors.

The elasticity and the sound wave anisotropy of hcp-metals, namely iron and cobalt have been investigated at high-pressure by very high resolution (meV) IXS. I will address the case of hcp-iron, the main constituent of the Earth's inner core, and report the direct experimental determination of the anisotropy in the propagation of longitudinal acoustic waves in textured sample above 100 GPa. Hcp-cobalt, here chosen a proxy for iron, has also been studied with the advantage to be