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Coherent diffraction microscopy: Present and future

Jianwei Miao[1], Changyong Song[2], Huaidong Jiang[1], Kevin Raines[1], Richard L Sandberg[3], Chien-Chun Chen[4], T. K. Lee[4], Thomas Earnest[5], Tetsuya Ishikawa[2], Henry C Kapteyn[3], Murnane M Margaret[3]

[1]University of California, Los Angeles, Dept. of Physics and Astronomy, PO BOX 951547, Los Angeles, CA, 90095-1547, USA, [2]SPring-8/RIKEN, 1-1-1, Kouto, Mikazuki, Sayo-gun, Hyogo 679-5198, Japan., [3]Department of Physics and JILA, University of Colorado and NIST, Boulder, Colorado, USA., [4]Institute of Physics, Academia Sinica, Nankang, Taipei 11529, Taiwan., [5]Physical Biosciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA., E-mail：miao@physics.ucla.edu

In 1999, researchers extended X-ray crystallography to allow the imaging of non-crystalline specimens by measuring the X-ray diffraction pattern of a non-crystalline specimen and then directly phasing it using the oversampling method with an iterative algorithm. The new imaging modality, called coherent diffraction microscopy or lensless imaging, has since evolved moving in three important directions. The first is the three-dimensional (3D) structural determination of non-crystalline materials. The second is towards the 3D imaging of whole cells at a resolution of 10 nm or better. The third is the potential of imaging single large protein complexes using extremely intense and ultrashort X-ray pulses. In this talk, we will review the principle of coherent diffraction microscopy, and present some applications of the imaging modality to nanoscience and biology by using synchrotron radiation, high harmonic generation and soft X-ray laser sources. Finally, we will discuss the future opportunity with X-ray free electron lasers.

Keywords: oversampling, coherent diffraction microscopy, lensless imaging

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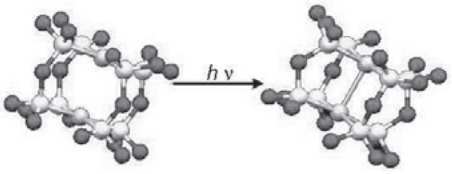
Time-resolved X-ray scattering of an electronically excited state in metal complexes in solution

Martin M Nielsen[1], Morten Christensen[1], Kristoffer Haldrup[1], Niels Harrit[1], Robert Feidenhans'l[1], Qingyu Kong[2], Marco Cammarata[2], Lo Russo Manuela[2], Michael Wulff[2]

[1]Niels Bohr Institute, University of Copenhagen, Centre for Molecular Movies, Universitetsparken 5, Copenhagen, Copenhagen, 2100, Denmark, [2]The European Synchrotron Radiation Facility, Grenoble, France, E-mail：meedom@nbi.ku.dk

The pathway taken of the atomic nuclei, while molecules are partaking in chemical reactions, and hence their intermediary molecular structures, is a fundamental question in chemistry, and a host of systems have been studied by laser spectroscopy down to the femtosecond time scale. However, while spectroscopic methods provide information on energy levels, direct structural information is not available. In the last few years, this gap of information has been bridged by X-ray scattering experiments on time scales down to picoseconds. Initially this has been made for crystalline systems with their inherent amplification of the scattered intensity and recently also for liquid systems, the natural environment for most chemical reactions. We here present results obtained from experiments performed at the time-resolved beamline ID09b at the ESRF, based on which we have successfully determined key structural parameters directly for the highly reactive excited state of the square-planar platinum compound tetrakis-μ-pyrophosphito-diplatinate(II) (PtPOP) in aqueous solution.



Keywords: time resolved, liquid scattering, data analysis

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Femtosecond X-ray crystallography of elemental solids: Coherent dynamics in bismuth and tellurium

Steven L Johnson[1], Paul Beaud[1], Gerhard Ingold[1], Ekaterina Vorobeva[1], Christopher J Milne[2], Faton S Krasniqi[1], Eeuwe S Zijlstra[3], Martin E Garcia[3], Maik Kaiser[1], Daniel Grolimund[1], Rafael Abela[1]

[1]Paul Scherrer Institut, Swiss Light Source, WSLA/107, Villigen PSI, Aargau, 5232, Switzerland, [2]Laboratoire de Spectroscopie Ultrarapide, Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland, [3]Theoretische Physik, Universitaet Kassel, Heinrich-Plett-Strasse 40, Kassel, 34132, Germany, E-mail：steve.johnson@psi.ch

Femtosecond laser excitation of the near-surface region of an optically opaque solid can create unique transient conditions that are far from thermal equilibrium. The properties of the resulting non-equilibrium state can be very different from those of more familiar thermodynamic phases. To better understand the structural evolution of laser-excited materials, we have used highly asymmetric femtosecond x-ray diffraction to observe the atomic motion in single crystals of bismuth and tellurium on time scales faster than their optical phonon periods. We observe coherent and incoherent structural dynamics that change as a function of distance from the surface of the crystal. In bismuth, we observe displacive excitation of the coherent A_{1g} optical phonon mode, a direct consequence of a sudden change in the quasiequilibrium structure of the unit cell due to electronic excitation of the system. Measurements of the Bragg diffraction from the (111) lattice planes at different angles of incidence allow us to extract the rates of electronic relaxation and diffusive transport. Other Bragg peaks also contribute information on the incoherent atomic motion caused be electronic softening of the acoustic and optical modes. As in bismuth, laser excitation of tellurium creates a large coherent population of a symmetric optical phonon mode. Unlike bismuth, the three-atom basis of tellurium makes an unambiguous measurement of the actual atomic motion more challenging. We show first measurements of the coherent structural response of the tellurium unit cell to intense electronic excitation, demonstrating a successful decomposition of the coherent motion into the Brillouin-zone-center optical modes of the lattice.

Keywords: time-resolved x-ray diffraction, time-resolved effects, laser radiation

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Electronic Grüneisen parameter and thermal expansion in ferromagnetic transition metals

Jianming Cao, Shouhua Nie, Li Junjie, Clinite Rick, Xuan Wang

Florida State University, Physics Department and National High Magnetic Field Laboratory, 1800 E. Paul Dirac Dr., Tallahassee, FL, 32310, USA,