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Coherent diffraction microscopy: Present and future

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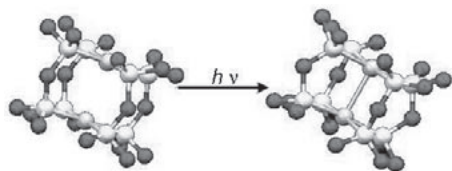
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Time-resolved X-ray scattering of an electronically excited state in metal complexes in solution

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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

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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 dispersive 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 by 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

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The Grüneisen parameter determines the magnitude of the system dimensional change in response to its thermal energy variation. Differentiating the various contributions to the Grüneisen parameter is of great importance to clearly understand the thermal expansion mechanism of solids. In particular, the electronic Grüneisen parameter (γ_e) characterizes the electronic contribution to the thermal expansion and is directly related to the electronic density of states at Fermi level. Here, we report the first measurement of electronic Grüneisen parameter γ_e of the ferromagnetic transition metal nickel using a novel approach of femtosecond electron diffraction (FED) [1]. In this measurement, the electronic thermal expansion was enhanced by ultrafast heating using femtosecond optical pulses. Then, its temporal evolution was differentiated from other thermal contributions by simultaneously monitoring the laser-induced ultrafast stress and structural dynamics in time domain with FED. This method overcomes the restriction of traditional low-temperature methods and offers a unique path to study electronic thermal expansion in magnetic metals. The measured γ_e above the Curie temperature indicates that the local magnetic moment that largely persists in the paramagnetic state of nickel does not contribute significantly to the thermal expansion [2]. Most interestingly, this value is significantly different from that measured in the ferromagnetic state. This difference implies not only its dependency on the magnetic ordering but also the existence of the ultrafast demagnetization process.

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Keywords: dynamics, thermal expansion, electron diffraction

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Ultrafast electron dynamics excited and probed with X-rays

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Function and dynamics in complex matter is often governed by disperse active sites, long range interactions and a large number of coupled degrees of freedom. Creating electronic excitations at these selected atomic sites we can monitor the ultra fast electron dynamics associated with charge transfer processes. Using the high brilliance femtosecond X-ray pulses from FLASH we can also create highly X-ray excited states. Here we study both the aspects of X-ray induced dynamics and the opportunities to excite and follow with femtosecond time resolved X-ray spectroscopic methods the wave packet dynamics in complex matter on the atomic scale.

Keywords: X-ray induced electron dynamics, X-ray free-electron laser, FLASH

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Performance tests on iterative phase-retrieval methods in higher dimensions

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Since the developing of the charge-flipping (CF) algorithm [1] as an ab-initio method for structure solution in crystallography, the usage of iterative phase-retrieval methods, like low density elimination (LDE) [2] or the phase determination by the principle of minimum charge [3], have become well established. Their extension to arbitrary dimensions [4] provides a comfortable and efficient tool for the reconstruction of the electron density distribution of modulated structures and quasicrystals (QCs). However, besides the success of these methods, intensive tests on the performance of such algorithms have not been conducted yet. The aim of this work is a systematical investigation of the limits of the CF and LDE algorithms with respect to QCs and approximant structures. For that purpose, diffraction data sets of selected QC models were calculated within certain limits. Such limits can be caused e.g. if the maximum diffraction angle is limited by the instrument setup. For a quantitative description, a figure of merit was specified in reciprocal and in real space. Characteristic differences of selected iterative phase-retrieval methods will be shown, e.g. a typical distribution of recovered phases was developed depending on their intensity and the chosen algorithm. Furthermore, it has been found, that only strong reflections will be retrieved with their calculated phase, while phases of weak reflections are randomly recovered. Several reasons and resulting features will be discussed.

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Keywords: quasicrystals, charge flipping, low density elimination

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Approximant structures for the AlCo based decagonal phases

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The AlCo-based alloy system is known to provide a variety of decagonal quasicrystals and recent atomic-scaled observations of HREM coupled with HAADF-STEM have revealed their structural features in terms of columnar clusters of atoms with local pentagonal symmetry. In particular, a variety of electron diffraction patterns observed in the Co-rich decagonal phases of the Al-Co-Ni alloy system, were featured by pentagonal or rhombic tilings composed of columnar clusters with a decagonal section of 2nm in diameter. Nearby the Co-rich decagonal phases in the AlCo-based alloy system, a variety of crystalline approximants with relatively complex structures are realized and the structural information for these materials serves the important information for the columnar structures with local pentagonal symmetry. The structures of W_2 -AlCoPd and W_2 -AlCoSi and τ^2 -AlCo phases are classified into this