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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 Cure 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 deference 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

MS.83.5

Acta Cryst. (2008). A**64**, C141

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 brillance 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 exciteand 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

MS.84.1

Acta Cryst. (2008). A**64**, C141

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

MS.84.2

Acta Cryst. (2008). A**64**, C141−142

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