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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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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

category and the present paper reports the results of single crystal structural analysis for these approximants. The present study reveals the fundamental atomic arrangement of the pentagonal columnar structure with 0.8nm periodicity and clarifies its linkage so as to form crystalline structures. Such structural information allows us to discuss the atomic structure of decagonal quasicrystals by reproducing the images of HREM and HAADF-STEM.

Keywords: alloy structure, single-crystal diffraction, quasicrystals

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New phenomena in epitaxial growth: Solid films on quasicrystalline substrates

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A quasiperiodic arrangement of atoms has only been realized in binary or ternary alloys, known as quasicrystals. These are complex intermetallics with long-range aperiodic order and non-crystallographic rotational symmetry (usually five-fold or ten-fold symmetry). The physical properties arising from the quasiperiodic arrangement of the metal atoms significantly depart from that of periodic alloys and have attracted a broad interest. A long standing issue has been to understand the relative influence of the quasiperiodic order on the physical properties of quasicrystals, independently from the complex chemistry associated with such alloys. This has been the starting point of recent attempts to grow new quasiperiodic systems by using quasicrystalline surfaces as templates to force a quasiperiodic structure in metal thin films deposited on such substrates. Here I will give an overview of the research conducted in the field of solid film growth on quasiperiodic surfaces. An atomistic description of quasicrystalline surfaces will be presented and discussed in relation to bulk structural models. Then the various phenomena occurring during thin film growth on quasiperiodic surfaces will be outlined. Emphasis will be placed on the nucleation mechanisms of the solid films, on their growth modes in relation to the nature of the deposited metals, on the possibility of alloying at the interface, and on the epitaxial relationships at the crystal-quasicrystal interfaces. We will also describe situations where the deposited elements adopt a quasiperiodic structure, which opens up the possibility of extending our understanding of the relation between quasiperiodicity and the physical properties of such structurally and chemically complex solids.

Keywords: surface science, quasicrystals, thin films

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Mesoscopic quasicrystalline and Archimedean tilings in polymer alloys

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Tilings and patterns are known not only to mathematicians and crystallographers, but also to designers and visual artists as the basis of decorative art appearing on furniture, curtains, wall papers, kilts, ceramics, ties, etc. In this talk, we show that star-polymers can produce elegant self-assembled periodic and quasiperiodic patterns without fabrication technique. We have been creating several complex but periodic patterns known as antique Archimedean tiling patterns, and finally, we have found evidence of a “polymeric quasicrystal” tiling for the first time [1]. Quasicrystals are the avant-garde structures that have noncrystallographic symmetry, and initiated a revolution of crystallography and solid-state physics in 1980's. Remarkably, our polymeric dodecagonal quasicrystal has a hundred times length-scale compared to metallic systems, and thus it approaches the scale of visible light, where a promising photonic application has been considered [2]. The present result indicates the universality of quasicrystalline order from atoms to polymers.

Reference:

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Atomic simulation and lattice dynamics of the ZnMgSc icosahedral quasicrystal

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The structure of the binary CdYb icosahedral quasicrystal was recently solved using a 6D modeling approach and synchrotron radiation data. The structure of the quasicrystal is described as a quasiperiodic packing of a large triacontahedron connected along 2- and 3-fold axis [1]. Going from the atomic structure to physical properties remains a challenging problem. Indeed, an accurate derivation of the physical properties requires to, (i) have a tractable Hamiltonian and (ii) specify a realistic and unique position and chemical spicity for each atom in the quasicrystal structural model. The whole procedure is illustrated on the example of icosahedral Sc-Mg-Zn alloy, starting from the derivation of effective pair potentials from first principle database, through “energetic” refinement of uncertain structural details, and finally comparative study of lattice dynamics for 1/1 and 3/2 approximants. The simulated dynamical response function reproduces perfectly the experimental one, measured by inelastic neutron and x-ray scattering [2]. In particular the differences observed between the quasicrystal and the 1/1 approximant are well accounted for. An analysis of eigen modes and their localization on clusters will be presented. It is also found that, except for the Sc icosahedrons, all cluster shells present a significant deviation from icosahedral symmetry, related to the relative orientation of the inner