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LASS carries out research in three areas: the development of X-ray methods, computational materials science and spectroscopy of nanomaterials. The following paragraphs summarise our main recent achievements.

Single-pulse, single-crystal diffraction at XFELs

4^{th} generation X-ray sources, the X-ray free electron lasers have unique radiation properties. They provide few femtoseconds long, monochromatic, coherent, focused hard X-ray pulses. Conventional measurements often unable to take advantage of these properties, necessitating development of fundamentally new experimental techniques potentially based on new measurement principles.

We have developed a new kind of diffraction measurement based on the Kossel lines. [1]. These lines are the consequences of diffraction and interference of the radiation originating from the secondary X-ray fluorescent source atoms within the sample. The Kossel lines have 2 unique properties: (*i.*) allow simultaneous measurement of all Bragg reflections of a single crystal, and (*ii.*) provide information not only on the amplitude, but also on the phase of the structure factors. We carried out a demonstration experiment at the European XFEL in Hamburg, Germany, and successfully demonstrated the feasibility of our fundamentally new experimental technique [1]. Kossel lines of a GaAs and GaP single crystals were measured in just 25 fs, and the electron density within the unit cell was determined via Fourier synthesis of the amplitude and phase information extracted from the profile of about 100 indexed Kossel lines (Figure 1).

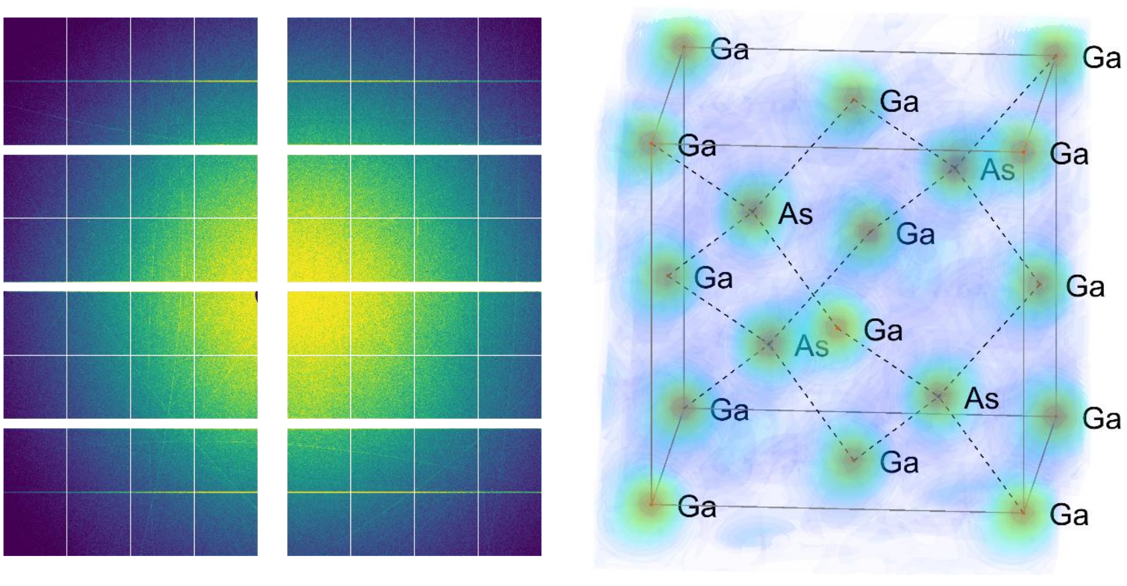

Figure 1. Kossel line pattern measured using a single 25fs X-ray pulse (left). Electron density of the unit cell obtained by direct Fourier synthesis (right).

Simulating peritectic coupled growth

An important group of our technically relevant materials, such as steels, are formed by the solidification of peritectic alloys. These alloys, similar to eutectic ones, can exhibit a rich variety of complex self-organizing solidification morphologies. We used phase-field modeling to examine the solidification of the NPG-TRIS peritectic model alloy [2], which was used in zero-gravity experiments on board the International Space Station. We determined the condition of steady-state coupled growth, identified the factors which affect its stability, and simulated 2D and 3D growth forms that were already observed in eutectic systems (Figure 2.).

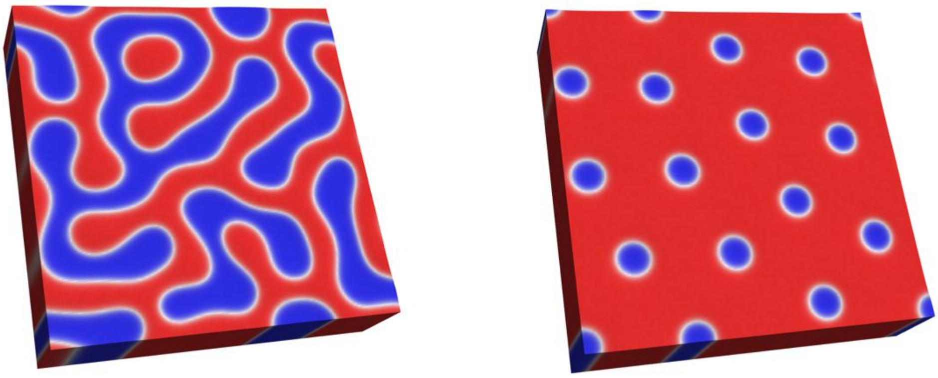

Figure 2. Growth forms in the peritectic NPG-TRIS alloy obtained by phase-field simulations. If the phase fractions of the solid phases (red and blue) are nearly equal, a random labyrinth-like lamellar pattern is preferred (left), while if the phase ratio is sufficiently different, rods of the minority phase form in the matrix of the majority phase (right).

Analysis of thermal boundary in natural convection

Heat transfer in turbulent fluids is traditionally estimated through measuring the thermal properties of the thermal boundary layer, as theories limited to describe this region. However, mostly it is done in a time and laterally averaged manner. We have established a novel Lagrangian method for time and spatially resolved tracking of the boundary layer [3]. The method may apply to heat transfer problems with complex boundaries (i.e. urban landscape thermal modeling). Ultimately, a characteristic time for the boundary layer dynamics is inherent in our approach that makes distinction to all previous works.

Model for the scattering scanning near-field optical microscopy (s-SNOM) process in nanotubes

Near-field infrared microscopy is an emerging method to extract spectroscopic information from nanostructures with spatial resolution of a few nanometers. Applications include mixtures of nanostructures or individual particles, but the basic description of the procedure is not fully clarified yet. We constructed a comprehensive analytical model for the scattering scanning near-field optical microscopy (s-SNOM) process in nanotubes. The model is based on the Mie scattering theory, extending it to non-spherical geometries and layered systems. This way, we could explain scattering from as complex entities as a molecule encapsulated in a boron nitride nanotube on a substrate. We used our previous measurements to validate the results [4]..

References :

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