Deciphering electron-phonon coupling by electron diffraction

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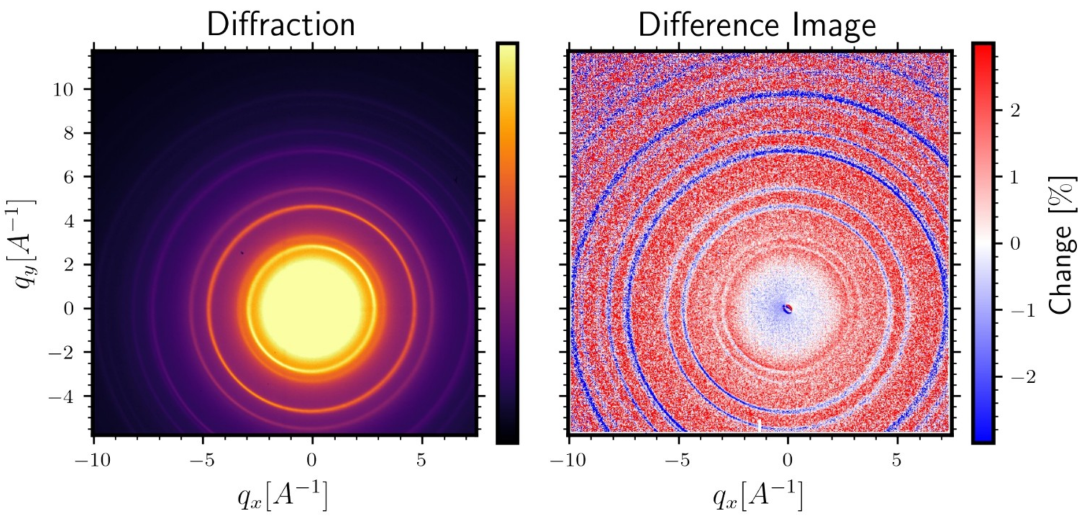
Electron-phonon coupling is the interaction between electrons and lattice vibrations (phonons) in a material. This coupling plays a critical role in many physical phenomena, such as electrical resistivity, superconductivity, and thermal conductivity and defines the material's properties, particularly its electrical and thermal behavior.

With ultrafast electron diffraction (UED) we can track atomic motion in real-time: A material is excited by an ultrafast laser pulse, which perturbs the electron system and generates phonons. A subsequent electron pulse is used to capture diffraction patterns of the material at different time intervals after excitation. By observing changes in the diffraction patterns (see image below), such as alterations in peak intensities or diffuse scattering, researchers can directly visualize how phonons evolve and interact with electrons on femtosecond timescales.

The goal of this study is to build a reliable framework to predict the manifestation of lattice vibrations in diffraction patterns from first principles in complex materials such as organic semiconductors. Starting from the calculating the phonon dispersion relation applying the “frozen-phonon” approach the Debye-Waller contribution and diffuse scattering through the full Brioullin-zone can be calculated.

This project provides an excellent opportunity for students interested in computational methods in experimental solid state physics and the bachelor and master lever.



Electron diffraction image (left) and difference diffraction image (right) of a polycrystalline aluminum film after laser excitation.

While the intensity in the Bragg reflection decreases due to incoherent motion of the atoms due to phonon population, the diffuse scattering background increases,

<u>Your Tasks</u>

- Calculation of phonon dispersion relations
- Developing tools to simulate diffraction patterns including lattice vibrations
- Comparison to available experimental data

<u>Requirements:</u>

- Don’t be afraid of math
- Basic programming knowledge goes a long way

  … don’t forget to have fun while you’re at it ;)

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