Investigating Beam-induced Atomic Motion

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Project Goal

Powerful X-ray sources with a high brilliance provided by synchrotrons are considered as ultimate tools for probing microscopic properties of materials. The influence of X-rays on hard condensed matter, however, has been neglected so far. It is therefore crucial to investigate beam-driven changes concerning the structure and the dynamics on a microscopic level to prevent any misinterpretations of experimental results. It also offers new opportunities to indirectly measure material-specific poperties, e.g. bonding properties.

Technique

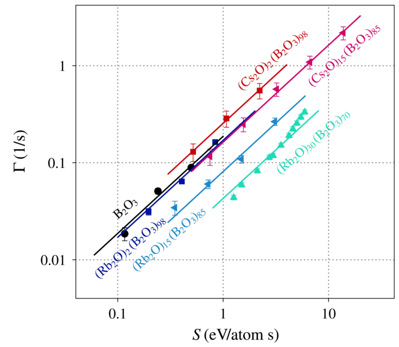
For examining the dynamical properties on an atomic level the technique of *X-ray Photon Correlation Spectroscopy* (XPCS) is used. Like a movie that consists of many frames, thousands of frames in a row were taken with a specific exposure time of the scattered X-ray photons that hit the detector and create the so-called *speckle pattern* in the reciprocal space. This movie of changing *speckle pattern* provide an insight into the atomic dynamics.

Observation

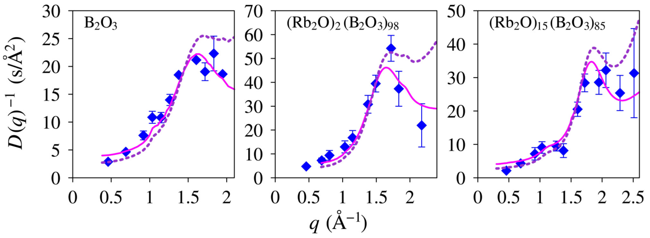
While the beam has negligible influence on the structure it changes the atomic dynamics. Varying the flux of the beam, that could be done by adjusting absorbers into the beam path, instantaniously and reversibly changes the dynamics. The dynamics is linearly dependent on the flux. It is also wave vector- , temperature- and material- dependent: While samples with ionic and covalent bonding types show this effect, the dynamics of metals does not change under irradiation.

Interpretation

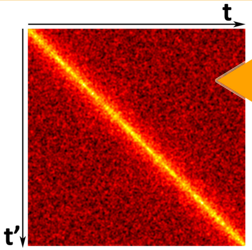
The photon bombardement of the beam causes radiolyses: Eletronic excitations with enegies large enough for atomic displacements. Metals, however, do not show flux-dependency since their electronic excitations delocalize faster. For different samples, e.g. oxide glasses or alkali oxide glasses, the effect of the flux-dependency varies due to various atomic compositions and bonding rigidities. The motion of the atoms corresponds to infinitesimal steps below the resolution of observation known as *Brownian Motion*.



The correlation rate Γ that is reciprocal to the atomic dynamics versus the dose rate *S*. The flux of the beam has different impact to various alkali oxide glasses: The higher the alkali content, the lower the flux impact.



The inverse of the diffusion D^{-1} versus the wave vector *q*. The pink line is modelling the data points via an *Interactive Brownian Motion* model, whereas the dashed purple line would correspond to a model of single jumps.



Two-time-Autocorrelation function:
If the crossing orange line does not change its width, this means that at fixed flux the dynamics remains stationary and is independent on the accumulated dose.

Movie of changing *speckle pattern* generated by XPCS