ESRF	**Experiment title:** Off-diagonal elements of the dielectric tensor of silicon by coherent inelastic x-ray scattering	**Experiment number:** HE-2274
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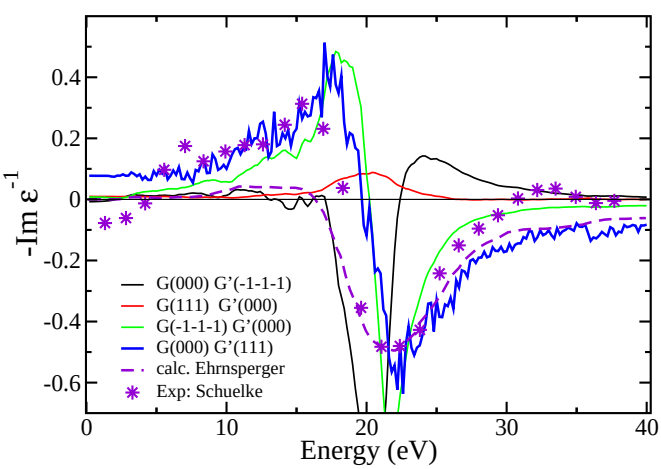
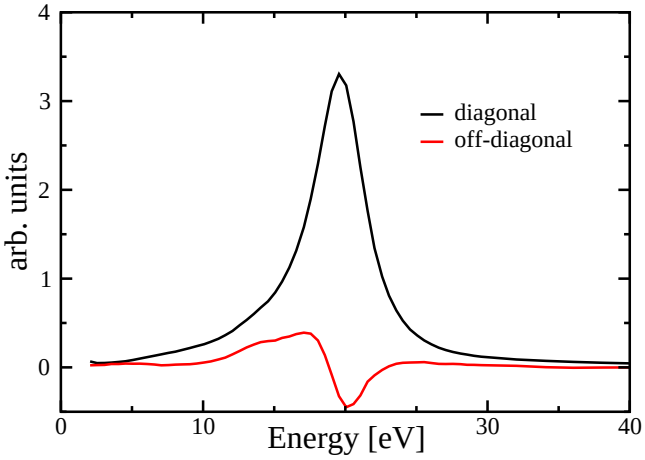
Report:

The aim of the experiment was to measure non-diagonal elements of the dielectric matrix of silicon. The experiment has been a sequel of experiment HE-1912 which measured the dynamic structure factor of Si [1]. It was found that the Adiabatic Local-Density Approximation (ALDA, also known as TDLDA) of the Time-Dependent Density-Functional Theory (TDDFT) describes the spectra for finite momentum transfer extremely well provided that the effects of finite lifetimes of electrons and holes be added. In addition, important coupling effects due to the atmic structure of the medium (local-field effects, LFE) were indentified. The excellent performance of the TDLDA stands in contrast with the result for zero momentum transfer where it fails. This left the open question if the TDLDA describes the off-diagnoal elements equally well, and, in turn, what is the role of the off-diagonal elements of the dielectric matrix for the problems encountered in the calculation at the reciprical lattice vector $(1,1,1)_{\mathrm{rec}}$.

In order to obtain some of the off-diagonal elements, coherent inelastic x-ray scattering experiments have been performed at ID16, using incoming photons of 8 keV and an energy resolution of 0.5 to 1.0 eV. Three different silicon single crystals have been employed in reflection (Bragg) geometry at room temperature. These consisted of energy scans at several values of momentum transfer performed simultaneously with the generation of a standing wave corresponding to Bragg conditions for a given reciprocal vector, ((111) or (220)). The procedure has been described in detail in by Schülke and Kaprolat [2,3]. The spectra have been recorded in the 2-100 eV energy range using momentum transfers between 0.7 $\mathrm{Å}^{-1}$ and 5 $\mathrm{Å}^{-1}$.





Left panel: Comparison with old experiment for q (0.9, 0.3, 0.3) 2 π/a of Ehrnsperger and Bross [4] along with our TDLDA calculation. Right panel: Preliminary result of the diagonal and the off-diagonal element for the first of the **q** vectors.

The momentum transfers measured where the following $((...)_{\mathrm{rec}}$ are the reciprocal coordinates):

- Crystal 1: $\mathbf{q} = 0.1$ [5,6,4] $\rightarrow$ $(0.50, 0.45, 0.55)_{\mathrm{rec}}$
- Crystal 2: $\mathbf{q} = 0.5$ [-1,3,1] $\rightarrow$ $(1.0, 0.0, 0.50)_{\mathrm{rec}}$
- Crystal 3: $\mathbf{q} = 0.25$ [-3,7,2] $\rightarrow$ $(1.125, -1.125, 0.50)_{\mathrm{rec}}$
- Crystal 3: $\mathbf{q} = 0.4$ [1,1,1] $\rightarrow$ $(0.40, 0.40, 0.40)_{\mathrm{rec}}$

The analysis of the experimental data under way using the approach of [3]. The analysis is not trivial due to certain calculations that are needed to extract the off-diagonal elements. Therefore, the analysis is not yet finished. Hence we show in the figures the only available previous results along with our calculation of the four off-diagonal elements concerned. The experimental result in the right panel preliminary and may change in the last stage of analysis, which is soon to be finished.

References

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