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Report:

The applications of silicon for microprocessors have encouraged the study of physical properties in silicon to the point that it can be considered one of the best known materials. The dielectric properties are especially relevant since the progressive miniaturisation of electronic components requires a state-of-the-art knowledge on quantum effects in the electrical conductivity, which already affect the fabrication of faster microprocessors.

The dielectric properties are described by the dielectric function $\varepsilon(\mathbf{q},\omega)$. The corresponding experimental observables are the absorption spectrum (proportional to the imaginary part of $\varepsilon(\mathbf{q},\omega)$) and the dynamical structure factor $\mathrm{S}(\mathbf{q},\omega)$ (proportional to the imaginary part of $\varepsilon^{-1}(\mathbf{q},\omega)$, also denominated loss function), that can be measured by inelastic x-ray scattering (IXS).

We have performed high-resolution room temperature IXS measurements of the dynamical structure factor $\mathrm{S}(\mathbf{q},\omega)$ of silicon at several momentum transfers along the [100] and [111] directions. The aim of the experiment was to ascertain the importance of local-field and excitonic effects in the plasmon spectrum and to distinguish them from the features originated due to interband transitions, the latter being hardly resolved in existing IXS measured reports [1]. The measurements were guided by first principles calculations of the loss function using a new formalism based on a combination of many body perturbation theory with time-dependent density functional theory in its local approximation for the exchange and correlation kernel (TDLDA) [2].

Measurements of $S(\mathbf{q},\omega)$ with x-ray photons of 7.9 keV energy and 200 meV energy resolution were performed for several q values along the [100]. The reduced number of sharp features found and the need of better statistics made us to change to an energy resolution of approx. 1 eV, which was employed for most of the measurements.

Figure 1 shows a comparison among the measured spectrum for q=0.53 a.u. along the [100] direction (200 meV resolution) and that reported in Ref. [1]. The presence of a shoulder at 15 eV and a peak at 7 eV becomes transparent in the new experimental data set. The shoulder can be attributed to exchange and correlation effects which are accounted for by our TDLDA calculation, whereas the interpretation of the small peak at 7 eV requires the consideration of excitonic effects which we are currently calculating using the Bethe-Salpeter formalism.

Figure 2 summarizes $S(\mathbf{q},\omega)$ measurements along the [111] direction. Since this is the bonding direction in silicon, a much richer fine structure is found for the plasmons. This has been already reported by Sturm and coworkers in Ref. [3], where they modeled the spectra with a Fano resonance resulting from the coupling of discrete plasmon states with the continuum of electron-hole-pair excitations. This resonance appears between 18 and 20 eV for q-values larger than 0.53 a.u. The analysis of the rich fine structure observed in these spectra, obtained with higher resolution than that used in [3], is still in progress.

Finally, we have performed tentative measurements of non-diagonal elements of the dielectric matrix using coherent inelastic x-ray scattering (CIXS). To our knowledge, this technique has not been employed for this purpose since the pioneering work by W. Schülke and A. Kaprolat [4]. It consists of the use of a standing wave field generated by setting the sample in Bragg geometry for a given G vector of the reciprocal lattice while simultaneously measuring the inelastic signal. This allows one to obtain information of the non-diagonal elements of the dielectric response matrix such as $S(\mathbf{q},\mathbf{G},\mathbf{G}',\omega)$. We have performed preliminary measurements for $\mathbf{G}_1 = (111)$ and $\mathbf{G}_2 = (111)$ and $\mathbf{q}_1 = 0.5(1,1,1) + 0.14(1,-1,0)$ and $\mathbf{q}_2 = (1,1,0) + 0.445(1,-1,0)$, following the recipe given in Ref. [4]. These data represent a unique set for comparison of the different theoretical approaches to the dielectric response matrix.

Summarizing, we have performed high resolution IXS measurements of the dynamical structure factor of silicon using as a guide state-of-the-art first principles calculations. A preliminary analysis shows a rich fine structure for the spectra obtained at momentum transfers along the [111] direction. Excitonic effects have become transparent due to the higher resolution employed compared to previous measurements. Non-diagonal elements of the dielectric matrix have been investigated as well.

References

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[2] F. Sottile, V. Olevano and L. Reining, Phys. Rev. Lett. **91**, 056402 (2003).

[3] K. Sturm, W. Schülke, and J. R. Schmitz, Phys. Rev. Lett. **68**, 228 (1992).

[4] W. Schülke and A. Kaprolat, Phys. Rev. Lett. **67**, 879 (1991).

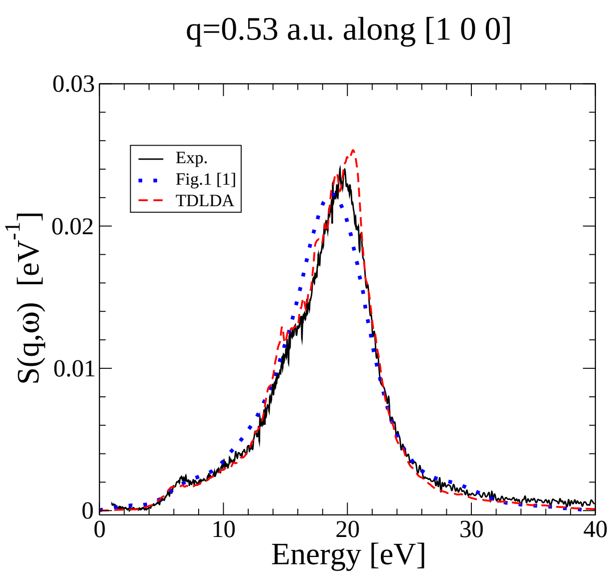
q=0.53 a.u. along [1 0 0]
Exp.
Fig.1 [1]
TDLDA
S(q,ω) [eV-1]
0.03
0.02
0.01
0
0
10
20
30
40
Energy [eV]

Fig. 1

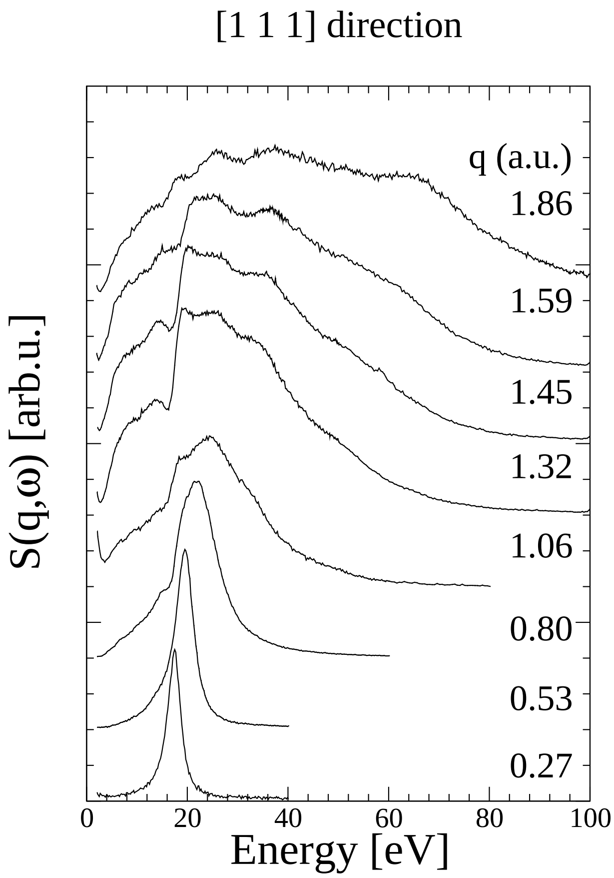
[1 1 1] direction
q (a.u.)
1.86
1.59
1.45
1.32
1.06
0.80
0.53
0.27
S(q,ω) [arb.u.]
0
20
40
60
80
100
Energy [eV]

Fig. 2