Albrecht *et al.* Reply: Cardona *et al.* [1] comment on a detail of Ref. [2]—an *ab initio* calculation of excitonic effects in silicon—namely, on a secondary peak in the theoretical spectrum, about 0.2 eV higher in energy than the calculated E_1 peak at 3.55 eV. Their experiment shows that if any structure exists near 3.8 eV, its amplitude must be less than 1% of the E_1 peak. Although not relevant to the main conclusion of Ref. [2], namely, that the inclusion of excitonic effects considerably improves the agreement between calculated and measured spectra, we agree that the transitions near 3.8 eV are overestimated in Ref. [2].

It is, however, worthwhile to discuss the origin of the secondary peak in the theoretical spectrum, since it is related to a quite general point concerning the calculation of optical spectra. In fact, this peak is already present in the LDA-RPA spectrum, which is computed using a grid of 2048 special k-points in the whole Brillouin zone (BZ) (dashed line in Fig. 1: the two peaks here appear, respectively, at 2.9 and 3.15 eV, because of the LDA underestimation of transition energies). By increasing the number of k-points in the BZ sampling this "double peak" line shape becomes smoother, yielding in the completely converged LDA-RPA spectrum a structureless plateau from 2.85 to 3.3 eV (full line in Fig. 1). The 3.15 eV peak, called P_1 in the following, becomes the higher-energy part of the plateau and comes from transitions around the Δ line. The lower-energy part of the plateau (the first peak at 2.9 eV) comes from a convolution of the E_0' and E_1 transitions, which are found correctly to be very close in energy in the calculation. For this reason, in Ref. [2] P_1 was identified with the structure discussed in Refs. [3,4], (see the shoulder in the derivative of ϵ_2 in Fig. 3 of Ref. [3]), which has been ascribed to the same origin in Ref. [4]. We can hence exclude the explanation proposed by the Comment's authors, namely, that the additional peak stems from a separation of the E_0' and E_1 transitions.

However, Fig. 1 shows that using a reduced number of k-points transforms the plateau into a fictitious double peak structure. Also in a completely converged exciton calculation this double peak structure might be washed out. It is therefore worthwhile to explore *how* the very limited number of k-points that can be taken into account in such calculations should be chosen. In Ref. [2] sets of special k-points [5] were used. However, it turns out that using random points, or at least a grid shifted off the high symmetry directions, is more efficient in avoiding the overestimation of the spectral structures. In fact, we have recalculated the spectrum including excitonic effects using a shifted grid of 256 k-points in the BZ. The peak P_1 is also present in this case but is less important than in the spectrum obtained with 2048 *special* points.

The concluding section of the Comment questions the exactness of surface optical properties calculations using relatively thin atomic slabs. The suggested effect of quantum confinement on the reflection anisotropy spectra (RAS) has however been shown to be irrelevant when reasonably thick slabs are used (20–30 Å), by recent calculations by some of us [6], using very thick atomic slabs (up to 170 Å). Instead, and coherently with our previous remarks on the calculations of $\epsilon(\omega)$ in the bulk, in Ref. [6] it was demonstrated that a much more important role is played by the BZ integrations. The lack of convergence of the BZ sampling, together with possible nonideal surface conditions in the experimental anisotropy measurements, is hence the most plausible explanation for the often reported discrepancies between the amplitudes of calculated and measured RAS spectra.

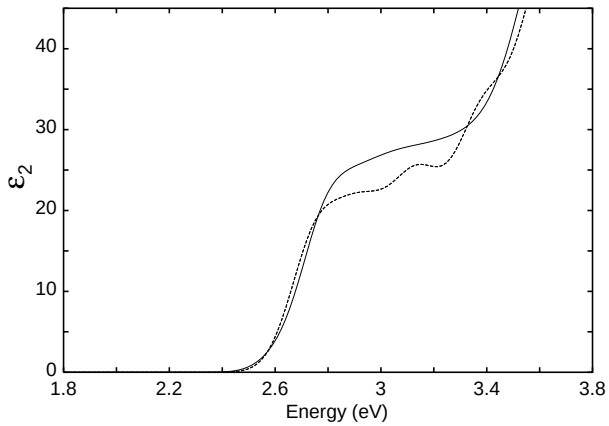

FIG. 1. Imaginary part of the dielectric function of bulk Si computed at the LDA-RPA level, using 2048 special k-points (dashed line) and 400 000 random k-points (full line) in the BZ. A Gaussian broadening of 75 meV has been used.

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