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MICROSCOPIC THEORY OF LATTICE DYNAMICS AND RECONSTRUCTION OF SEMICONDUCTOR SURFACES

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Abstract.—On the basis of a microscopic theory of surface density response including local-field and excitonic effects we calculate the phonon spectrum of an ideal Si(111) slab. A drastic enhancement of the non-local response is obtained for wavevectors corresponding to 2x1 and 7x7 superstructures, signalling an excitonic insulator instability of the metallic dangling bond surface state. The coupling of the resulting charge-density wave to the lattice produces a soft surface mode with atomic displacements supporting the ionic buckling model.

In this contribution we present a) a calculation of the phonon spectrum for an 8-layer ideal Si(111) slab starting from an accurate description of the surface electronic states and b) a detailed study of the implications for a microscopic understanding of the surface 2x1 and 7x7 reconstructions.

It has already been established that in a Wannier or LCAO basis for the wave functions, the non-interacting surface polarizability is of the separable form \( \chi = \chi^A_1 \). The separability enables one to solve the integral equation for the density response \( \chi = \chi^A + \chi^{XC} \), which determines the electronic contribution to the dynamical matrix given by

\[
D^E_{\alpha\beta}(\kappa, \hat{q}) = -\frac{1}{M} \sum_{ss'} F^S_{\alpha}(\kappa, \hat{q}) \left\{ N^{-1}(\hat{q}) + \chi^{XC}(\hat{q}) \right\}^{-1}_{ss'} F^S_{\beta}^{\dagger}(\kappa, \hat{q}),
\]

Here \( \alpha \) and \( \beta \) denote Cartesian coordinates and \( \kappa \) an ion in the 3-D basis of the slab. \( F^S_{\alpha}(\kappa, \hat{q}) \) corresponds to the force experienced by the ion \( \kappa \) due to interaction through the ionic potential with the density wave As in direction \( \alpha \). \( N^{-1} \) is the inverse non-interacting polarizability and \( \chi^{XC} \) is the Coulomb interaction matrix which includes both RPA local-field effects as well as electron-hole interaction. In Fig. 1 we present the phonon spectrum in the (0,1) direction obtained for an ideal 8-layer slab of Si(111). In the region where \( q < 1/2 \), being 1 the thickness, we obtain phonon instabilities related to violation of infinitesimal rotational (unrelaxed surface) and translational (a surface acoustic summation was not implemented) invariance. On the other hand, the interplay between local-field and excitonic effects...
produces an instability of surface modes at the zone boundary. An analysis of the eigenvectors of these modes, which are elliptically polarized in the sagittal plane and strongly localized in the outmost layer, shows that the displacements of the surface atoms give rise to a "buckled" surface, supporting thus Haneman's\(^7\) model for the 2x1 surface reconstruction.

In order to obtain a better understanding of the mechanism which produces a softening of the surface modes at \(q_{BZ}^{r}\), we concentrate on the top layer of the slab and take into account only the dangling-bond (DB) orbitals. In Fig. 2 (a) we show the contribution to the susceptibility from the non-interacting electron-hole system. The band structure gives rise to maxima near to wavevectors that correspond to the 7x7 reconstruction due to "nesting" of the Fermi surface.\(^8\) But no structure corresponding to the 2x1 superstructure is observable. The RPA local-field effects give a large correction (Fig. 2(b)) due to the extremely localized nature of the DB-orbitals. The features present before disappear and no electronic instability is observable. Beyond RPA, the system shows a strong tendency to an excitonic insulator instability when electron-hole attraction is considered. In this approximation the excitation energy of the system is lowered giving an enhancement of density response (Fig. 2(c)) and a tendency of the DB's to form a CDW. We can distinguish two features connected with commonly observed superstructures. First, we obtain a saddle-point at L. This enhancement of the susceptibility is responsible for the surface phonon instabilities at the L point (Fig. 1). But being a saddle-point, the
corresponding 2x1 superstructure should be still unstable against other configurations. In fact we observe that the next local maximum appears for a wavevector nearly corresponding to the 7x7 reconstruction. Another maximum appears at J, corresponding to a (\sqrt{3}x\sqrt{3})30^\circ superstructure, which is occasionally observed\(^9\).

The coupling of the CDW with the lattice, given by the form factor \(F_\alpha^{\kappa,q}(\kappa,q)\) determines the type of reconstruction. We observed that the coupling factor of the DB-CDW to displacements parallel to the surface is zero at the zone boundary. The only contribution for displacements parallel to the surface comes from interactions of the DB's with the "back bonds" which are much smaller than the first ones. This fact indicates that the CDW can almost only couple with displacements perpendicular to the surface as corroborated in the full calculation, discarding thus the "covalent bonding" model.

References