Zeitschrift: Helvetica Physica Acta
Band: 62 (1989)
Heft: 6-7

Artikel: Surface crystallography and lattice dynamics : GaAs(110) VS Si(111) 2x1
Autor: Santini, P. / Ruggerone, P. / Miglio, L.
DOI: https://doi.org/10.5169/seals-116120

SURFACE CRYSTALLOGRAPHY AND LATTICE DYNAMICS: GaAs(110) VS Si(111) 2x1

P. Santini, P. Ruggerone, L. Miglio and G. Benedek,
Dipartimento di Fisica dell'Università, via Celoria 16,
I-20133 Milano, Italy

The GaAs(110) surface is the most extensively studied one for heteropolar semiconductors: a well settled scheme for its relaxation is available[1] which consists in a nearly bond length conserving rotation of the surface chains by a tilt angle of about 30°. This configuration originates a striking crystallographic similarity between this surface and the Si(111) 2x1, where tilted chains are produced by the 2x1 reconstruction[2].

We extend the bond-charge-model approach which we used for Si(111) 2x1 [3] to calculate the lattice dynamics of a 23 layers GaAs(110) slab: The cores positions at the two surfaces are modified according to the relaxation pattern, and the surface bond charges are positioned where the charge density maps display their maxima. Static equilibrium conditions are imposed on the surface cores and bond charges and no fitting procedure is here used.

The calculated surface phonons (see fig.1) show a quite good agreement with the experimental data[4-7], confirming the reliability of our approach. However, we are here interested just in comparing the dispersion curves of GaAs(110) to the ones of Si(111) 2x1 (see fig.1 and fig.2). In both systems a 10 meV flat branch is present, consisting in a normal-to-the-surface vibration of the topmost surface chains: Its frequency position at zone border with respect to the Rayleigh wave is determined by the chain tilt. A striking similarity in the dispersion relations is also found for the optical modes (longitudinal vibrations of the topmost chains) starting in Γ at 24.9 meV in GaAs and 52.5 meV in Si: In our opinion this is actually a dynamical fingerprint of the surface chain configuration.

Finally, the different substrate orientations have a remarkable effect on the surface modes that are deeply penetrating into the bulk. The high-energy modes above the bulk bands in Si, for instance, involve vibrations of stiff sub-surface structures (five-fold rings): They are missing in the GaAs case since only regular six-fold structures are here present.

References

1. G. Quian, R.M. Martin and D.J. Chadi, PRB 37, 1303 (1988).
2. K.C. Pandey, PRL 49, 223 (1982).
3. L. Miglio, P. Santini, P. Ruggerone and G. Benedek, Surf. Sci. 211, 335 (1989).

4. U. Harten and J.P. Toennies, Europhys. Lett. 4, 833 (1987).
5. R.B. Doak and D.B. Nguyen, J. Electr. Spectr. 44, 205 (1987).
6. U.del Pennino, M.G.Betti, C.Mariani and I.Abbati, Surf.Sci. 211 (1989).
7. P.Santini, L. Miglio and G. Benedek, U. Harten, P. Ruggerone and J.P. Toennies, to be published.

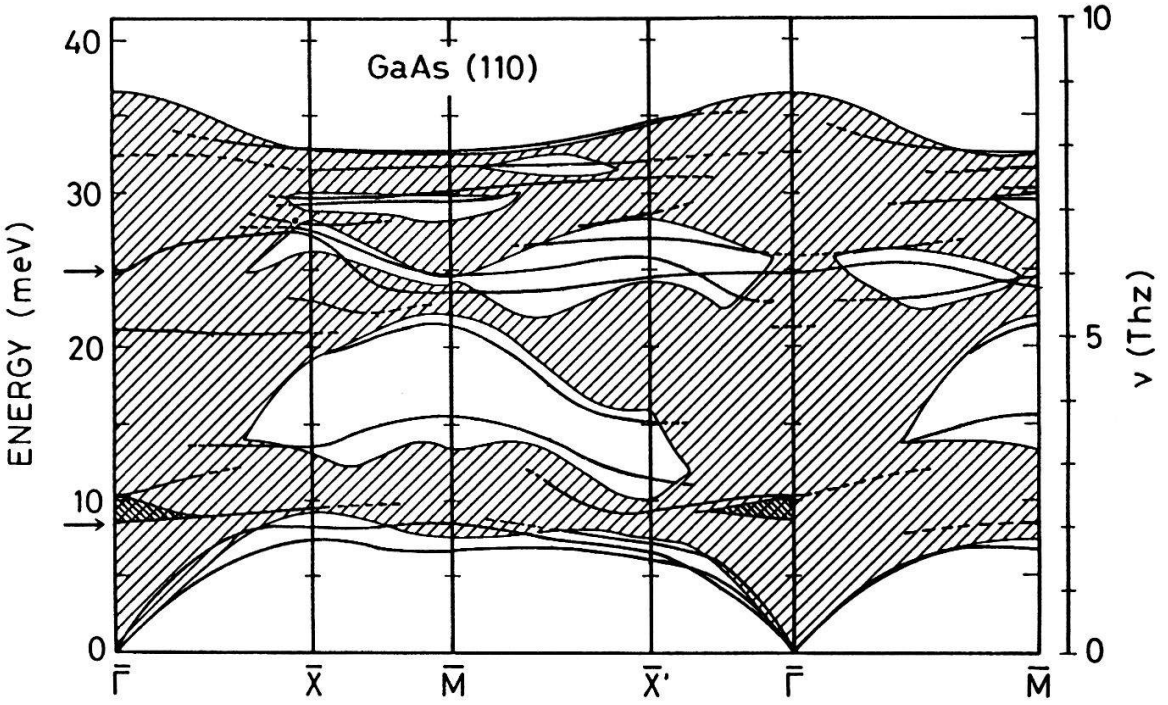

Fig.1

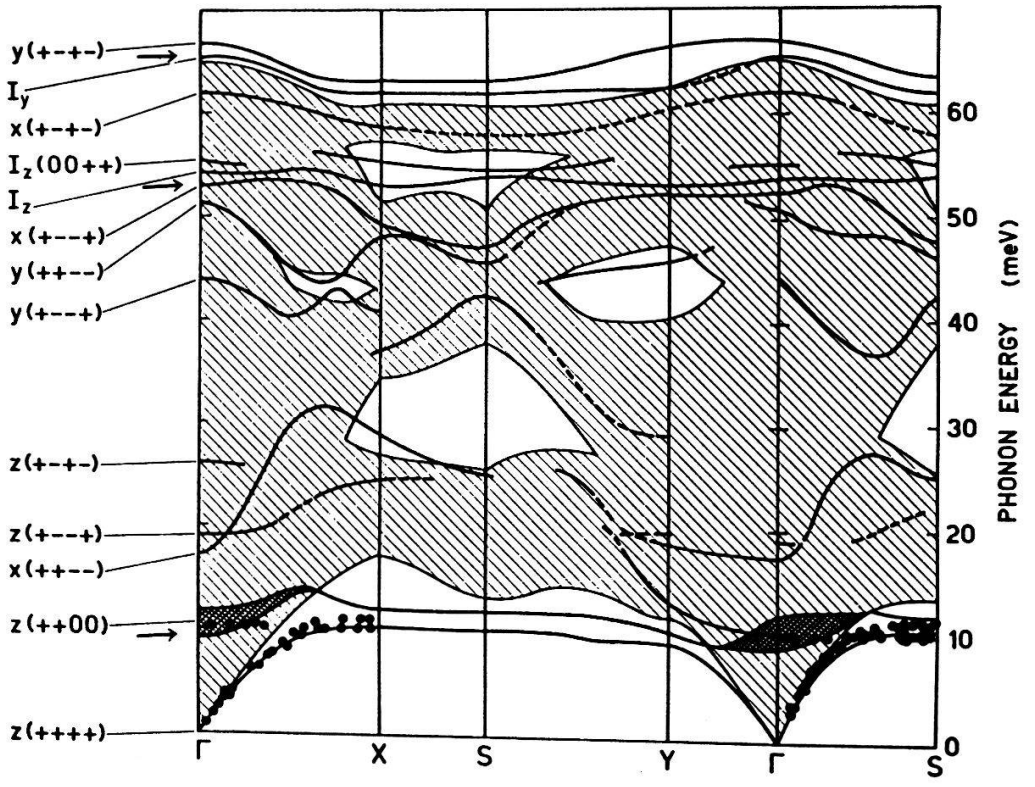

Fig.2