Lattice vibrations in mixed semiconductors

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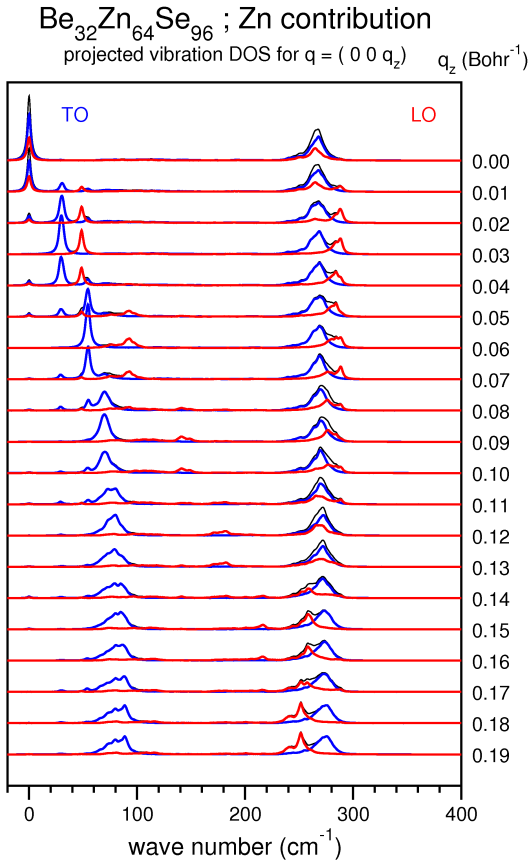
Solid solutions within zincblende- or wurtzite-type compounds find many applications because they allow to continuously tune lattice parameters, elastic properties, or electronic characteristics (band gap values etc.) of semiconductor devices. The study of vibration spectra helps to identify different ordered phases (for example, when dealing with ternary and quaternary semiconductors used in photovoltaics[1]) or, when applied to genuine solid solutions, to reveal the distribution of stress, or an extent of ordering.[2] However, this information comes about in a concealed form and, for its extraction, needs to resort to first-principles calculation results.

The calculations described in the present contribution are done in the frozen-phonon approach, using the SIESTA code[3] on supercells of 64 to 192 atoms. The aspects of alloying were treated in twofold way. Either (at small or "critical" concentrations), relevant structural patterns were identified (isolated impurities, pairs of interacting impurities, extended chain-like structures), and their impact on vibration spectra was inspected. Or (for "general" intermediate concentrations), several special quasirandom structures were constructed.

The immediate results of calculations are phonon modes (a discrete spectrum and eigenvectors) at the Γ point of the supercell used. For a sufficiently large supercell, this information is rich enough to allow projecting out "spectral functions" resolved in **q** values within the underlying Brillouin zone of the prototype (e.g., zincblende) lattice - see the figure on the right for the (Be,Zn)Se system. This allows to recover the "traces" of phonon dispersion in mixed crystals, also detectable e.g. by inelastic neutron scattering.[4] Otherwise, using a projection technique onto given symmetry coordinates, an *a posteriori* "approximative" symmetry analysis of phonon modes is possible on a mixed system.[5]



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2. O. Pagès, A.V. Postnikov, A. Chafi, D. Bormann *et al*., *Eur.J.Phys.B* **73**, 461 (2010).
3. http://icmab.cat/leem/siesta/ and references to basic papers therein , notably J.M. Soler, E. Artacho, J.D.Gale, A. García *et al*., *J.Phys.Cond.Matt.* **14**, 2745 (2002).
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