Meaningful analysis of lattice vibrations in mixed and complex semiconductors

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First-principles study of lattice dynamics is commonly done by applying frozen-phonon approach to supercells. In practical simulations of mixed (pseudobinary) semiconductors of, say, zincblende type, the size of supercells may easily amount to several tens of atoms, in order either to cover non-trivial quasirandom structures, or to explicitly include structural patterns of interest (clustered or chained impurities, pronounced tendencies for ordering, etc.) In parallel to this, a number of nominally ordered mixed semiconductors exist whose unit cells reach comparable sizes *per se*. In either case, a phonon calculation yields a large and confusing set of eigenvalues and eigenvectors the analysis of which, beyond constructing the density of modes resolved into atomic species, is not obvious. Fortunately, some insight can be gained by applying different projection techniques of eigenvectors, thus emphasizing the properties of interest. Examples are *i*) identification of "genuine" zone-center modes, helpful for comparison with infrared or Raman spectra [1]; *ii*) attribution of phonon modes by symmetry, even when symmetry relation hold only "approximatively" [2]; *iii*) extraction of dispersion (**q**-dependent) trends in vibration branches of mixed systems, visible in experiments but "nonexistent" in calculation (because of the formal lack of translation invariance) [3]. This approach will be illustrated on a number of cases including (Zn,Be)Se of different composition and under different conditions, and photovoltaics-relevant materials $Cu_2ZnSnSe_4$ and Cu_2SnSe_3. The calculation have been done by the SIESTA method; however, the projection techniques outlined are not related to any specific implementation of the frozen-phonon technique.

1. A. V. Postnikov *et al*., *Phys.Rev. B* **71**, 115206 (2005).
2. A.V. Postnikov and N.B. Mortazavi Amiri, *Phys.stat.solidi A* **210**, 1332 (2013).
3. M. N. Rao *et al*., to be published in *Phys.Rev.B* (2014).