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Raman scattering on phonons/phonon-polaritons of disordered semiconductor mixed crystals

Due to their high purity and their simple (cubic) structure and constituents (atoms), the pseudo-binary disordered $A_{1-x}B_xC$ semiconductor alloys set a benchmark to explore how physical properties are impacted by disorder in a percolation context. In terms of modelling one is tempted by the virtual crystal approximation (VCA), in which the actual A and B substituents are replaced by a virtual $A_{1-x}B_x$ atom with physical properties averaged over those of A and B depending on the composition x. By construction the VCA generates smooth variations with x of all physical properties: “the world is linear”. In fact, the physical properties of most importance for semiconductors, *i.e.*, the lattice constant and the optical band gap, actually obey linear-like variations with x. Presumably the reason is that such physical properties are integral in character and hence operate a natural average on the alloy disorder. Now, what about the local physical properties, such as the bond force constant, that governs the lattice dynamics? Generally, the lattice dynamics is interesting to address the effect of alloying, in that, through its diversity, it offers a unique playground to assign the relevant length scales at which operate various kinds of disorders induced by alloying, from quasi-infinite phonon-polaritons wavelengths probed by inelastic light (Raman) scattering down to minimal phonon wavelengths of twice the lattice constant achieved by inelastic neutron scattering.

Such extended studies of the lattice dynamics of semiconductor alloys are conducted within a long-standing international collaboration presently formalized into the so-called ViSA-IRP consortium (Vibrations of Semiconductor Alloys – International Research Partnership). This consortium notably puts forward an original percolation scheme [1] beyond the VCA to explain the Raman spectra of cubic $A_{1-x}B_xC$ semiconductor alloys. This can be grasped within a generic dual Raman signal per bond (A-C or B-C) reflecting a sensitivity of bond vibrations to their local (AC- or BC-like) environment. The VCA→Percolation change of paradigm raises a series of issues: (i) In principle, the duo can be used to elucidate the nature of the A→B substitution as to whether this is ideally random of due to clustering / anticlustering. Besides, (ii) one may well wonder how the duo behaves on approach to a pressure-induced structural transition, with three possible scenarios: convergence, divergence, parallelism. Last, (iii) It is interesting to test how/whether the percolation scheme for the dual Raman modes transfers under lowering the crystal symmetry from cubic to hexagonal. Such issues are investigated in the phonon-polariton [2] and phonon [3] regimes by combining (high-pressure) forward/backward Raman scattering and inelastic neutron scattering, with *ab initio* phonon calculations in support.

[1] O. Pagès *et al*. Physical Review B 86 (2012) 045201
[2] H. Dicko et al. Scientific Reports 9 (2019) 7817
[3] T. Alhaddad *et al*. Scientific Reports 15 (2025) 1212