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THE PERCOLATION SCHEME FOR THE VERY BASIC UNDERSTANDING OF THE RAMAN SPECTRA OF MIXED CRYSTALS: APPARENT UNIVERSALITY AND POSSIBLE APPLICATION

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Generally, while dealing with mixed crystals, the crucial issue is to determine whether the atom substitution is ideally random or due to local clustering/anti-clustering. In the latter case, the next issue is to estimate the deviation from random substitution via some relevant order parameter. Raman scattering is interesting with respect to the raised issues because it probes the force constant of a chemical bond, which is a local property. As such, it is presumably sensitive to the local environment of a bond. Moreover, Raman scattering is conveniently operated at the laboratory scale, being non-destructive, fast, and relates to the crystal in volume. However, if we refer to the admitted models for the description of the abundant Raman spectra of the mixed crystals with cubic structure, worked out at the emergence of such systems in the sixties, namely the modified-random-element-isodisplacement (MREI) model and the cluster model, they both fail to account for the natural complexity of the Raman spectra of most random mixed crystals, not to mention about the non-random ones. Basically the MREI model falls short of explaining the natural complexity in question, while the cluster model overestimates it by far. Over the past decade we have introduced a novel model to discuss the Raman spectra of the mixed crystals with cubic structure, the so-called percolation model that seems to apply universally. Moreover, as this model distinguishes between the vibrations of like bonds depending on whether they vibrate in like or foreign environment, it offers a possibility to formalize any trend towards local clustering/anti-clustering (like environment favored/disfavored) via the Raman intensities. In this communication we provide a comprehensive overview of the percolation scheme covering various vibrations addressed in a Raman experiment (the purely-mechanical TO modes as well as the polar LO and phonon-polariton ones), supported by *ab initio* calculations.

Biography

Olivier Pagès has completed his PhD in Solid State Physics on "Study by Raman scattering of the electronic band bending at the interface between semiconductor compounds" from Université Paul Sabatier (Toulouse III, France). He then conducted Postdoctoral studies at the Birkbeck College (London University, UK) for 1.5 years on "Dielectric approaches of percolation phenomena occurring in highly complex binary polymeric mixtures of the insulating-conducting type". He is presently the Director of the Laboratoire de Chimie et Physique – Approche Multi-Echelle des Milieux Complexes (LCP-A2MC) de l'Université de Lorraine (Nancy-Metz, France). His field of research is concerned with the introduction of a percolation-based approach for the very basic understanding of the vibrational properties of the mixed crystals that can be viewed as the most simple out of complicated systems. He has published more than 65 papers in reputed journals on the subject.

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