Vibrational excitations in structures with topological and lattice disorder

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We present a review of a theoretical study of vibrational excitations in disordered materials using an analytical (CPA) and numerical approaches [1-4]. The structural models were: (i) realistic models of vitreous silica and germania constructed by classical molecular dynamics; (ii) models of a single-component "metal" glass with dominant icosahedral order; (iii) lattice models with force-constant disorder. Topics studied include: (i) single plane wave and wave packet propagation and the related Ioffe-Regel crossover; (ii) the origin of the boson peak in the topologically disordered icosahedral glass and disordered lattices with force-constant disorder (the boson peak is due to disorder-induced level-repelling and mode-hybridization effects on states near the lowest van Hove singularity of the corresponding crystalline approximant); (iii) the vibrational localization in disordered lattices by means of multifractal analysis, in analogy to the study of the Anderson localization-delocalization transition for electrons in disordered systems (the phase diagrams for vibrational localization in vector models have been established and scaling properties of critical states have been analysed); (iv) the high-disorder mechanical instability involving negative vibrational eigenvalues and the origin of the zero-frequency spectrum singularity in disordered lattices.

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