

Poster Presentation

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Lattice dynamics and macroscopic properties in complex metallic alloys

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Complex metallic alloys are long-range ordered materials, characterized by large unit cells, comprising several tens to thousands of atoms [1]. These complex alloys often consist of characteristic, cluster building blocks, which in many cases show icosahedral symmetry. Numerous complex phases are known, that can be described in a rather simple way as the periodic or quasi-periodic packing of such atomic clusters. The lattice dynamics of CMAs has been the subject of both theoretical and experimental investigations in view of their interesting macroscopic properties such as low thermal conductivity. In aperiodic crystals in the higher wave-vector regime, theory predicts that the lattice modes are critical: they are neither extended as in simple crystals nor localized as in disordered systems [2]. Experimentally phonons have been studied in different CMAs systems like clathrates, approximant-crystals and quasicrystals. For all of them, acoustic modes are well-defined for wave-vectors close to Brillouin zone centres, but then broaden rapidly as the result of coupling with other excitations [3]. We will present a combined experimental and atomistic simulation study of the lattice dynamics of the complex metallic alloy Al₁₃Co₄ phase [4], which is a periodic approximant of the decagonal phase. Particular attention will be paid to the differences between the periodic and 'quasiperiodic' directions. Inelastic neutron scattering measurements carried out on a large, single grain on a triple-axis spectrometer will be compared to simulations, focussing on the dispersion relations and the intensity distribution of the $S(Q,\omega)$ scattering function, which is a very sensitive test of the model [3]. Simulations are performed with DFT methods and empirical, oscillating, pair potentials [5]. In addition, thermal conductivity calculations, based on the Green-Kubo method, will be compared with measurements, which show a weak anisotropy [6-7]. In this way, the structure-dynamics-properties relation for CMAs is thoroughly explored.

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