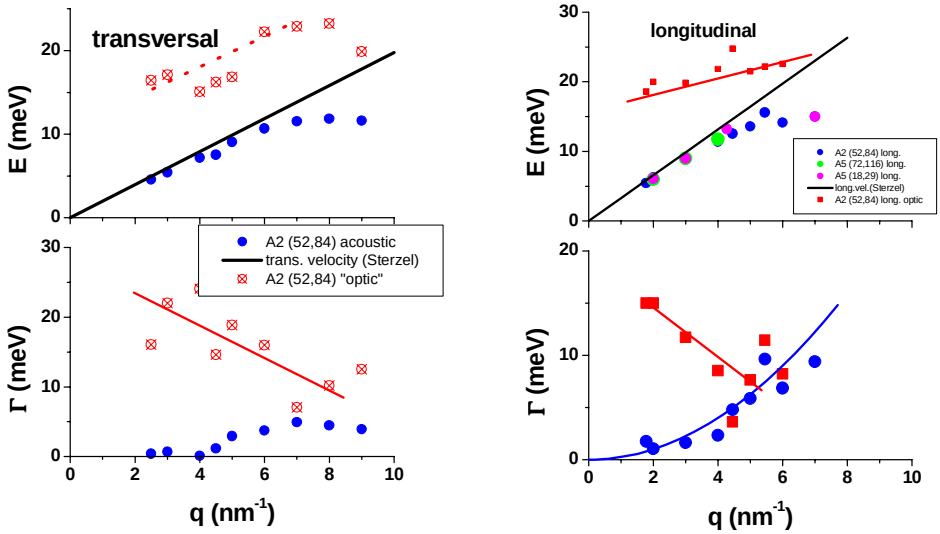
Vibrational properties (phonon dispersion and density of states) in quasi-crystals

BRAND, R.A., VOSS, J., KRISH, M., CHUMAKOV A. and RÜFFER R.
Institute of Physics, Universität Duisburg-Essen, ESRF, Grenoble France

Quasicrystals (QCs) are alloy compounds with non-crysataalographic icosahedral (i-) or decagonal (d-) point symmetry. This new type of long-range but non-periodic order has led to the discovery of interesting dynamical properties [1]. It has been shown that the elementary lattice excitations in QCs can be classified into phonons and phasons. The phonons may be marginally localised ("critical").

Single-grain samples of several QC systems are available. We have used such samples to study the phonon dispersion ($\omega(q)$) in i-AlPdMn [2] and i-MgZnY [3]. The latter results are shown in the figure below. The start of the LA and TA branches were found in agreement with the measured sound velocities, but both quickly flatten out for $q > 4$ nm^{-1}. In addition, the line width $\Gamma(q)$ for the TA mode increases strongly above this point. For the LA mode, it seems that the increase in $\Gamma(q)$ is quadratic in q, such as is found in glasses. Very broad optical branches were found in i-AlPdMn and i-MgZnY as well except for the TO branch of i-AlPdMn seems to be missing. An initial study of the TA and LA branches in i-AlCuFe was also performed and similar results were found.



The iron-partial vibrational density of states $g_{Fe}(E)$ was studied in several iron-containing QCs using i-AlCuFe and d-AlNiFe. These results were compared to results obtained by inelastic neutron scattering on isotope-doped samples. It was found possible to extract the elemental-specific g(E) for each component [2]. The resulting true total g(E) is in good agreement with the anomalous results of the lattice contribution to the specific heat $C_{latt}(T)$. The elemental-specific contributions identify low energy non-Debye excitations on mainly Cu as the origin of the anomalous $C_{latt}(T)$, a result which correlates well with studies of the phason dynamics for Cu [3] and Fe [4].

References

[1] R.A. Brand et al., in "Quasicrystals", ed. H.-R. Trebin (Wiley-VCH, Weinheim 2003).
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