

Phonon Spectroscopy in Quasicrystalline Al-Cu-Fe

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Introduction

Quasicrystals are a new class of materials showing long-range rotational order but exhibiting symmetries that are not in agreement with the space groups of three-dimensional crystallography. Investigations concerning the lattice dynamics of these materials are still rare. Inelastic neutron scattering experiments have focused mainly on the determination of the dispersion of acoustic modes. Optic modes in quasicrystals have received less attention so far. However, measurements of the phonon density of states using nuclear resonant scattering revealed the presence of high-energy excitation (ca. 30 meV).¹ On the other hand, the temperature dependence of the specific heat at low temperatures shows deviations from the Debye law suggesting the existence of low-energy nonacoustic modes below 10 meV.

Methods and Materials

We used high-resolution inelastic scattering of x-rays for our investigation on the lattice dynamics in quasicrystalline materials.² These experiments were performed at the APS beamline 3-ID. Since our first test experiments in February 2000 showed promising results, we continued these measurements in June 2000. The sample was a single-domain Al-Cu-Fe quasicrystal cut perpendicular to the five-fold axis. The Bragg reflection 18,29 was chosen as starting point for our measurements. The quasicrystal was aligned in order to observe longitudinal phonon modes propagating along the five-fold symmetry axis. Inelastic spectra gained at different momentum transfer are shown in Fig. 1.

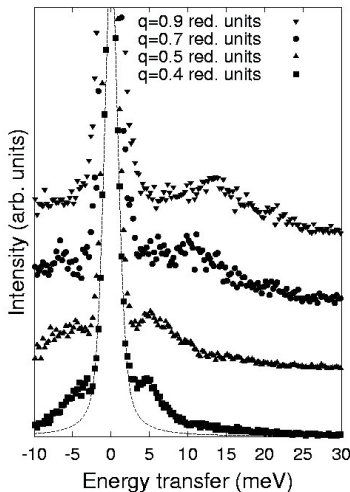


FIG. 1. Inelastic x-ray scattering from a single domain sample of quasicrystalline Al-Cu-Fe, gained at different momentum transfers. The dashed line represents the instrumental resolution function.

Results

Data were collected in an energy range from -10 meV to 40 meV.¹ The energy resolution during the experiments was 2.2 meV. We were able to gain inelastic spectra at five different momentum transfers from 0.4 to 1.1 reduced units, which correspond approximately to 0.14 to 0.4 \AA^{-1} . Besides the strong elastic contribution,

all spectra clearly show excitations in the energy range below 20 meV. The spectra collected at higher momentum transfers show a shift of all excitations to higher energies. Furthermore, an increased broadening of the excitations for larger momentum transfers can also be noticed. All inelastic spectra show obviously the existence of modes that are additional to the expected longitudinal acoustic mode, see Fig. 2. These excitations are most probably due to low-energy optical modes or due to transverse acoustic modes propagating perpendicular to the five-fold axis.

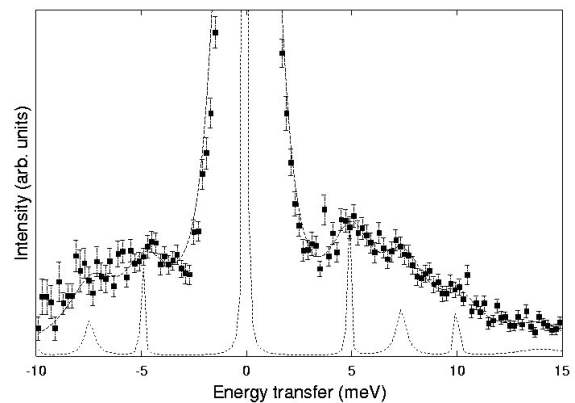


FIG. 2. Spectrum taken at a momentum transfer of 0.5 reduced units. The solid line is a fit to the data using damped harmonic oscillator functions, convoluted with the spectrometer resolution function. The dashed line corresponds to the fit after deconvolution.

Discussion

The experiments showed that high-resolution inelastic x-ray scattering is a feasible method for the investigation of lattice dynamics in quasicrystalline materials. We were able to detect excitations that were not revealed with common methods, like inelastic neutron scattering. Since the intensity of the phonon excitations is low compared to the intensity due to elastic scattering, further measurements using longer counting times are required to improve the statistics.

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References

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