

Diffuse Scattering and Phasons in the i-Zn-Mg-Sc Phase and its 1/1 Approximant

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Phasons modes are excitations characteristic of the quasicrystalline state. In the same way than phonons modes lead to thermal diffuse scattering, phason modes lead to diffuse scattering in the diffraction pattern. This diffuse scattering can be calculated in the framework of the hydrodynamic theory of icosahedral phases.

Diffuse scattering has been extensively studied in the i-AlPdMn phase. It has been shown that most of the observed diffuse scattering is due to phason modes, which are interpreted as pre-transitional fluctuations.

We present an extensive room temperature study of the diffuse scattering in the i-ZnMgSc quasicrystal and its 1/1 periodic approximant. For this purpose, absolute scale measurements of the X-ray diffuse scattering have been carried out on the D2AM beam line (ESRF). Whereas the diffuse scattering measured in the 1/1 approximant can be accounted for by the thermal vibrations (TDS), a supplementary contribution to the signal is observed in the quasicrystal. This extra contribution is larger for reflections having a larger Q_{per} component, indicating that it is due to phason modes. This demonstrates that although both phases share the same clusters, phason modes are a characteristic of the quasiperiodic long range order. Using the absolute scale measurement, we find that the amount of diffuse scattering is about four times smaller in the i-ZnMgSc than in the i-AlPdMn phase. This demonstrates the high structural quality of the i-ZnMgSc phase, which is also evidenced by the large number of high Q_{per} reflections observed in the diffraction pattern.

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