The atomic structure of quasicrystals is now well understood in the CdYb[1] and the isostructural Zn(Mg)Sc system. Both the quasicrystal (i-MgSc) and its 1/1 periodic approximant (Zn₆Sc) are described by a packing of large triacontahedral units on a quasiperiodic and a bcc lattice, respectively. The triacontahedral cluster is built up by the close packing of large (Sc) and small (Zn) atoms arranged on successive shells of approximately icosahedral symmetry, except for the innermost one which is a tetrahedron. In the 1/1 approximant the tetrahedra occupy six different orientations above the transition temperature (Tc) of 160 K. Below Tc they are ordered in an anti-parallel way along the (110) direction [2,3]. Combining quasielastic neutron scattering as a function of temperature and atomic scale simulation using oscillating pair potentials [4], we show that above Tc the disorder is dynamic in nature. The Zn tetrahedron behaves as a single 'molecule' which reorients constantly on a time scale of a few ps. Due to the close packing of the constituting atoms, these tetrahedron reorientations induce large distortions of the successive icosahedral shells (of the order 0.8 Å) resulting in an exceptional dynamical flexibility (down to T=160 K) unique for such intermetallic compounds. A similar dynamics is observed in the quasicrystal and is certainly playing an important role in the mechanism that stabilizes the quasiperiodic long range order.


Quasicrystal, dynamics, simulation