

QC3 Tetrahedron Dynamics in the i-ZnMgSc quasicrystal and its 1/1 periodic approximant Zn₆Sc H. Euchner,^{af} T. Yamada,^b R. Tamura,^b T. Ishimasa,^c S. Rols,^d H. Schober,^d M. Mihalkovic,^c M. de Boissieu,^{fa} *ITAP, Universität Stuttgart, Germany,* ^b*Tokyo University of Science, Tokyo, Japan,* ^c*Hokkaido University, Sapporo, Japan,* ^d*Institute Laue Langevin, Grenoble, France,* ^e*Slovak Academy of Sciences, Bratislava, Slovakia,* ^f*SIMAP, Grenoble-INP, CNRS, Université Joseph Fourier, St. Martin d'Herès, France*
E-mail: euchner@itap.physik.uni-stuttgart.de

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 (T_c) of 160 K. Below T_c 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 T_c 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.

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Quasicrystal, dynamics, simulation

QC4 Quasicrystal and Approximant Surfaces: Structural Determination and Pseudomorphy. Julian Ledieu, *Institut Jean Lamour, Université de Lorraine, UMR7198 CNRS, Ecoles des Mines, Parc de Saurupt, 54042 Nancy, France*
E-mail: Julian.ledieu@ijl.nancy-universite.fr

Over the last 20 years, intensive efforts have been dedicated to the study of quasicrystal surfaces [1]. With only few exceptions, a consensus has emerged that quasicrystal surfaces should be considered as bulk-terminated. The selection of bulk planes as surface terminations obeys experimentally established rules. Compared to surfaces of "classical" crystalline materials, aperiodic surfaces offer a wealth of structurally and chemically inequivalent sites. Their particular electronic structure and topography have led to unusual growth phenomena [2]. Now, the growth of approximant systems, which are large unit cell complex metallic alloys close in composition to a related quasicrystalline phase, allows the direct comparison of structural and growth phenomena on related periodic and aperiodic surfaces. Following a summary of the main results obtained on quasicrystal surfaces, we will report the recent work performed on Al-based approximant surfaces. For both type of systems, nucleation phenomena will be presented along with the pseudomorphic growth of single-element thin films.

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