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Nuclear and magnetic structure of $CaCu_2O_3$

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We have investigated the structural and magnetic properties of the spin-ladder compound, $CaCu_2O_3$. A full data set was collected at 6 K using the E5, four-circle diffactometer at the BERII reactor, at the Hahn-Meitner Institute, Berlin. The refinement of the crystal structure was carried out with the program Xtal 3.4. A total of 1576 (473 unique) reflections were collected, allowing the crystal structure of $CaCu_2O_3$ to be successfully refined in the orthorhombic space group Pmmn with a residual R_F=0.038(R_W=0.034). In this structure the Ca-atoms are located at the Wyckoff position 2a(1/4,1/4,z), the Cu- and O1-atoms at 4f(x,1/4,z) and the O2-atoms at 2b(1/4,3/4,z). We have determined the positional parameters x and z of the copper atoms with high accuracy. In contrast to the results of Ruck et al. [1] all these positions were found to be fully occupied. Furthermore while the positional parameters of the atoms do not show significant changes down to low temperature, the atomic thermal vibrations are strongly reduced at lower temperature. The Cu^{2+} ions of $CaCu_2O_3$ possess spin-1/2 and become magnetically ordered below the Néel temperature T_N=25.5(0.5) K. We have found that the magnetic propagation vector is in fact incommensurate and given by **k**=(0.43,1/2,1/2) so that the magnetic satellites are generated by the rule $(hkl)_M=(hkl)_N \pm \mathbf{k}$. A total of 45 magnetic (9 unique) reflections were collected and the determination of the magnetic structure is in progress.

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Keywords: low-dimensional magnetism, neutron diffraction, single crystal diffraction

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An analysis on the synthesis of icosahedral quasicrystal based on AlMgMn complex metallic alloys

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Though several classes of quasicrystals have been discovered, still the criteria of synthesis and their stability region in the phase diagram are not fully understood. It is often realized that in some alloy systems there is a close relationship between the quasicrystals and the crystalline intermetallic phases as in both the cases the clusters resembles closely. In case of Mg-based system, the relationship between the quasicrystals and the typical Frank-Kasper phase in terms of clusters is well recognized for the synthesis of metastable quasicrystals. Often, based on e/criteria, the search for quasicrystals appears to be possible depending on the alloy system. In the present study, attempts will be made to critically review the basis of synthesis, and analyze the binary and ternary intermetallic phases in Al-Mg alloys for the possible formation of quasicrystalline phases. Al-Mg alloys are known to be light and corrosion resistant alloys. It is found that in case of the composition based on $Al_{18}Mg_3Mn_2$ phase, quasicrystals formation is highly favorable during rapid solidification. It should be emphasized that this phase is known as T-phase in literature and it contains 184 atoms with a FCC lattice parameter of 1.453nm, isostructural to $Al_{18}Mg_3Cr_2$. The manganese atoms take the icosahedral co-ordination. There is some similarity with the Bergman phase of $Mg_{32}(AlZn)_{49}$. However, the clusters in both the cases are not quite similar. The analysis of the rapidly solidified Al-Mg-Mn phase suggests that quasicrystal in Al-Mg-Mn phase does not belong to the Bergman class rather it conforms to the Mackay class of quasicrystals. Attempts will be made to rationalize the basis of synthesis and stability region of quasicrystals and related crystalline approximant phases.

Keywords: quasicrystals, complex metallic alloys, rapid quenching

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Atomic arrangement of Al-Co-Ni Co-rich quasicrystal and W(AlCoNi) crystalline approximant

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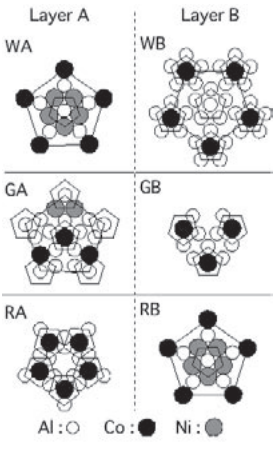
The structure of Al-Co-Ni Co-rich quasicrystal has been studied by scanning tunneling microscopy (STM) combined with high-angle annular detector dark-field scanning transmission electron microscopy (HAADF-STEM). STM observation of the surface compositional dependence of Co and Ni for Al-Co-Ni Co-rich quasicrystal has identified the 0.47 nm Co cluster and the 0.29 nm Ni cluster, respectively. From the STM images of the clean Co-rich surface, it is concluded that multiple main clusters is essential to explain the structure. From these results, three main clusters are proposed for both A and B stacking layers, as shown in Figure 1. These clusters are partly based on the Hiraga model [1]. Moreover, we have identified that the three main clusters have a tendency to form a boat-type cluster. It is also identified that the boat-type cluster forms 4 different tiling patterns: 5 boat pentagon, 5 boat star-shape, 8 boat twin-star, 3 boat head-inside. We have also applied the boat cluster to the HAADF-STEM image of W-(AlCoNi) crystalline approximant to successfully identify the atomic arrangement.



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Keywords: quasicrystals, structure determination, STM