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Atomic-scale electron microscopy and spectroscopy of AlMnPd quasicrystal

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Quasicrystals are aperiodically long-range ordered solids that exhibit rotational symmetries incompatible with conventional periodic lattice order. Their structure is often described according to a hyperspace crystallography, which interprets the quasicrystal as a periodic structure embedded in a hyperspace. This mathematical recipe enables to calculate the diffraction intensity of any quasicrystal model structures, and accordingly the quasicrystal structures can be determined by the x-ray diffraction analysis along the similar manner for periodic crystals.

Al-Mn-Pd alloys form a thermodynamically stable decagonal quasicrystal, a planar realization of the quasiperiodic order. Its structure had been intensively studied by single-quasicrystal X-ray diffraction [1], [2] and high-resolution phase-contrast electron microscopy [3], [4], which led to the established model structure that reasonably satisfies the both observations. In the present work, we have revisited the decagonal Al-Mn-Pd by aberration-corrected ultrahigh-resolution scanning transmission electron microscopy (STEM), and immediately find that the observed Z-contrast is significantly different from that expected from the existing model structures. The observed contrast cannot be reproduced by the simulation based on the model structure proposed by x-ray analysis [2], forcing to modify the local chemical order of Al/Mn/Pd. During the course of study, we particularly emphasize an effective use of electron energy-loss spectroscopy (EELS) at atomic-scale, which has been successful for identifying the Mn and Pd sites that are hardly distinguished based on the Z-contrast intensity alone. The present results strongly demonstrate that the direct observation of real-space atomic configurations is indispensable to determine the quasicrystal structure conclusively [5].

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Effect of Ti addition on the hydrogen storage properties of nanoquasicrystal-glass composites in $(Zr_{69.5}Al_{7.5}Cu_{12}Ni_{11})_{100-x}Ti_x$ alloys

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The high number of potential interstitial sites for hydrogen and the favourable hydrogen-metal chemistry make Zr-Al-Cu-Ni quasicrystalline alloys a promising material for the hydrogen storage applications [1]. The alloy $Zr_{69.5}Al_{7.5}Cu_{12}Ni_{11}$ is of special interest for studying the influence of hydrogenation on the microstructure of these quasicrystalline alloys [2]. We have investigated the effect of Ti addition on the quasicrystalline phase formation and indentation characteristics of $Zr_{69.5}Al_{7.5}Cu_{12}Ni_{11}$ alloy [3]. The addition of Ti changes the morphology of quasicrystals. It is therefore imperative that a systematic examination of hydrogen storage properties in a given system is carried out.

In the present study, the hydrogen storage properties of $(Zr_{69.5}Al_{7.5}Cu_{12}Ni_{11})_{100-x}Ti_x$ (x=0, 4 and 12) nanoquasicrystal-glass composites have been investigated. The investigation will be focussed on the phase formation and microstructural changes with addition of Ti and their correlation with hydrogen storage properties of Zr-Al-Cu-Ni alloys. It has been found that the hydrogen uptake capacity and the absorption kinetics of the composites increase with addition of Ti. The hydrogen storage capacity is found to be 1.20 wt. %, 1.38 wt. % and 1.56 wt. % for the alloys with x=0, 4 and 12 respectively. The increase in the hydrogen uptake capacity may be attributed to the grain refinement of quasicrystals resulting due to Ti addition. The hydrogen decomposition behavior of $(Zr_{69.5}Al_{7.5}Cu_{12}Ni_{11})_{100-x}Ti_x$ (x=0, 4 and 12) nanoquasicrystal-glass composites has been investigated by using temperature programmed desorption (TPD) experiment. The TPD experiments indicate that the addition of Ti reduces the maximum desorption temperature of hydrogenated ribbons.

The microstructural changes during hydrogenation have also been investigated. The structural characterization of the hydrogenated ribbons reveals an expansion of the quasilattice with hydrogenation. After hydrogenation, a broad hump along with weaker peaks in the X-ray diffraction pattern has been observed. Transmission Electron Microscopy (TEM) investigations exhibited microstructural changes during hydrogenation. It has been observed that microstructural and morphological changes alter the hydrogen storage properties of nanoquasicrystal-glass composites.

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Ion beam analyses of Al(Si)-Cu-Fe approximant thin films

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Quasicrystalline materials exhibit properties that are very different from conventional metallic materials. They are metallic alloys, and show high hardness and stiffness but low electrical and thermal conductivity. The coefficient of friction and surface energy of the quasicrystalline materials are also very low [1]. Both structure and physical properties of a higher order approximant crystal are similar to those of a quasicrystal.

In this work, multilayered Al-Cu-Fe thin films have been deposited by triple-target unbalanced high vacuum magnetron sputtering onto Si substrates. The multilayer periods are ranging from Λ=2 nm to Λ=400 nm, with nominal layer thicknesses ratios of 7:2:1 to maintain a global chemical composition corresponding to the icosahedral quasicrystalline phase. The number of periods was varied from N=1 to N=50 with total film thicknesses up to 400 nm.

Isothermal annealing was performed on all samples for temperatures up to 800 °C using an in situ high-temperature X-ray diffraction (XRD) furnace. The composition of the multilayer sequences before and after annealing was investigated using time-of-flight elastic recoil detection analysis (ToF-ERDA) and Rutherford backscattering