

X-RAY STUDYING AMORPHOUS → QUASICRYSTAL TRANSFORMATIONS IN SPUTTERED Ti-Zr-Ni FILMS

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In recent years much attention has been paid to the study of composite materials, which are partially crystallized systems consisting of amorphous matrix and embedded nanoparticles of crystalline phase. In this work we have considered the structure transformations that occur during annealing in Ti-Zr-Ni system contained 42 at.% Ti, 40 at.% Zr and 18 at.% Ni. With such composition quasicrystals can form in the system [1,2]. Ti-Zr-Ni films of micron thickness were prepared by magnetron sputtering in Ar atmosphere. As-prepared samples were confirmed as amorphous by X-ray diffraction (XRD). XRD patterns revealed 2-3 broad haloes. For investigation process the samples were annealed in vacuum at temperatures from 100 to 400°C with an interval of 50 degrees during 60 min. After each annealing step XRD spectra were obtained by DRON-3M installation with Cu K α radiation source and crystal-monochromator in the range of $2\theta = 20 - 150^\circ$. As temperature increased XRD line shape gradually changed, against the background of the halo sharper peaks appeared. To find quantitative structure characteristics of amorphous samples the method of radial distribution function (RDF) construction has been used [3]. For multi-component alloys this method allows us to get mean values of radii of nearest coordination spheres and coordination numbers. New Profile Program has been used to analyze RDF curve. Also we have evaluated the shortest interatomic distance using Ehrenfest's relation [3]. Quasicrystal XRD peaks positions we have calculated using method proposed by Cahn[4]. With satisfactory coincidence of the bar diffractogram of the quasicrystal with the maxima of the experimental diffractogram, the quasicrystallinity parameter could be estimated from the value of the fitting parameter.

Joint analysis of structural characteristics obtained using various calculation methods allows us to draw the following conclusions. In the initial state, the samples contain regions with different composition and different short-range order. There are nanoregions with icosahedral short-range order, which can be considered as nuclei of quasicrystalline phase. Upon heating, the sizes of the quasicrystallinity regions increase, and the following size effect is observed: in films with smaller thickness the phase transformations appear at higher temperatures.

References

1. Davis J. P., Majzoub E. H., Simmons J. M., Kelton K. F. Ternary phase diagram studies in Ti-Zr-Ni alloys// *Materials Science and Engineering*. – 2000. – 294-296. – p. 104 – 107.
2. Huang H., Meng D., Lai X. et al. TiZrNi quasicrystal film prepared by magnetron sputtering//*J. Vacuum*. – 2015. – v. 122. – p. 147-153.
3. Skryshevskii A.F. *Structure Analysis of Liquids and Amorphous Solids*. Moscow: High School. – 1980. – 328pp.
4. Cahn J. W., Shechtman D. Indexing of icosahedral quasiperiodic crystals//*J. Mater. Res*. – 1986. – vol. 1, N.1. - p.13-26