Nanocomposites and nanomaterials

CRYSTAL STRUCTURE OF THE $TbCu_5Al_7$ COMPOUND

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Rare-earth based materials are one of the most investigated due to their widespread potential applications such as permanent magnets [1], magnetocaloric systems [2], hydrogen storage materials [3] and other applications. Crystallite size reducing up to nano-scale provides an opportunity to improve the properties of material [4, 5]. Therefore, investigation of new phases as a first step of the nano material preparation is important task for researcher. In this work we present results of investigations of the $TbCu_5Al_7$ ternary compound.

In references [6] the authors presented information concerning the existence of the $TbCu_5Al_7$ ternary compounds and the $ThMn_{12}$ structure type was proposed without any crystallographic data.

The sample was prepared by arc melting of the elements with further annealing at 600°C. Crystal structure of the this compound was successfully refined by the Rietveld method using the X-ray powder pattern of the $TbCu_5Al_7$ sample collected on the Guinier Huber G 670 diffractometer ($CuK\alpha_1$ radiation). The structure was successfully solved in the : *I*4/*mmm*, $ThMn_{12}$ structure type, Pearson symbol, *tI*26, $a = 8.70178(4)$, $c = 5.12573(3)$ Å; $R_I = 0.0467$; $R_P = 0.0780$; $R_{wp} = 0.0818$. Atomic coordinates as well as isotropic displacement parameters are are summarized in Table.

Tabl. 1. Atomic coordinates and isotropic displacements parameters of the $TbCu_5Al_7$ compound

Atom	Site	*x*	*y*	*z*	B_{iso}, Å^2
Cu1	8*f*	1/4	1/4	1/4	0.66(2)
*M**	8*j*	0.2803(1)	1/2	0	0.46(4)
Al	8*i*	0.3451(2)	0	0	0.56(4)
Tb	2*a*	0	0	0	0.54(2)

*Mixed occupation.
M = 0.143(3) Cu + 0.857(3) Al

Crystal structure of this compound can be consider as "cluster" formed from Cu and Al atoms around Tb. Packing 20 vertex polyhedrons are represented in Figure.

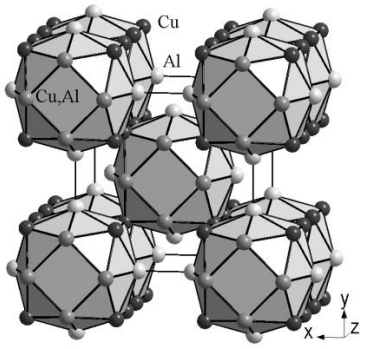

Fig. Polyhedron packing in the structure of $TbCu_5Al_7$ ternary compound

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