Abstract

The investigation of the system Th-Ni-B prompted a novel ternary compound ThNi$_{12}$B$_6$. X-ray structure analysis of single crystals obtained by mechanical fragmentation of an as cast alloy revealed a fully ordered CeNi$_{12}$B$_6$-type structure (space group Cmc$_2$$_1$, No. 36; a = 0.95638(1) nm, b = 0.73852(1) nm, c = 1.10195(1) nm; R$_{F2}$ = 0.0305).

Density functional calculations (DFT) have been performed comprising heat of formation, electronic band structure and density of states, Fermi surface via Wannier functions, phonon band structure and density of states, phonon and electronic contributions to the specific heat and the elastic constants C$_{ij}$. Comparing the parameters evaluated from DFT with the experimental data, overall satisfactory agreement has been achieved.

Electrical resistivity, magnetic susceptibility and specific heat manifest a Pauli paramagnetic, metallic behaviour for ThNi$_{12}$B$_6$ without any anomalies, in close match with the isotypic homologue LaNi$_{12}$B$_6$.

Static and dynamic hardness measurements show rather high values; Young’s modulus is in the range of 240 GPa. The Debye temperature, $\theta_D = 490$ K, gained via elastic constants, is slightly higher than the values estimated from specific heat or electrical resistivity data. A rather low coefficient of thermal expansion, $\alpha = 5.5\times10^{-6}$ K$^{-1}$, was extracted from the temperature dependent length change.
Figure I: Rietveld refinement (CuKα) for the sample specimen with nominal composition ThNi$_{12}$B$_6$ (as cast condition). Atom parameters were taken from the single crystal X-ray-refinement as presented in Table 1 of the paper.