

SUMMARY

The aim of this thesis is an experimental mineralogical research of the Sb-Te-Ni ternary system using silica glass tube method. The emphasis is placed on determining the crystal structure of ternary phase Ni_2SbTe_2 , which was founded as 6 μm grain by Vavřin a Frýda (1998) at the Kunratice Cu-Ni deposit (North Bohemia).

The crystal structure of Ni_2SbTe_2 , prepared at 800 °C (terminated by quenching), determined from X-ray single crystal diffraction data, is hexagonal, NiAs type with lattice parameters $a = 3.91085(18)$ Å, $c = 5.24897(31)$ Å. The antimony and tellurium atoms occupy the crystallographic position $2c$, the position $2a$ is occupied by nickel atoms.

The crystal structure of Ni_2SbTe_2 , prepared at 400 °C (terminated by slow cooling to 50 °C within the interval of 22 hours), is hexagonal with lattice parameters $a = 3.91106(21)$ Å, $c = 15.6960(10)$ Å. The antimony and tellurium atoms occupy different crystallographic positions, antimony $2c$ and tellur $4f$. The resultant structure is a layered structure with the alteration of layers (Te-Ni-Sb-Ni-Te-).

The situation in the case of crystal structure of Ni_2SbTe_2 at 400 °C (terminated by quenching) is more complicated. The powder diffraction pattern corresponds to the disorder (high temperature) phase; nevertheless, it was possible to observe weak reflections near $1/3$ and $2/3$ of the distance between sharp diffractions on the photographs of reciprocal planes $h0l$ obtained from electron diffraction (SAED). These weak diffractions systematically shifted from $1/3$ to the left and from $2/3$ to the right, i.e. closer to the sharp diffractions.

It was not possible to determine all phase relations in the Sb-Te-Ni system at 400 °C. Ni_2SbTe_2 - NiTe_2 , NiTe_2 - Sb_2Te_3 a Ni_2SbTe_2 - Sb_2Te_3 form tie-lines. The phase Ni_2SbTe_2 forms a solid solution with end members having a composition of 42,1 % Ni, 13,0 % Sb, 44,9 % Te and 43,0 % Ni, 28,4 % Sb, 28,6 % Te (at. %) at 400 °C. The most characteristic feature is a small change of the nickel content as well as significant differences of the antimony and tellurium content.