Investigation of $Zr_{1-x}Ce_xNiSn$ Thermoelectric Material

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The increasing of the thermoelectric power factor $Z^*(x)$ values while doping *n*-ZrNiSn intermetallic semiconductor with Ce atoms was obtained for the first time. It was found that Ce atoms are in Ce^{4+} valence state that generated structural defects of donor nature in the crystal.

Attempts to get thermoelectric materials with high efficiency conversion of thermal energy into electrical by doping *n*-ZrNiSn with rare-earth metals (R) have failed [1] because the default valence state in rare earth metals is R^{3+}. As a result, in the crystal substitution of Zr atoms by R ones generates the acceptor structural defects. It caused a drift of the Fermi level from the conduction to the valence band and decreasing of resistivity and thermopower coefficient values.

Taking into account the feature of Ce to change the valence state from Ce^{3+} to Ce^{4+}, the crystal and electronic structures, temperature and concentration dependences of magnetic susceptibility, electrical resistivity and thermopower coefficient of $Zr_{1-x}Ce_xNiSn$ thermoelectric material were investigated in the ranges: K, $x = 0.01–0.10$, $H \leq 10$ kOe.

A complex mechanism of the compensation degree change in $Zr_{1-x}Ce_xNiSn$ was revealed as a result of the simultaneous reduction in the number of defects with donor nature (Ni atoms in 4*a* positions of Zr) and generation of defects with donor nature in the same positions due to substitution of Zr atoms by Ce in Ce^{4+} valence state. Investigated solid solution $Zr_{1-x}Ce_xNiSn$ is a promising thermoelectric material.

1. V.A. Romaka, V.V. Romaka, Yu.V. Stadnyk. *Intermetallic semiconductors: properties and applications* // Lvivska politekhnika, Lviv, 2011, 488 p.