



STUDY OF SEMICONDUCTING THERMOELECTRIC MATERIAL $\text{Er}_{1-x}\text{Zr}_x\text{NiSb}$

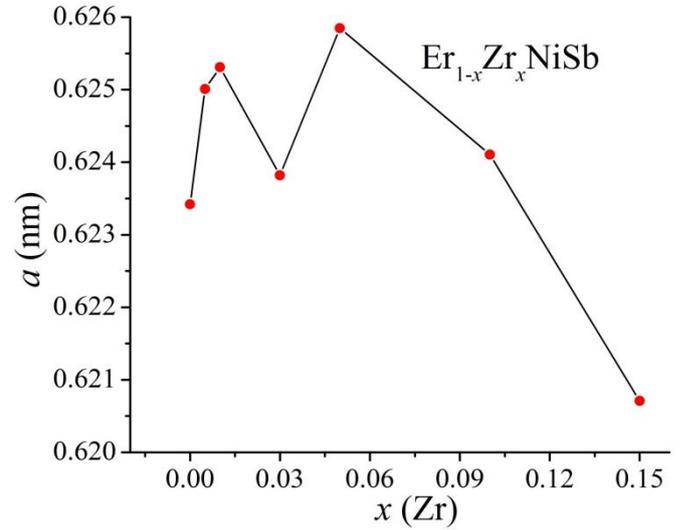
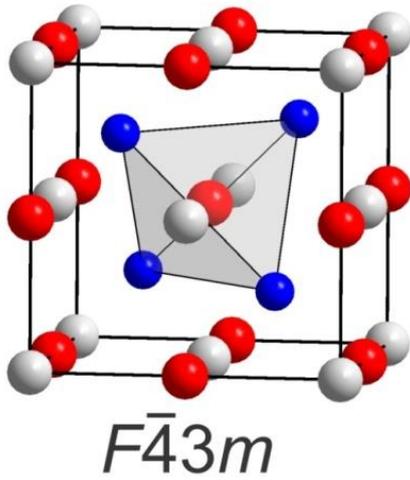
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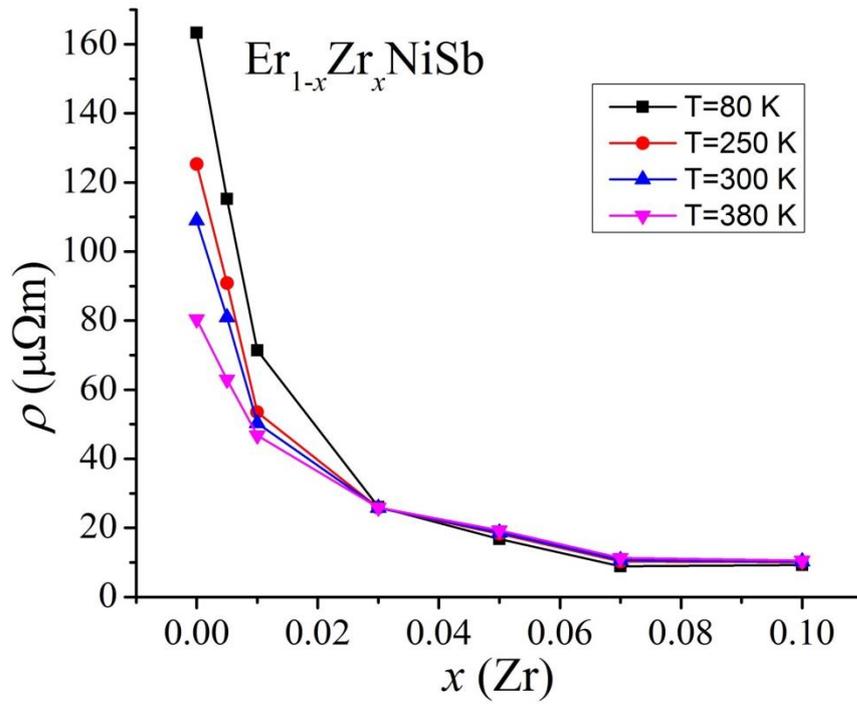
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RNiSb compounds (R-rare earth metal) and corresponding solid solutions with the MgAgAs structure type (space group $F\bar{4}3m$) are semiconductors and promising thermoelectric materials.

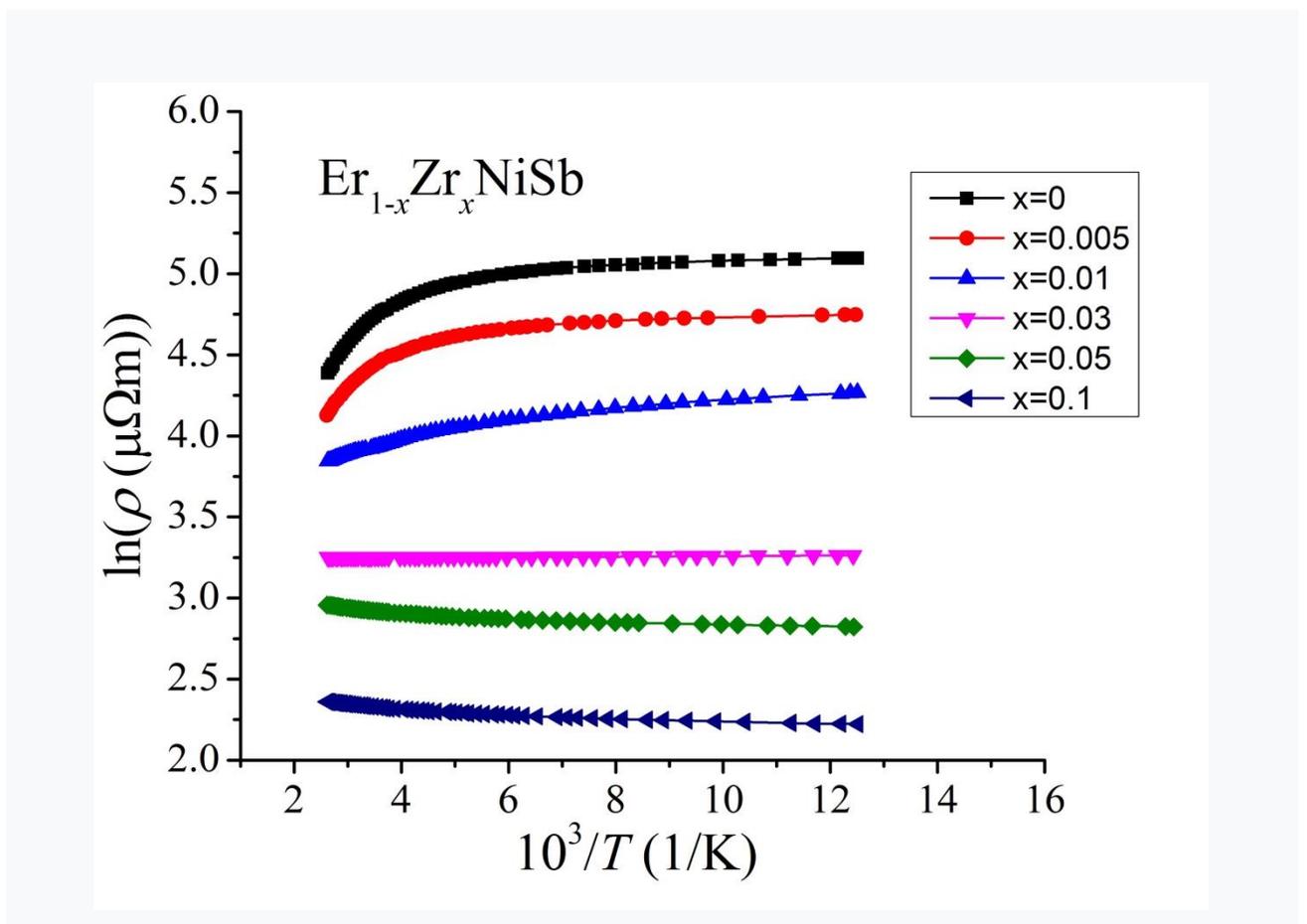
The structural, kinetic, energy state and magnetic characteristics of the $\text{Er}_{1-x}\text{Zr}_x\text{NiSb}$ ($x=0-0.10$) solid solution were investigated. Structural studies of $\text{Er}_{1-x}\text{Zr}_x\text{NiSb}$ showed that impurity Zr atoms can partially occupy different crystallographic positions in the ErNiSb structure and generate the structural defects of the different nature.



Temperature dependencies of electric resistivity $\ln(\rho(1/T))$ and thermopower coefficient $\alpha(1/T)$ of $\text{Er}_{1-x}\text{Zr}_x\text{NiSb}$, $x=0\div 0.03$, are typical for compensated semiconductors with activation parts which indicates the location of the Fermi level ε_F in the band gap. Positive sign of the thermopower coefficient $\alpha(T,x)$ of the ErNiSb compound showed the hole-type of the conductivity and location of the Fermi level near the valence band at a distance $\varepsilon_1^\rho=45.2$ meV. Introduction in the ErNiSb compound the lowest concentration of the Zr atoms ($x=0.005$) does not change the thermopower coefficient sign, results in a decreasing of the resistivity values and depth of the the Fermi level up to $\varepsilon_1^\rho=39.8$ meV. For a p -type semiconductor, this is possible when the concentration of acceptors increases and the concentration of free holes become higher. Thus, at $x=0.005$ Zr atoms do not occupy $4a$ position of the Er atoms and the donors are not generated.

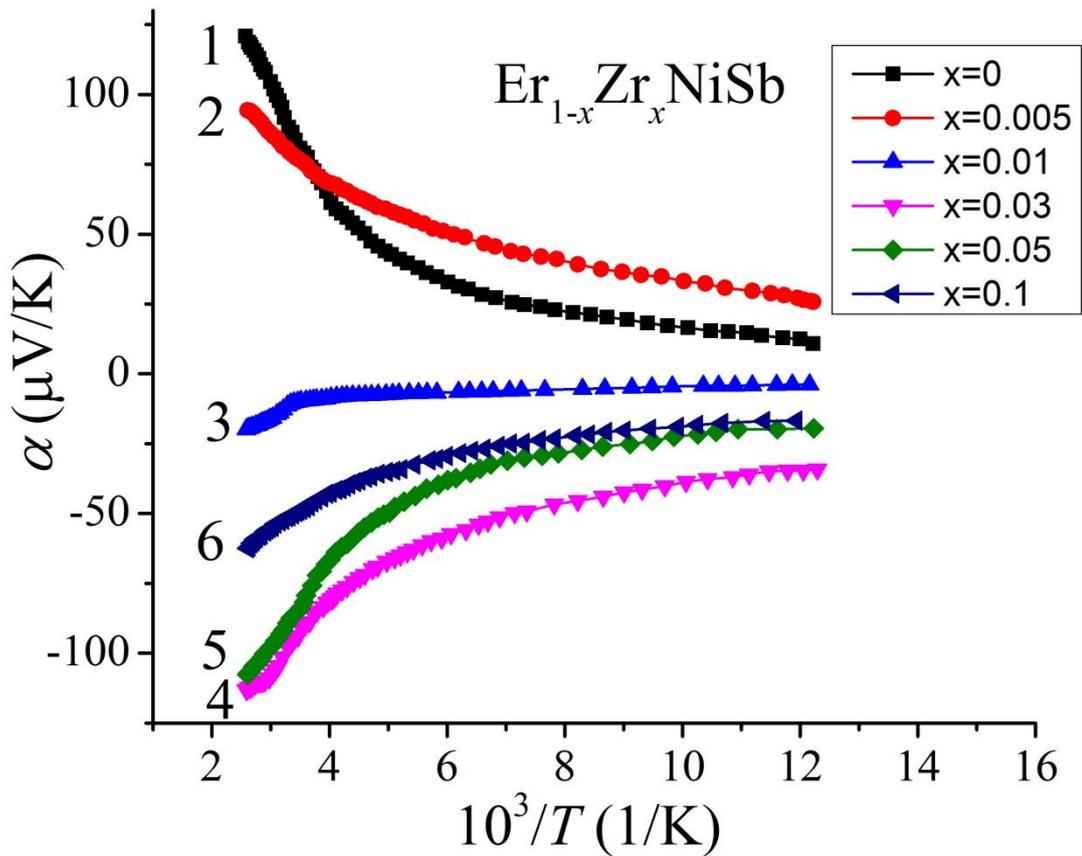


Variation of electric resistivity values with Zr content in the Er_{1-x}Zr_xNiSb solid solution



Temperature dependence of the electric resistivity for Er_{1-x}Zr_xNiSb solid solution

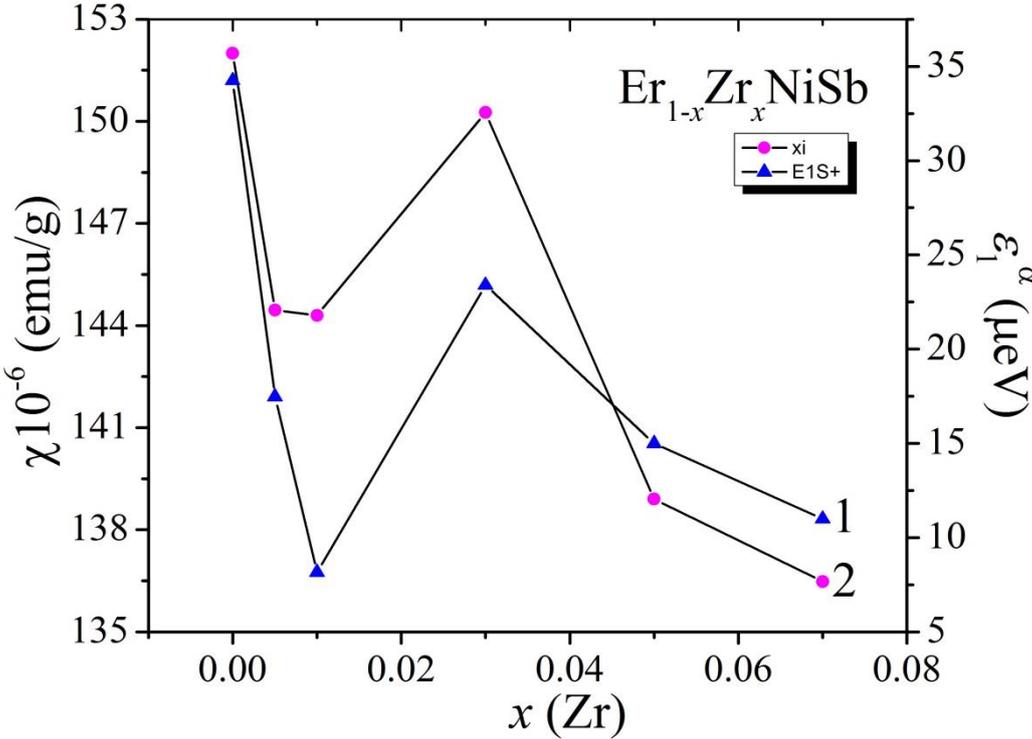
At $x=0.01$ the sign of the thermopower coefficient $\alpha(T,x)$ of $\text{Er}_{1-x}\text{Zr}_x\text{NiSb}$ is negative at all temperatures and electrons are the main charge carriers. At $x=0.01$ the Fermi level lies near the conduction band at a distance 6.7 meV. At higher Zr content ($0.01 < x$) the sign of the thermopower coefficient $\alpha(T,x)$ remains negative at all temperatures and activation parts on $\ln(\rho(1/T))$ dependencies disappear through metallization of the conductivity.



Temperature dependence of the thermopower coefficient
for $\text{Er}_{1-x}\text{Zr}_x\text{NiSb}$ solid solution

Magnetic susceptibility measurements $\chi(x)$ of $\text{Er}_{1-x}\text{Zr}_x\text{NiSb}$ at 300 K confirmed the simultaneous generation of the structural defects of the acceptor and donor nature. $\text{Er}_{1-x}\text{Zr}_x\text{NiSb}$ samples are Pauli paramagnets, their magnetic susceptibility is determined by free electrons and

proportional to the electron density at the Fermi level $g(\epsilon_F)$. There is a complete correlation in the behavior of $\chi(x)$ and $g(\epsilon_F)$ for $\text{Er}_{1-x}\text{Zr}_x\text{NiSb}$.



Magnetic susceptibility (2) and activation energy vs Zr content
for $\text{Er}_{1-x}\text{Zr}_x\text{NiSb}$ solid solution