

MECHANISM OF DEFECT FORMATION
IN HEAVILY Y-DOPED n -ZrNiSn.
I. CRYSTAL AND ELECTRONIC
STRUCTURES

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S u m m a r y

Crystal and electronic structures of an intermetallic semiconductor ZrNiSn heavily doped with an Y impurity ($N_A^Y \approx 3.8 \times 10^{20} \div 4.8 \times 10^{21} \text{ cm}^{-3}$) have been studied. It is shown that the doping of n -ZrNiSn is accompanied by the ordering of a crystal structure. Impurity atoms occupy the positions of Zr atoms only, generating acceptor-type defects. By detecting the conductivity transition "dielectric-metal," the existence range of a solid solution $\text{Zr}_{1-x}\text{Y}_x\text{NiSn}$ and the dependences between the solid solution concentration, on the one hand, and the direction and the rate of Fermi level drift, on the other hand, have been established.