Structure and Properties of α- and β-CeCuSn: A Single Crystal and Mössbauer Spectroscopic Investigation

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Two modifications of CeCuSn were prepared from the elements: the high-temperature (β) modification crystallizes directly from the quenched sample, while the low-temperature (α) modification is formed after annealing at 700 °C for one month. Both modifications were investigated by powder and single crystal X-ray diffraction. We find for β-CeCuSn the ZrBeSi-type structure, space group $P6_3/mmc$, a = 458.2(1), c = 793.7(2) pm, w$R2$ = 0.0727, 148 F^2 values, 8 variable parameters. In the case of α-CeCuSn we find the NdPtSb-type structure, space group $P6_3mc$, a = 458.4(1), c = 785.8(2) pm, w$R2$ = 0.0764, 233 F^2 values, 11 variable parameters. The copper and tin atoms build up layers of ordered $[Cu_3Sn_3]$ hexagons. The layers are planar in β-CeCuSn, however, with highly anisotropic displacements of the copper and tin atoms. In α-CeCuSn a puckering effect is observed resulting in a decrease of the c lattice parameter. Both modifications of CeCuSn exhibit antiferromagnetic ordering, but there is a considerable difference in their magnetic behaviour. Anomalies in the physical properties of the α- and β-modifications of CeCuSn have been detected by Mössbauer spectroscopy and magnetic and specific heat measurements, which serve to explain the structure-property relations.

Key words: Stannides, Crystal Structure, Magnetism