

EXPERIMENTAL STUDY AND THERMODYNAMIC MODELLING OF Co-Se-Sn TERNARY SYSTEM

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The ternary Co-Se-Sn system has been investigated experimentally to determine the phase equilibria and the microstructure of the alloys formed at different temperatures (400, 600 and 1000 °C). Samples of various compositions were prepared by melting, annealing, and quenching techniques and characterized using scanning electron microscopy, X-ray diffraction and thermal analysis. The combined experimental results confirmed the presence of several binary phases in this system, including Co_3Sn_2^1 , CoSn_2^1 , CoSe^2 , Co_9Se_8^2 , CoSe_2^2 , SeSn^3 and one ternary phase $\text{Co}_2(\text{SnSe})_3^4$.

Furthermore, a new thermodynamic description of this system was introduced using the CALPHAD (CALculation of PHase Diagrams) approach to predict and describe the phase equilibria, including the development of new models for phases CoSe , Co_9Se_8 and CoSe_2 . The models and thermodynamic description were verified by comparing the predicted phase diagrams with the experimental data obtained in this study.

The experimental and modelling results obtained in this study provide new insights into the behaviour of the Co-Se-Sn system and can be applied in the design and optimization of Co-based alloys for various industrial applications, such as magnetic storage media, high-temperature materials, and thermoelectric devices.

References

1. Ishida, K., Nishizawa, T., *The Co-Sn (cobalt-tin) system*. J. Phase. Equilib. 12, 88–93 (1991).
2. Komarek, K.L., Wessely, K., *Das System Kobalt-Selen*. Monatsh. Chem. 103, 896–906 (1972).
3. Sharma, R.C., Chang, Y.A., *The Se-Sn (selenium-tin) system*. Bull. alloy phase diagr. 7, 68–72 (1986).
4. Laufek, F., Navrátil, J., Plášil, J., Plecháček, T., Drašar, Č., *Synthesis, crystal structure and transport properties of skutterudite-related $\text{CoSn}_{1.5}\text{Se}_{1.5}$* . J. Alloys Compd. 479, Issues 1–2, 102–106 (2009).