THERMODYNAMIC MODELING OF PHASE EQUILIBRIA IN Mg-Ca-Li-BASED SYSTEMS

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Modern materials science is confronted with the challenge of developing novel structural materials that combine low density, high strength, significant ductility, and chemical resistance, which are in demand in the aerospace, transportation, and energy sectors. In this context, Light High-Entropy Alloys (LHEAs) are considered particularly promising. However, the LHEAs developed to date are predominantly aluminum-based and contain a large quantity of brittle intermetallic compounds, which limits their practical application.

The core scientific problem lies in the development of fundamentally new approaches for the design and synthesis of aluminum-free LHEAs, capable of minimizing the formation of phases that degrade mechanical properties and ensuring an optimal balance of hardness, strength, ductility, and corrosion resistance.

This study addresses the following interrelated tasks: performing thermodynamic modeling of phase equilibria in (Ca,Sr,Ba)MgLi systems to substantiate optimal compositions; optimizing melting techniques to minimize the loss of low-melting-point components; conducting a comprehensive investigation of the phase and chemical composition of the obtained samples using X-ray diffractometry, electron microscopy, and EDS analysis; determining mechanical properties and corrosion resistance; and formulating recommendations for the creation of new LHEAs for high-tech industries.

A key objective of the project is the thermodynamic modeling of phase equilibria in the selected systems using modern algorithms (CALPHAD). This approach enables the prediction of probable phases, their composition, and relative fractions at various temperatures and component concentrations.

This work utilizes the capabilities of the FactSage 8.0 software package, within which a proprietary user database is being developed to describe the investigated Mg-Ca-Li-based systems. Phase diagrams of the simulated systems have been constructed. Furthermore, the Scheil-Gulliver model is employed to simulate the solidification behavior of the melts in the studied systems.

This modeling serves as the foundation for the well-founded selection of experimental compositions and the optimization of synthesis conditions.

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