A Dual Approach to Ni-Cr Superalloys: Thermodynamic Modeling with JMatPro and Superconductivity Prediction via McMillan Formalism

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Abstract:

Nickel-chromium-based superalloys, particularly high entropy alloys (HEAs), represent a transformative class of materials known for their exceptional mechanical, thermal, and superconducting properties. This study focuses on a comprehensive evaluation of the thermodynamic and superconducting characteristics of such alloys. Thermodynamic properties have been systematically analyzed using JMatPro, enabling precise computation of phase stability, mixing behavior, and entropy contributions. These computational results offer valuable insights into the energetic and structural arrangements that govern alloy stability and formation. Concurrently, the superconducting properties have been investigated through McMillan's formalism, applying electron-phonon coupling theory to predict key superconducting state parameters, including the transition temperature (TC), Coulomb pseudopotential (μ*), and electron-phonon interaction strength (λ). The outcomes highlight the potential of Ni-Cr-based HEAs in exhibiting robust superconductivity even under high disorder, along with favorable thermodynamic profiles, making them promising candidates for advanced functional applications in energy and electronics.

Keywords:

High entropy alloys (HEAs), nickel-chromium superalloy, McMillan formalism, superconductivity, transition temperature.