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Dissertation Report

ON

CALCULATION OF ENTHALPY OF FORMATION OF INTERMETALLICS IN Ni-Al-Zr SYSTEM USING DENSITY FUNCTIONAL THEORY

Submitted in partial fulfilment of the requirements of the degree of

Master of Technology

In

Materials Engineering

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Abstract

Nickel based superalloys are the most important materials in aerospace and turbine applications. To improve their properties elements like Zr are added to influence properties. For the prediction of properties can be done by implementing ICME approach of integrating useful information from multiple modelling techniques at different scales. In, the present work the enthalpy of formation of NiAl and Ni_3Al is predicted in consideration with Zr solubility. To predict this, Wagner Schottky model is used. The enthalpies of formation of point defects were determined from first principle calculations. Using these, the site preference of Zr in NiAl and Ni_3Al was predicted. It was found that Zr prefers the Al sublattice for all cases in both NiAl and Ni_3Al. After this the enthalpies of formation of intermetallic with ternary Zr solubility was determined. A qualitative estimate of the effect of Zr on the elastic properties of NiAl

Keywords: Nickel Aluminides; Point defects; First principles calculation; Enthalpy of formation