

DISSERTATION REPORT

ON

Thermodynamic Optimization of Ni_3Al , NiAl , FCC and Liquid Phase in Ni-Al System

Submitted in partial fulfilment of the requirements

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(Physical Metallurgy)

By

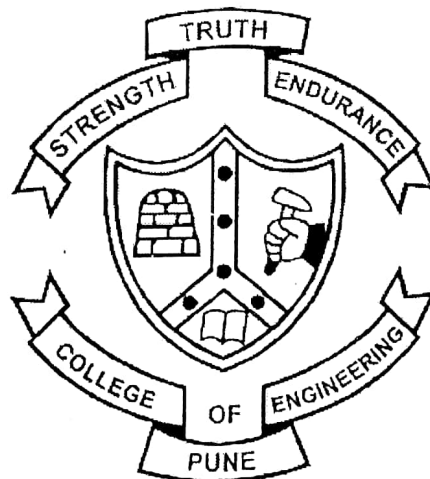
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Abstract

Alloy phase diagrams are useful to metallurgists, materials engineers, and materials scientists for development of new alloys for specific applications and design and control of heat treatment procedures for specific alloys that will produce the required mechanical, physical, and chemical properties. The Ni-Al system has been extensively studied due to wide use of Ni based superalloys for high temperature application. The superalloys are complex and costlier containing more than 10 elements such as Al, Ti, Ta, Nb, Cr, Co, Mo, W, Re and Ru for better properties. Recently, intermetallic based eutectic alloys in Ni-Al-Zr system with only three cheaper alloying elements has shown very good high temperature properties which are potential candidate material for high temperature application in place of Ni based superalloys. The Ni-Al-Zr ternary phase diagram with recent experimental data by Gunjal et. al. can be constructed theoretically for better understanding of microstructure morphology evolution and alloy development.

The computational assessment can be possible by combining binary systems such as Ni-Al, Al-Zr and Ni-Zr but with consideration of solubility of Zr in Ni_3Al and NiAl and Al in Ni_5Zr and Ni_7Zr_2 . The available assessment of Ni-Al system by previous researchers considered very complex free energy models for these phases which is very difficult to add solubility effect in it. So, the present work deals with reassessing Ni-Al phase diagram with simple two sublattice models for Ni_3Al and NiAl . The optimization of model parameters of liquid, FCC, Ni_3Al and NiAl has been done in PARROT module of Thermocalc software with respect to high temperature phase fields of Ni-Al system. The invariant reaction related to NiAl and Ni_3Al phase with liquid and FCC solid solutions are fitted with reasonable match. The thermochemical data such as enthalpy of mixing, activity or chemical potential, constitutional data such as liquidus, solidus and solvus temperatures shows reasonable agreement between experimental and calculated by present assessment.

Key words: Phase diagram, Thermodynamic and thermochemical properties, CALPHAD.