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Experimental and First Principles Study of the Ni-Ti-W System

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Abstract. Nickel based superalloys are structural materials with a chemical composition and structure which has been developed to enable good high temperature performances leading to a wider range of applications. Their unique properties are due to their microstructure characterized by the coexistence of L1₂-ordered intermetallic precipitates like Ni₃Al or Ni₃Ti - γ' phase - in a face-centered cubic nickel based solid solution matrix, (Ni) - γ phase. Solid solution strengthening at high temperatures can also be provided by the addition of refractory alloying elements, like tungsten, W. Therefore, the mechanical properties behaviour of the alloys is very strongly related to their composition and microstructures.

The purpose of this work is to study the effect of composition and microstructures in a series of Ni-rich prototype alloys, Ni_{100-2x}-Ti_x-W_x (in which x is in at.%), in order to understand and ultimately optimize the performance of these materials. The adopted strategy was to combine experimental studies using Neutron Diffraction, Electron Probe Micro Analysis – EPMA, Differential Scanning Calorimeter – DSC and micro-hardness measurements, with first principles calculations for structure optimization and Gibbs energies at different temperatures, for each phase, leading to thermodynamic assessment.

Introduction

Ni-based superalloys are widely used for high-temperature applications due to their excellent mechanical properties for high temperature applications. Their unique properties are due to their microstructure characterized by the coexistence of a disordered Ni based austenitic solid solution matrix, with a face centred cubic (fcc) lattice (structure A1) - γ phase, which is hardened primarily by the precipitation of the Ni₃X type compounds [1]. The structural characteristics of these intermetallic compounds depend of the alloying composition.

It has been shown that coherent γ' phase, L1₂ ordered structure, Ni₃Al or Ni₃Ti precipitates, can be destabilized and the formation of lower strength Ni₃Ti with D0₂₄ structure, η phase, promoted when the content of Ti is high [2]. The D0₂₄ hexagonal crystal structure is closely related with the cubic face centered, L1₂, as the site occupation by Ni and Ti in hexagonal basal planes and the {111} fcc planes are the same [3].

The existence of a η phase has been associated to a deleterious effect on alloy's strength and ductility, but it is also pointed out that keeping some amounts of it during processing is a way to control grain size [2]. Grain size is an important factor in hardening, it is well known that strengthening is inversely proportional to the grain size; this is due to the existence of grain boundaries as sources of dislocations and barriers to deformation [4].

Tungsten besides being commonly used as a solid solution strengthener in nickel-base superalloys [5] is known to be useful in retarding the formation of the Ni₃Ti – D0₂₄ η phase, since it partitions preferably to the (Ni) - γ phase [6]. Therefore, high-temperature mechanical properties of nickel-base superalloys are further enhanced by moderate additions of tungsten. High levels of the

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