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Experimental and theoretical study of lattice relaxation around refractory atoms in nickel

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Abstract

The lattice relaxation around Mo, Ru, Hf, Ta, W and Re in Ni is investigated by means of X-ray absorption spectroscopy. For all of the investigated concentrations the substitutional lattice position is confirmed except for the higher Hf concentration where different phases are observed. An outward relaxation of the neighboring atoms is detected with clear trends of increasing nearest neighbor distances with decreasing valence for the 5d impurities, and separate trends for the 4d impurities. Ab initio supercell calculations within the linearized augmented plane wave formalism are used to complement the experimental results and allow for a better interpretation of the experimental trends in terms of the electronic structure of the impurity.

Keywords: Extended X-ray absorption fine structure (EXAFS, XANES); Nickel alloys; Augmented plane wave method (FLAPW)

1. Introduction

While in many important applications of metals and intermetallic phases the properties of materials can be tailored by introducing suitable alloying elements, the local structure and possible lattice relaxation around these elements is in general not very well known. Nickel-base superalloys are of significant technological importance, due to their very high strength (shear resistance and flow stress) at high temperatures, as compared to usual alloys such as steels. The last generations of superalloys include refractory elements, e.g. Mo, W, Ru, or Re, that help enhance their superior mechanical properties and corrosion resistance [1]. The strengthening effect is not fully understood in terms of the underlying mechanism, and efforts have been made to correlate it to structural, electronic or bonding features of the impurity system [2–4].

Ni-base superalloys consist of a face-centred cubic (fcc) Ni solid solution matrix (γ phase) in which the strengthening γ' phase (Ni_3Al-type) is dispersed. The lattice mismatch between the two phases is found to be an important parameter in controlling the properties of the superalloys [5–7]. It appears that one way of altering the lattice mismatch is by doping with refractory elements, which incorporated either into the γ or γ' phase, or into both, can contribute to the overall contraction or expansion of the corresponding lattice. The clustering of the refractory elements has also been attributed as one of the possible mechanisms of solid solution strengthening [2].

In the following we present the results of a combined, experimental and theoretical determination of the local structure around Mo, Ru, Hf, Ta, W and Re in nickel. In some model γ phases of Ni-base superalloys the addition of small amounts of Re, Mo, Ru and W were shown to affect short-range order (SRO) which is reflected by peaks of the $\{1\,1/2\,0\}$ type. The SRO is approximately stable up to 600 °C and then decreases gradually up to about 1000 °C where it finally vanishes [8,9]. To date, the lattice

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