Superlattices and Microstructures 52 (2012) 834–843

Contents lists available at SciVerse ScienceDirect

Superlattices and Microstructures

journal homepage: www.elsevier.com/locate/superlattices

Characterization of lattice defects for $L1_2$–Ni_3Al involving the ordering process via the microscopic phase field method

Jing Zhang *, Zheng Chen, Xiujuan Du, Cheng Chen, Tao Yang

State Key Laboratory of Solidification Processing, School of Material Science and Engineering, Northwestern Polytechnical University, Xi'an Shaanxi 710072, China

ARTICLE INFO

Article history:
Received 6 April 2012
Accepted 10 July 2012
Available online 20 July 2012

Keywords:
Lattice defect
Ordering
Microscopic phase field
Temperature dependence

ABSTRACT

The quantitative and temporal-evolutional advantages of the microscopic phase field are used to study the lattice defects of the $L1_2$–$Ni_3Al(\gamma')$ phase in a ternary Ni–Al–V system. The temporal evolutional process of the occupancy of each individual atom conforms to classical nucleation processes, where the occupancy is constant at the incubation period, and then fluctuates up or down during segregation and equilibrium at the coarsening period. The α sublattice of the $L1_2$ structure is almost completely occupied by regular Ni_{Ni} with a small amount of antisite defect Al_{Ni} and the substitutional defect V_{Ni} at the equilibrium state. By sharp contrast, the β sublattice is predominantly occupied by regular Al_{Al}, as well as the non-negligible antisite defect Ni_{Al} and substitutional defect V_{Al}. Regular atoms have a negative correlation with temperature; hence, the defects are positive. By comparison, the β sublattice, which accommodates most of the defects in Ni_3Al, is more sensitive to temperature than the α sublattice. The results are generally in line with comparisons reported by other scientists.

1. Introduction

$L1_2$–Ni_3Al, a Cu_3Au-type (Fig. 1a) intermetallic compound, has attracted attention in both theoretical and experimental [1–4] fields because of its abnormally low density, high-temperature strength, excellent corrosion resistance, and oxidation resistance. However, some undesirable characteristics hinder the Ni_3Al compound from being a generally useful engineering material. Mechanical properties can be enhanced by defect control and alloying; hence, studies on the defects and alloying effects of Ni_3Al involving temperature and its ordering process are necessary [5–7].

* Corresponding author. Tel.: +86 029 88476023.
E-mail address: jingzhang@nwpu.edu.cn (J. Zhang).

0749-6036/$ - see front matter © 2012 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.spmi.2012.07.008

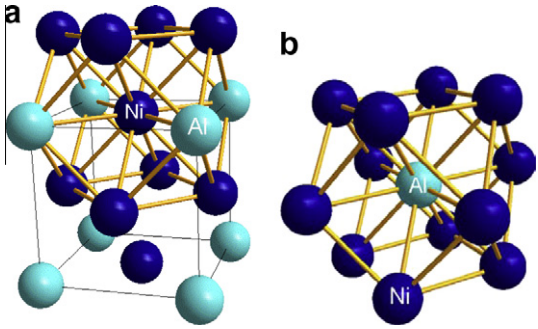

Fig. 1. Coordination sphere of Ni and Al in Ni_3Al phase. Ni atom connects with other eight Ni atoms and four Al atoms within coordination sphere (a), whereas an Al atom sealed by twelve Ni atoms is isolated from one another in a perfect $L1_2$ structure (b).

Table 1
Formation energy for antisite defect of Ni_3Al (E_f: formation energy, A_B: anti-structure atom A/vacancy on B site).

$E_f(V_{Ni})$	$E_f(V_{Al})$	$E_f(Ni_{Al})$	$E_f(Al_{Ni})$	Method
1.64	1.87	−0.14	0.46	EAM [11]
1.419	2.478	1.674	0	Al-rich EAM [12]
1.683	3.213	1.440	0	Al-rich Ab initio [12]
1.628	1.850	0.837	0.837	Stoichiometric EAM [12]
1.863	2.673	0.720	0.720	Stoichiometric initio [12]
1.837	1.222	0	1.674	Ni-rich EAM [12]
2.043	2.133	0	1.440	Ni-rich ab initio [12]
1.47	1.91	0.58	0.54	EAM [13]
1.84	2.74	0.89	0.89	Ab initio LDA-FLAPW(frozen) [14]
1.95	2.81	0.99	0.99	Ab initio LDA-VASP(frozen) [14]
1.46	2.12	0.72	0.72	Ab initio GGA-VASP(frozen) [14]
1.50	2.00	0.51	0.51	Ab initio GGA-VASP(relaxed) [14]
1.646	2.408	0.832	0.602	EAM [15]
1.47	1.92	0.56	0.59	EAM [16]
1.47	1.91	0.54	0.58	EAM [17]
1.42	1.65	0.31	1.02	Many-body potential [18]
1.48	2.14	0.31	0.66	Many-body potential [19]
1.87	2.65	0.69	0.75	First-principles [20]

In recent years, theoretical studies on Ni_3Al alloy have revealed that the dominant defects in the intermetallic are antisite defects. The existence of the antisite defect constructs an antisite-bridge diffusion tunnel for atomic diffusion on one side. Furthermore, it damages the long-range order, which most probably leads to the solid solution failure or facilitates the phase transition and invalidates the second phase strengthening on another side. The theoretical studies listed in Table 1 show that the deviation from stoichiometry produces anti-structure atoms on both the α sublattice (nickel sites, Al_{Ni}) and β sublattice (aluminum sites, Ni_{Al}), whereas the vacancy concentration (nickel sites, V_{Ni}; aluminum sites, V_{Al}) is generally very small. Experimental measurements, such as the positron lifetime spectroscopy conducted by Badura-Gergen et al. [8] and Würschum [9], and XRD performed by Nic and Mikkola [10], provide an experimental justification for the aforementioned arguments.

The temperature-dependent antisite defect of Ni_3Al shows an Arrhenius law type positive trend with an elevated temperature studied by Minshin [12] using the embedded atom method. This viewpoint is supported by Fu et al. [20] using the first-principle method, de Koning et al. [21] via atomistic simulation, and Badura-Gergen et al. [8] through a positron-annihilation spectroscopy experiment. For the alloying effect, the mechanical properties are enhanced with the alloying element vanadium (V). Mekhrabov et al. [22] studied the atomic ordering characteristics of Ni_3Al intermetallic. They pointed