Materials Science and Engineering A 539 (2012) 38–41

Contents lists available at SciVerse ScienceDirect

Materials Science and Engineering A

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

The effects of alloying elements on generalized stacking fault energies, strength and ductility of γ'-Ni_3Al

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ARTICLE INFO

Article history:
Received 17 September 2011
Accepted 19 December 2011
Available online 18 January 2012

Keywords:
Ni-based superalloys
First-principles
Strengthening
Alloying elements

ABSTRACT

Using first-principles calculations, we study the effects of the alloying elements Re, Ta, W, Ru and Ti on the generalized stacking fault energies, strength and ductility of γ'-Ni_3Al. The element Re effectively increases three kinds of generalized stacking fault energies on the (1 1 1) plane inducing more strength and less ductility of Ni_3Al than the other elements. Quantificational analyses of bonding strength between alloying elements and their neighbor atoms reveal the electronic mechanism underlying these effects.

1. Introduction

Nickel-based single-crystal superalloys are widely used structural materials in turbine engines due to their superior high-temperature mechanical properties [1]. The main structure of these alloys is the precipitation of the ordered γ'-Ni_3Al phase with $L1_2$ structure, which is coherently embedded in a solid solution matrix of the γ-Ni phase. γ'-Ni_3Al, with its anomalous temperature dependence of the yield stress, is largely responsible for the strength of superalloys and their resistance to deformation at high temperatures [2,3]. Therefore, a study of the mechanical behaviors of γ'-Ni_3Al should partially reflect the global properties of Ni-based superalloys.

The configuration and movement of dislocations play a key role in understanding plastic deformation and mechanical properties of crystalline solids. One example is the existence of glissile and sessile configurations of the $\langle\bar{1}\,0\,1\rangle\{1\,1\,1\}$ dislocation in Ni_3Al leading to the anomalous yield behavior [4–6]. One perfect $\langle\bar{1}\,0\,1\rangle\{1\,1\,1\}$ dislocation in Ni_3Al will dissociate into two partial $a/2\langle\bar{1}\,0\,1\rangle\{1\,1\,1\}$ dislocations containing an anti-phase boundary(APB) fault, as Fig. 1 shows. The $a/2\langle\bar{1}\,0\,1\rangle\{1\,1\,1\}$ dislocation will further dissociate into two $a/6\langle\bar{1}\,\bar{1}\,2\rangle(1\,1\,1)$ Shockley partial dislocations separated by complex stacking faults (CSF). The $\langle\bar{1}\,0\,1\rangle\{1\,1\,1\}$ dislocation will also dissociate into two $a/3\langle\bar{2}\,1\,1\rangle(1\,1\,1)$ dislocations bounding a superlattice intrinsic stacking fault (SISF).

Fundamentally, the large-scale properties of materials can be traced to the small scale [7,8]. Plastic deformation on the macroscopic scale is influenced by electronic structure (or bonding) on the atomic scale. In the Peierls–Nabarro model, the core structures and properties of dislocations in many materials [9–12] have been investigated by combining density functional theory (DFT) with elasticity theory using the concept of generalized-stacking fault (GSF) energy (or |Ã surface) introduced by Vitek [13,14]. In addition, Rice [15–18] introduced the unstable stacking fault energy, γ_{us}, to evaluate brittle vs. ductile response in fcc and bcc metals in terms of the competition between dislocation nucleation and Griffith cleavage at a crack tip. γ_{us} is the maximum energy encountered on the GSF energy surface during rigid sliding along a slip plane, in the Burgers vector direction. Parameters for the GSF energy surface obtained from DFT calculations can also be used to evaluate twinnabilities in nanocrystalline metals [8,19–21]. Therefore, GSF energies contain many important solid-state parameters, which bridge the gap between electronic structures and dynamics of dislocations.

To acquire extraordinary properties, more than 10 alloying elements are added to nickel-based single-crystal superalloys, including Co, Cr, Ti, Ta, Mo, W, Re and Ru. Experimental results [22–24] have confirmed that the elements Ta and Ti preferentially partition to the γ'-Ni_3Al in superalloys, whereas W distributes averagely between two phases. Besides, although Re and Ru preferentially partition to the γ-Ni, some Re and Ru still enter into the γ'-Ni_3Al. The effects of these elements on the GSF energies of γ'-Ni_3Al are still unclear. The abilities of these elements altering

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doi:10.1016/j.msea.2011.12.112

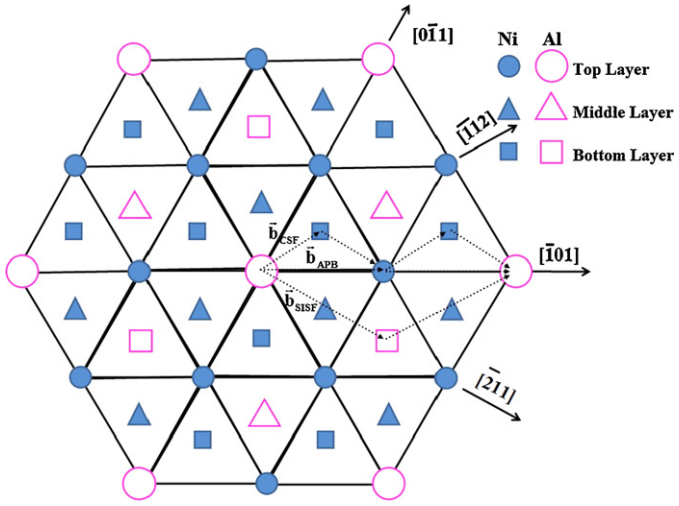

Fig. 1. Illustration of three successive (1 1 1) planes of Ni_3Al and the Burger's vectors of forming three kinds of planar faults. Filled blue figures stand for Ni atoms, open pink figures stand for Al atoms (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article).

the strength and ductility of Ni_3Al need to be evaluated, which is fundamental and essential for alloy design. In this paper, we perform first-principles calculations to explore the effects of Re, Ru, Ta, Ti and W on GSF energies, surface energies and Rice-criterion ductility in γ'-Ni_3Al. The results shed light on the strengthening mechanism of these alloying elements in Ni_3Al. We also explain the electronic mechanism underlying the effects via quantificational analyses of bonding strength between alloying elements and their neighbor atoms.

2. Computational method and models

Our DFT calculations were carried out with the plane-wave based Vienna ab initio simulation package (VASP) [25,26] using the projector augmented wave method [27,28] and the generalized gradient approximation in the parametrization by Perdew et al. [29]. Plane waves were included up to a cutoff energy of 350 eV, which yields convergent results. The convergence accuracy of the total energy was chosen as 10^{-5} eV in the relaxation of electronic degrees of freedom. The structures of the models were relaxed until the maximum force was less than 0.02 eV/Å. We used the Monkhorst–Pack scheme for k points sampling [30]. To calculate planar fault energies, we used supercells by introducing displacement on the (1 1 1). Ni_3Al is a close-packed structure with an arrangement of three successive planes along the <1 1 1> direction as shown in Fig. 1. An APB, CSF and SISF on the (1 1 1) plane were formed by shearing $a/2\langle\bar{1}\,0\,1\rangle(1\,1\,1)$, $a/6\langle\bar{1}\,\bar{1}\,2\rangle(1\,1\,1)$ and $a/3\langle\bar{2}\,1\,1\rangle(1\,1\,1)$ respectively. To eliminate the interactions of parallel faults, we introduced a vacuum region of 12 Å to separate the parallel faults. The supercells containing 12 layers along the <1 1 1> direction and 96 atoms in total, and the 16 atoms in the top and bottom layer are fixed during relaxation to avoid surface reconfiguration. An $8 \times 5 \times 1$ k-mesh was used for the k points sampling. Based on the hypothesis of dilute alloys, we set up a single-impurity model [7] to evaluate the effects of various alloying elements. In this model, one alloying element substitutes for an Al atom in the slip plane.

3. Results and discussion

Table 1 summarizes the unstable stacking fault energies in each slip system and alloying system. Fig. 2(a) shows the effects of alloying elements on GSF in the $\langle\bar{1}\,0\,1\rangle(1\,1\,1)$ slip system. From the

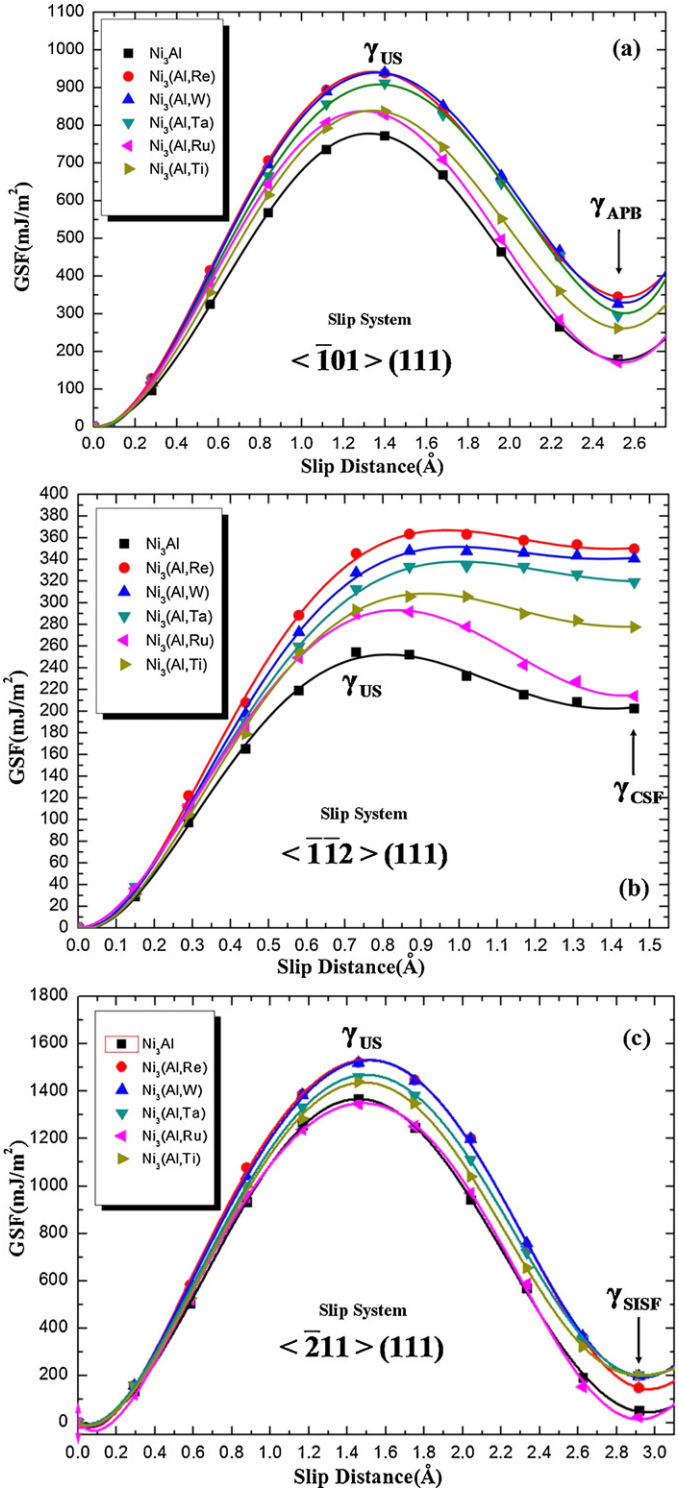

Fig. 2. The effects of alloying elements on the GSF energies in each slip system and alloying system.

results, we concluded that Re remarkably increases the unstable stacking fault energy in the $\langle\bar{1}\,0\,1\rangle(1\,1\,1)$ slip system of Ni_3Al. The abilities of other elements to raise the unstable stacking fault energies are in the order: W>Ta>Ti>Ru. The effects of alloying elements on GSF in the $\langle\bar{1}\,\bar{1}\,2\rangle(1\,1\,1)$ slip system in Fig. 2(b) are similar to those in the $\langle\bar{1}\,0\,1\rangle(1\,1\,1)$ system. Re promotes the unstable stacking fault energy most. Other alloying elements are also in the order: W > Ta > Ti > Ru. Fig. 2(c) presents the effects of alloying elements on GSF in the $\langle\bar{2}\,1\,1\rangle(1\,1\,1)$ slip system. The improvements of the unstable stacking fault energies caused by alloying elements are