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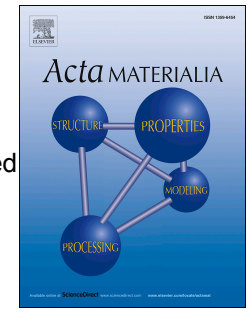

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First-principles modeling of superlattice intrinsic stacking fault energies in Ni_3Al based alloys

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High-throughput quantum mechanics based simulations have been carried out to establish the change in lattice parameter and superlattice intrinsic stacking fault (SISF) formation energies in Ni_3Al-based alloys using the axial Ising model. We had direct access to the variation in SISF energies due to finite compositional change of the added ternary transition metal (TM) element through constructing large supercells, which was equally necessary to account for chemical disorder. We find that most added TM ternaries induce an important quasi-linear increase in the SISF energy as a function of alloying composition x. The most pronounced increase corresponds to Fe addition, while Co addition decreases the SISF energy monotonically. Our results shed light on the role played by TM elements on strengthening $L1_2$ Ni_3Al precipitates against stacking fault shear. The data are of high importance for designing new Ni-based superalloys based on computational approaches.

Keywords: First-principles; Ni superalloys; Alloys; Stacking faults; Dislocations

I. INTRODUCTION

Nowadays high-performance aero-engines owe their exceptional high-temperature mechanical properties to Ni-based superalloys consisting of a large volume fraction of ordered γ' ($L1_2$) Ni_3Al precipitates coherently embedded in a matrix of γ-Ni (fcc Ni) phase[1]. The shear strength of these precipitates resulting from order strengthening and the anomalous temperature dependence of the yield stress (*critical resolved shear stress* CRSS) give rise to Ni-based superalloys extraordinary strength and deformation resistance at high-temperatures[2].

In contrary to the situation at high temperatures ($\geqslant$ 950 °C[3]) and low stresses where the micromechanism of creep is characterized by dislocations activity of type $a/2\langle 1\bar{1}0\rangle\{111\}$ restricted to the γ channels, experiments[3–5] have shown that at intermediate-temperatures (750 − 850 °C) and high stresses ($\geqslant$ 500 MPa) the micromechanism of creep is quite different. Reports in the literature[3–5] established that during the primary creep process the deformation occurs by shearing the γ' precipitates – so called *stacking fault shear* – by dislocation ribbons of overall Burgers vector $a\langle 11\bar{2}\rangle$ [3–5].

It was Leverant and Kear[6] who made the first observation that primary creep deformation occurs by the movement of dislocation ribbons of net Burgers vector $a\langle 11\bar{2}\rangle$, which was later supported by transmission electron microscopy (TEM) studies. Now it is known that the mechanism of formation of the $a\langle 11\bar{2}\rangle$ dislocation ribbons involves the reaction of $a/2\langle 1\bar{1}0\rangle\{111\}$ dislocations in γ, which are dissociated into their Shockley partials. A typical reaction might then be given by[5]

$$a/2[011] + a/2[\bar{1}01] \rightarrow a/3[\bar{1}12] + a/6[\bar{1}12] \quad (1)$$

If the applied stress is sufficient, the $a/3[\bar{1}12]$ dislocation is able to enter the γ', leaving a superlattice intrinsic stacking fault (SISF) behind it and the remaining $a/6[\bar{1}12]$ at the γ/γ' interface.

The SISF energy is known to play an important role in the structure and energetics of dislocations formed by slip processes. There is strong evidence that SISFs and SESFs, characterized by low fault-energies relative to other stacking fault configurations, are the main planar fault energies through which shearing of the γ' phase happens under high-applied-stress and low-intermediate-temperatures creep conditions[5, 7–9] (Primary creep). The knowledge of the variation of these fault energies upon alloying is extremely important to have a better understanding of the shearing of the strengthening γ' phase in nickel-base superalloys which is crucial for developing physics-based deformation models of the aerospace and power generation systems.

The transmission electron microscopy technique used to determine the planar fault energies is known to involve assumptions, and consequently produces sometimes inaccurate values, particularly for the SISF energies – see Ref. 10 and references therein. The experimental technique relies on measuring the width of the stacking fault ribbon which is inversely proportional to the fault energy[11–13]. Accordingly, it is accompanied by difficulties related to thin film effects, short length ribbons (comparable to errors) and uncertainty in applying corrections. Moreover, the experimental determination of fault energies depends heavily on the type of elasticity theory applied.

On the other hand, *ab initio* quantum mechanics based methods are powerful tools that can be harnessed to enhance the mechanical properties of complex multicomponent Ni-base superalloys *via* probing the variation of the stacking fault energies upon adding a specific ternary element with composition x to the Ni_3Al based-systems. There are several factors giving rise to the complexity of Ni-base superalloys: the wide variety of alloying elements

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