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Influence of dilute solute substitutions in Ni on its generalized stacking fault energies and ductility

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ABSTRACT

We determine effects of substitutional solutes belonging to 3d, 4d and 5d transition metal (TM) series on volume, intrinsic stacking fault energy (ISFE), unstable stacking fault energy (USFE) and ductility parameter of Ni using first-principles calculations based density functional theory (DFT), considering both ferromagnetic (spin-polarized) and non-magnetic states of Ni. For each of the TM series, we find that volume exhibits a minimum for substitutional elements with half-filled *d*-orbitals (5 *d*-electrons). Reduction in ISFE of Ni is seen with all the solute additions except for Pd (in the non-magnetic case). Inclusion of spin-polarization has a pronounced effect on the fault energies and results in increase in both ISFE as well as USFE. In the non-magnetic case, USFE exhibits maxima for alloying with elements having five electrons in *d*-orbital. Except for Zr and Pd, substitution of other elements enhanced cleavage energy of Ni. Differences in the fault energies on alloying have been explained based on the electronic structure of the alloys. There exists a correlation between change in volume and change in USFE with substitutional alloying. It is envisaged that the exhaustive data generated here would not only form necessary input to multi-scale microstructural modeling, but also help in evolving simple recipes for design of new alloys.

1. Introduction

The excellent creep strength of Ni-based single crystal superalloys (NBSCs) is mainly attributed to the individual as well as the combined effect of the two phases namely γ (matrix, solid solution based on Ni) and γ′ (precipitates with $L1_2$ structure based on ordered intermetallic Ni_3Al) [1]. Various solutes added to the system, depending on the thermodynamics and the prevailing kinetics, partition preferentially into γ or γ′. These solutes mainly provide either solid solution strength or enhance the precipitation strengthening or both depending on the composition of the two major phases and their inherent nature. NBSCs find application especially at elevated temperatures because of their ability to retain strength at the high operating temperatures. The dominant deformation mechanism of creep at these temperatures is very sensitive to the stacking fault energy (SFE) of the composite system.

It is well established that the dislocation movement in FCC materials is facilitated by the dissociation of perfect dislocations of type $1/2[\bar{1}\,1\,0]$ into Shockley partials $1/6[\bar{1}\,2\,\bar{1}]$ and $1/6[\bar{2}\,1\,1]$ on the (1 1 1) plane [2] (Fig. 1 a). Since the partials are not lattice vectors, the FCC stacking sequence (…ABCABC…), is locally disturbed in the region between the partials and the faulted region is known as intrinsic stacking fault (ISF). The associated energy cost due to the presence of this planar fault is known as the intrinsic stacking fault energy (γ_{is}). γ_{is} is inversely related to the spacing between the partials, *d* [2]. Hence, it determines the ability of dislocations to glide on the intersecting slip planes and directly correlates with strengthening of materials. Lower γ_{is} (wider spacing between the partials) retards the possibility of cross slip and reduces the steady-state creep rate $\dot{\varepsilon}$ with a widely used empirical relation [3,4], $\dot{\varepsilon} \approx \mathbf{\Gamma_{SF}^{n}}$, where Γ_{SF} ($=\gamma_{is}$/Gb) is the normalized γ_{is}, with G being the shear modulus, $\boldsymbol{b}$, the Burgers vector, and, n, an empirical parameter with a value around 3–4 [5].

Generalized stacking fault (GSF) energy surface or the γ-surface is widely used to evaluate the SFE and is defined as the energy per unit area for sliding one part of the crystal over the other on any slip plane [6]. Locations corresponding to minima in the γ-surface correspond to stacking faults and maxima determine the energy barriers during slip along a given direction on the slip plane [7]. The lowest among these barriers in a family of various possible paths is the unstable stacking fault energy (γ_{us}), and is proportional to the energy release rate needed for nucleation of dislocation on that plane. γ_{us} is an important microscopic energy that correlates with the ideal shear strength of the

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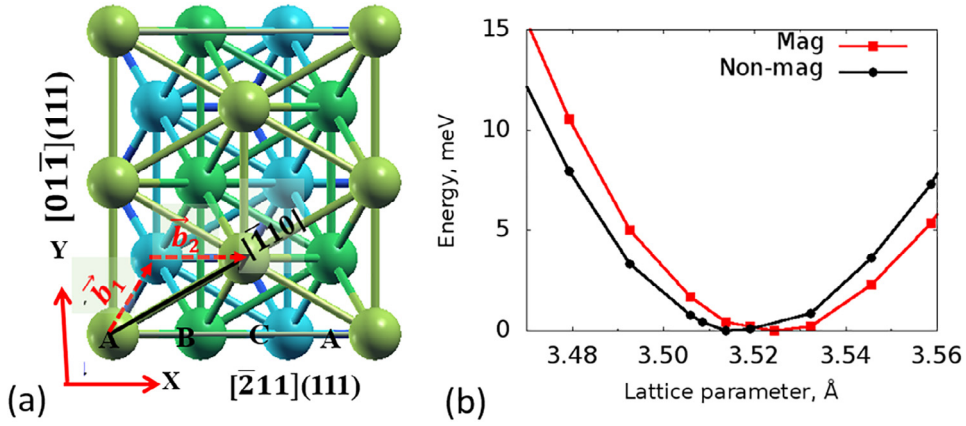

Fig. 1. (a) Schematic two-dimensional presentation of {1 1 1} plane (with different color of atoms) representing the stacking sequence of FCC and dissociation of Burgers vector of a perfect dislocation $\vec{b} = 1/2[\bar{1}\,1\,0]$ into two Shockley partials $\vec{b_1} = 1/6[\bar{1}\,2\,\bar{1}]$ and $\vec{b_2} = 1/6[\bar{2}\,1\,1]$ and (b) variation of energy as a function of lattice parameter for non-magnetic and magnetic states of Ni.

materials.

γ_{is} itself can be engineered through alloying with different substituent elements. Such substitutions affect the γ_{us} as well as change the atomic volume of the phases. Volume change associated with the solute addition not only plays an important role in the solid solution strengthening but also modifies the lattice mismatch (δ) between the γ and γ′, which directly affects the precipitation hardening as well as order strengthening [1]. Solute addition also affects the intrinsic ductility of the material. Ductility is a macroscopic property and according to Rice [7], it depends on the competition between processes of nucleation of dislocations blunting a crack tip and crack propagation through cleavage. Rice [7] defined a dimensionless ductility parameter (D) as $D = 0.15G_c/\gamma_{us}$, where G_c is the Griffith work or energy needed to create two new surfaces ($G_c = 2\gamma_s$, where γ_s is the surface energy). A system is said to be ductile if $D > 1$, and larger values of D indicate higher ductility.

Numerous theoretical and experimental studies have been carried out to gain better understanding of the effects of solute substitution on various properties, such as lattice parameter, γ_{is} and γ_{us} of Ni. For example, Siegel calculated the GSF of Ni alloyed with Nb, W, Mn, Fe and Cu and evaluated a measure of twinnability of the above alloys [8]. Datta et al. addressed the surface effects on stacking faults by analyzing nanofilms of Al, Cu and Ni [9]. Shang et al. explored the effects of alloying elements on the SFE of dilute Ni-base superalloys and their temperature dependence [10]. However, to the best of our knowledge, a systematic study of effects of alloying on volume changes, γ_{is}, γ_{us} and ductility of Ni is lacking. We present here first-principles DFT calculations to gain understanding of the effect of substitutional solute element belonging to 3d, 4d and 5d transition metals (TM) on the planar faults and associated properties. In our comprehensive analysis, we consider nickel in both ferromagnetic (spin-polarized) and non-magnetic states.

2. Computational details

Our calculations to simulate effects of solutes have been done within DFT using Quantum Espresso package [11] with a Plane Wave Self Consistent Field (PWSCF) approach. Plane wave basis truncated with an energy cutoff of 25 Ry was used in representation of Kohn-Sham wave functions and that with 200 Ry for representation of density. Ultrasoft (US) pseudopotentials [12] were used along with a generalized gradient approximation (GGA) for the electron correlation and exchange energy with the Perdew-Burke-Ernzerhof (PBE) functional [13]. Uniform mesh of (3X3X2) k-points was used in sampling Brillouin zone integration (of supercells) after performing a series of calculations with different meshes to test for the convergence of results [14]. Hellman-Feynman forces and stresses on atoms were used to optimize crystal structures, through minimization of total energy with the Broyden-Fletcher-Goldfarb-Shanno (BFGS) scheme. It is assumed that convergence to optimized structure is achieved when either the difference in the total energy between successive self-consistent cycles is less than 10^{-5} eV or the average force in the system is less than 0.02 eV/Å. We used non-magnetic and spin-dependent DFT calculations here.

We constructed a supercell with three orthogonal directions along [0 1 $\bar{1}$], [$\bar{2}$ 1 1] and [1 1 1] direction and having of six (1 1 1) layers (i.e., with the stacking sequence ABCABC along the [1 1 1] corresponding to close-packed FCC structure). This system with 96 Ni-atoms (consisting of 16 atoms in each layer) was completely relaxed, with the flexibility to change its cell size also, to obtain the equilibrium volume corresponding to minimum energy structure. In order to calculate the fault energies, shear deformation along ⟨1 1 2⟩{1 1 1} was simulated by suitably displacing the image of the supercell along the [$\bar{2}$ 1 1] direction, and allowing the positions of the atoms in the outer planes to relax along directions only perpendicular to the fault plane. For the displacement corresponding to a Burgers vector $\vec{b_p} = 1/6[\bar{2}\,1\,1]$, an energy minimum was found corresponding to an ISF, and the corresponding energy penalty γ_{is} is estimated as

$$\gamma_{is} = \frac{E_f - E_o}{A}$$

where E_f and E_o are the energies of the faulted and undeformed structures, and A is the area of the slip plane in the supercell on which fault has been generated. For pure Ni system, after a series of refined calculations, the first maximum of the GSFE was found at the slip corresponding to the translation of 0.56 $\vec{b_p}$ and its energy is used to obtain γ_{us}. In order to find out the effect of solutes, one of the Ni atoms on the shearing plane was substituted with an atom of alloying element from the 3d (Ti, V, Cr and Co), 4d (Zr, Nb, Mo, Ru and Pd) and 5d (Ta, W, Re and Ir) transition metal series and the procedure of estimating equilibrium volume and the defect energies was repeated for each substitution. This allows us to explore the effect of dilute alloying of about 1% on the mentioned fault properties. The calculation of ductility parameter requires the Griffith work, G_c as input. The procedure adopted here is essentially the same as described in Kumar et al. [15] but by considering essentially the same supercell as described above and with (1 1 1) as the plane of separation or cleavage.

3. Results

3.1. Changes in volume upon solute substitution

Typical variation in energy of the systems, after subtracting the minimum energies corresponding to the equilibrium lattice parameters,