



First-principles calculations of generalized-stacking-fault-energy of Co-based alloys



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ABSTRACT

The generalized-stacking-fault-energy (GSFE) curve for pure Cobalt and Co-9 at.% X solid-solution alloys (X = Cr, W, Mo, Ni, Mn, Al, Fe) have been successfully calculated by rigidly shearing an fcc crystal at a (111) plane along a [11–2] slip direction in two processes using first-principles density-functional-theory (DFT), provide a highly accurate modeling and a fairly good agreement with available experimental and other theoretical results in the literature. The objectives of this study are to provide a useful guideline for the Co-based alloy design with superior performances and new insight for understanding the nature of the fcc to hcp phase transformation. Evaluation of the GSFE values is based on the ratio of the stable and unstable stacking fault energy, the twinnabilities with three criterions for crack tip twinning, grain boundary twinning and inherent twinning, as well as the predicted critical twinning stress. It concludes that alloying with Cr, W and Mo atoms are expected to bring a significant increase in the tendency of the dominant deformation mechanism for the formation of partial dislocations and mechanical twinning of pure Co. The investigation regarding the electronic structure, such as interlayer distance distortion between a faulted and perfect fcc structure, atomic bonding, charge density distributions and density of states (DOS) in the present work can describe why and how alloying atoms change the GSFE values of Co-based alloys.

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1. Introduction

Co-based alloys or superalloys have an excellent resistance to various forms of wear and high strength over a broad range of temperatures. These alloys mostly used in aerospace, nuclear and petrochemical industries especially in aero-engine combustor components [1]. The high wear resistance of Co-based alloys is thought to be due to the transformation of metastable face-centered cubic (fcc) structure of cobalt to the low temperature hexagonal close-packed (hcp) structure on the application of high shear stresses during sliding. The shear-induced alignment of the hcp basal plane significantly reduces friction and improves galling resistance [2]. A thin and easily shear layer can form at the sliding surface then strain hardened the Co-based alloy. The wear-induced fcc to hcp transformation involves the coalescence of stacking fault in the subsurface regions [2,3].

Stacking fault (SF) is an important type of planar defect and resulted from the incorrect stacking sequence of lattice plane in a

crystal. A measure of the energy cost to shear two adjacent atomic planes about each other are the stacking fault energy (SFE) [4]. Stacking fault energy is a critical intrinsic material parameter that significantly affects the plastic deformation behavior and mechanical properties. Low-SFE materials, like Co-based alloys, enables the formations of high densities of SFs and twins, which promote partial dislocation accumulation then enhance both the ductility and fracture toughness without compromising high strengths [4,5]. The kinetic process of partial dislocation movements is controlled by SFE (γ), and $\gamma \propto 1/R$, where R is the width of separation between partial dislocations. Hence, a lower SFE corresponds to a larger distance of separation between dissociated partials, resulting in reduced cross-slip and climb [6].

Recent researches [7–9] indicate that the generalized-stacking-fault-energy abbreviated as GSFE, dictate the competition between slip and twinning or the plastic deformation mechanism, rather than the SFE itself. The physical interpretation of GSFE represents the energy penalty between two adjacent planes during various degrees of inelastic shear deformation in a particular slip direction on a given slip plane, representing the nature of slip and involving the stable, unstable stacking and twin fault energies [6,10]. The unstable SFE γ_{us} is the first maximum energy on the GSFE curve

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that represents the energy barrier to creating a stacking fault. As the partial dislocation starts to propagate, the GSFE decreases to the minimum value referred to stable SFE γ_{sf} and create a stacking fault defect. Then, the ratio of stable and unstable SFE (γ_{sf}/γ_{us}) is the parameter to understand the dominant deformation mechanism, whether the extended partials or full dislocations. Similarly, the observation of twin nucleation is dependent on the ratio of unstable-twinning and unstable SFE (γ_{ut}/γ_{us}). The unstable-twinning SFE γ_{ut} is the second maximum energy on the GSFE curve that represents the energy barrier to creating a micro-twin defect. In particular, the GSFE curve can be used to predict the solid-solution strengthening and model of phenomena linked to dislocations, plastic deformation, crystal growth and phase transition [6,11,12]. The fcc to hcp phase transformation of Co-based alloys occurs during plastic deformation at room temperature by shear in the $a/6[11-2]$ slip system on (111) planes (a is the lattice constant), also referred as strain-induced martensitic transformation (SIMT). Co-based alloys with lower generalized-stacking-fault (GSF) energy in the $a/6[11-2]$ slip system indicate a great tendency to form stacking faults. The formation of the stacking fault in fcc crystal on a close-packed (111) stacking plane ABCABC produces the hcp nucleus stacking BCBC in the fcc matrix, which is regarded as the beginning of fcc to hcp phase transformation [12].

Successful modeling depends heavily on the precision of obtained GSFE values. First-principles density-functional-theory (DFT) calculations are capable of providing highly accurate structural modeling with little or no experimental input [13]. Since experimental determination of GSFE value is almost at present not possible, the first-principles calculation has been widely used in various cases. For example pure fcc metals, including Ni [14], Cu [15] and Al [9], and also pure hcp metals, including Mg, Ti, Zn and Zr [16]. Only a limited number of papers have analyzed GSFE values for alloys such as for; Ni [14], Al [17], Fe [18], Mo [19] and Mg alloys [6,20]. Such calculations have not been carried out for pure Co and Co-based alloys, except for binary Co-33%Ni alloys by Chowdhury et al. [1]. Then, the GSFE values of pure Co and binary Co-X alloys with Ni, Cr, W, Mo, Al, Fe and Mn as the alloying atoms will be calculated in the present study.

Pure Co is known to crystallize in two phases with fcc and hcp lattices γ - and ϵ -phases, respectively. The experimental stable SFE (γ_{sf}) of the fcc Co is in the range from 13.5 to 18.5 mJ/m² at temperatures 500–710 °C [21]. Some authors consider the SFE of Co–Cr–Mo alloys is in the range from 10 to 30 mJ/m² [22], even to be negative because of the metastability of γ -phase (fcc) at room temperature [23]. In principle, alloying atoms could disturb the local environment of matrix atoms, and then it is a common practice to modify SFE by the useful alloying element addition [20]. Alloying atoms tend to segregate to the stacking faults due to chemical interaction, and the SFE becomes negative as the alloying atoms segregate to such a high concentration (known as Suzuki segregation [24]). Many researchers revealed that certain alloying elements could significantly lower the SFE of different alloys from the experiments or theoretical simulation. For example, Co–Ni based superalloy [25], Co–Ni–Cr based superalloy [26] and Mg–Zn–Y alloy [27].

From a solid state physics standpoint, the alloying atoms induced an atomic volume mismatch that contributes to the hardening effects. The alloying atoms can alter the fault energy landscape in the alloy structure and affects the tendency of competing crystal deformation mechanisms (such as full or partial dislocations, stacking faults and twinning faults) and fcc to hcp transformation [1]. This type of transformation in binary Co–Ni alloys leads to a good shape memory effect (SME) and such a combination with the ferromagnetism of fcc and hcp phase renders the potential to serve as function materials in wide ranges of application [28].

The objective of this study is to provide a useful guideline for the Co-based alloy design with superior performances. Then it is necessary to examine how alloying atoms alters selected mechanical property of Co by evaluation of GSFE values. The assessment is placed on the deformation mechanism tendency of a metal to undergo full or partial dislocations, deformation twinning and twinnabilities. Evaluation of the twinnabilities with three criterions for crack tip twinning proposed by Tadmor and Bernstein [7], grain boundary twinning suggested by Asaro and Suresh [29], and inherent twinning for perfect fcc materials without crack tip or grain boundary proposed by Li et al. [30]. Furthermore, the tendencies in the GSFE values and an actual relationship with alloying atoms were analyzed regarding the electronic structure, such as density distributions surrounding the solute atoms, interlayer distance and density of states (DOS).

2. Computational details

In the present work, the calculation of total energy was performed by the Cambridge Sequential Total Energy Package code (CASTEP) [31] based on density-functional-theory (DFT) [32]. The exchange–correlation functional was Perdew–Burke–Ernzerhof (PBE) [33] version of the generalized gradient approximation (GGA). Fully optimized geometry is an essential precondition of calculation (atoms moved until reach minimum energy and forces are zero at different volume). The relaxation was terminated based on convergence parameters. The convergence parameters as follows: total energy tolerance 10^{-5} eV/atom, force tolerance 0.03 eV/Å, maximum stress component 0.05 GPa, and maximum displacement 0.001 Å. After enough volumetric relaxation and energy convergence test, the Monkhorst–Pack [34] scheme k-points grid sampling is set as 36 irreducible k-points ($11 \times 11 \times 1$) in the Brillouin zone and the plane wave energy cut-off is 400 eV. The calculations used a spin-polarized approximation which uniformly distributed over the space for pure Co and also for all the alloying elements due to its ferromagnetic nature of Co-based alloy. The predicted spin magnetic moment for Co is 1.65 μ_B /atom. A full optimization of the supercell was performed to acquire the equilibrium structure and to obtain the total energy versus volume (E - V) data points.

The differences in total energies associated with the perfect structure and the related defect structure have been calculated to model the GSFE curve from first-principles. An infinitely large structure is ideal for the calculations. However, it is a common practice in the first-principles calculation packages to repeat a finite size supercell infinitely with periodic boundary condition (PBC). Fig. 1(a) shows the geometry of the computational cell that used in the present work. The $1 \times 1 \times 1$ supercell was created from the fcc unit cell of pure Co in $[11-2]$, $[-110]$ and $[111]$ directions. Then, the $1 \times 1 \times 4$ supercell was used for the first-principles calculations consist of 22 atoms with 11 layers and ABCABCABCAB stacking sequence of close-packed (111) planes. Fig. 1(b) shows the top view geometry of an (111) plane in the present work with the distinct stacking sequence A (light blue atoms), B (red atoms) and C (dark blue atoms). Perfect or full dislocations in an fcc structure occurs predominantly in the close-packed (111) planes and the $[10-1]$ directions from A to A positions (green arrow), define the lattice vector $b_1 = a/2[10-1]$ (a is the lattice constant). The easiest path for an atom to slip between adjacent A positions is to slip to a B position first then to final A position (yellow arrow). Then, it is advantageous for full dislocations with Burgers vector b_1 to split into two partial dislocations with Burgers vectors $b_2 = a/6[11-2]$ and $b_3 = a/6[2-1-1]$ connected by an SF ribbon.

The GSFE values were calculated by rigidly shearing a studied supercell at a (111) plane along a $[11-2]$ slip direction in two pro-

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