Computational Materials Science 126 (2017) 103–107

Contents lists available at ScienceDirect

Computational Materials Science

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

First-principles investigation on slip systems and twinnability of TiC

Tengfei Li [a], Tianmo Liu [a,*], Liqiong Zhang [a], Tao Fu [b], Hongmei Wei [a]

[a] College of Materials Science and Engineering, Chongqing University, Chongqing 400044, China
[b] College of Aerospace Engineering, Chongqing University, Chongqing 400044, China

ARTICLE INFO

Article history:
Received 23 July 2016
Accepted 19 September 2016

Keywords:
Generalized stacking fault energy
Slip system
Twin
First-principle calculation

ABSTRACT

The slip systems and comparative twinnability of TiC have been investigated in term of generalized stacking fault energy curves and the relevant energy properties by the density functional theory based first principles calculations. The possible slip systems of three low index planes were taken into consideration in TiC. When a pre-existing twin fault was considered, it was found that the slip in the twin plane had the much lower unstable stacking fault energy which might induce the alteration of the deformation mechanism and result in the enhancement of toughness.

1. Introduction

Transition metal carbides, nitrides and borides have been widely used due to their superior mechanical, physical and chemical properties [1–3]. As a typical transition metal carbide, TiC has been applied to many fields, such as protective coating materials for cutting tools [4], aerospace structural components [5], and strengthening phases in other structural materials [6], because of its high melting point, high hardness and high-temperature oxidation resistance [7,8]. However, its applications are limited by its intrinsic brittleness [9]. In order to improve the toughness of this class of materials, many methods have been developed to improve their ductility while maintaining high hardness, such as adding a small quantity of alloying elements [10,11], even making pseudobinary alloys [12–14], and introducing twin structures [15,16]. To engineering the toughness of this class of materials, a thorough insight into the defect behavior, such as dislocation and twin, is crucial. The generalized stacking fault (GSF) energy established by Vitek [17], represents the extra energy for a perfect crystal to cut across a slip plane into two parts which are subjected to a relative displacement along an arbitrary vector and rejoined. The GSF curve and the relevant energy properties could be applied to model a lot of phenomena linked to dislocations [18], plastic deformation [19,20], and deformation twinning [21].

In this work, we use density function theory to calculate the GSF energy curves for different planes. The obtained unstable stacking fault energies of different slip systems have been made quantitative comparisons to determine the preferred slip system. Furthermore, the twinning boundary energy of TiC has been computed. The GSF energy curve for {1 1 1} twin plane is also obtained.

2. Methodology

The density functional theory calculations were performed using the Vienna ab initio simulation package (VASP) [22,23], with the projector augmented wave (PAW) [24,25] basis set, employing the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional [26]. The different Monkhorst-Pack k-point meshes for the Brillouin-zone integration were applied for the different supercells, with linear k-point separation less than 0.04 $Å^{-1}$ along each periodic direction in reciprocal space [27]. A planewave kinetic energy cutoff of 450 eV was used for the planewave expansion of the wave functions in the supercell calculations. Ti $3d^3 4s^1$ and C $2s^2 p^2$ electrons were regard as valence electrons in the used pseudopotentials. A thickness of 10 Å vacuum was embedded into the surface supercell to avoid the interaction between the slab and its periodic images [28]. During the relaxations, all structures were relaxed to an energy convergence of 10^{-5} eV, meanwhile, the maximum force on each atom was less than 0.01 eV/Å. The optimized lattice constants of bulk TiC ($Fm\bar{3}m$, a = 4.334 Å) agreed well with the experimental values of 4.324–4.35 Å [29–31] and theoretical values of 4.33–4.333 [32–34], respectively, verifying the accuracy obtained from the proposed parameters.

The GSF energy established by Vitek [17], represents the extra energy for a perfect crystal to cut across a slip plane into two parts which are subjected to a relative displacement along an arbitrary vector and rejoined. However, it needs to pay particular attention

* Corresponding author.
E-mail address: tmliu@cqu.edu.cn (T. Liu).

http://dx.doi.org/10.1016/j.commatsci.2016.09.028
0927-0256/

to choosing the sliding vectors for the crystalline ceramic materials such as TiC, which contains more than one element and has special atomic arrangement. TiC has a rock-salt (B1) crystal structure with (0 0 1), (1 1 0) and (1 1 1) as its low index planes which are considered as the possible slip planes in this work (Fig. 1). In order to explore the preferred slip systems in this material, all possible slip systems will be considered. As shown in Fig. 2, it displays the atomic arrangements of the (0 0 1), (1 1 0) and (1 1 1) planes of TiC from the different perspectives. In the top-view graphs, the considered possible slip systems are also indicated. For the top-view images of the (0 0 1) and (1 1 0) planes, the uppermost layer is considered, while the top-two layers for the (1 1 1) image. When a slip has occurred, the image of the slipped part should be overlapped. Hence, the following slip systems will be taken into account: {1 0 0}⟨1 0 0⟩, {1 0 0}⟨1 1 0⟩, {1 1 0}⟨1 0 0⟩, {1 1 0}⟨1 1 0⟩, {1 1 0}⟨1 1 1⟩, {1 1 0}⟨1 1 2⟩, {1 1 1}⟨1 1 0⟩ and {1 1 1}⟨1 1 2⟩ slip systems. As mentioned before, the dense {1 1 1} twins have been detected in TiC [15,16,35,36]. For the {1 1 1} plane slip, a pre-existing twinning fault configuration was also considered which involved two kinds of twin boundary structures: Ti-type and C-type [15]. During the GSF energy calculations, a vector x along the slip direction was applied when shifting the upper part supercells rigidly. Under the slip vector, DFT calculations were performed by relaxing all atoms only along the z-axis. Furthermore, it was also taken into account for {1 1 1} plane slip that the slip displacement was applied between two neighboring Ti layers at the interface, allowing the C atoms to relax between them [37]. The GSF energy was obtained as:

$$\gamma_x = (E_x - E_0)/\ A \tag{1}$$

where $\boldsymbol{\gamma_x}$ was the GSF energy for slip vector x; E_x and E_0 were the energies of the supercell with slip vector x, and with x = 0, respectively; A was the area of the slip plane.

As shown in Fig. 3(a) and (b), twin models were constructed to calculate the {1 1 1} twin boundary energies of TiC. The twin boundary energies are the energy costs of unit area of the boundary between the crystallographic twin and its corresponding normal stacking structure. It quantifies the stability of the twin [38] and could be theoretically calculated by

$$\zeta = (E_{twin} - E_{bulk})/\ A \tag{2}$$

where E_{twin} is the total energy of the twin model, E_{bulk} is the total energy of corresponding perfect bulk scaled to the supercell size and A represents the area of the twin boundary.

3. Results and discussions

A correct interpretation of the nature of slip in a crystalline material requires the GSF energy curve, involving both stable and unstable stacking fault energies [39]. The stable stacking fault energy, i.e., intrinsic stacking fault energy, γ_{is}, is the local energy minima on the GSF energy curve. It can be applied to interpret dislocation splitting widths, which represents the possibility of the splitting of perfect dislocation into partials [40,41]. The unstable stacking fault energy, γ_{us}, is the maximum energy of the GSF energy curve, which is used as a criterion for dislocation nucleation by denoting the lowest energy barrier for dislocation nucleation [42,43].

The DFT results of GSF energies as a function of displacement fraction along the ⟨1 0 0⟩ and ⟨1 1 0⟩ directions in {1 0 0} plane are shown in Fig. 4a. For both ⟨1 0 0⟩ and ⟨1 1 0⟩ directions, there is a single maximum point in each GSF energy curve which implies the unstable stacking fault energy for the given slip system. Furthermore, the unstable stacking fault energy (2.94 J/m^2) of {1 0 0}⟨1 1 0⟩ slip system is much lower than that of the {1 0 0}⟨1 0 0⟩ slip system, signifying that a dislocation energetically prefer to nucleate along ⟨1 1 0⟩ direction for {1 0 0} plane. While for the {1 1 0} plane, the directions of ⟨0 0 1⟩, ⟨1 1 0⟩, ⟨1 1 1⟩ and ⟨1 1 2⟩ were considered as shown in Fig. 4b. Obviously, the slip system of {1 1 0}⟨1 1 0⟩ has the lowest stacking fault energy (2.28 J/m^2) which agrees well with the previous DFT result (Table 1) [44]. For the ⟨1 1 1⟩ and ⟨1 1 2⟩ directions, there is a pair of minimum points symmetrically located in the GSF energy curve, which implies the intrinsic stacking fault energy, in sharp contrast to the others slip systems. It corresponds to a stable structure for a stacking fault during the slip process. It should be noted that the ⟨1 1 2⟩ direction is secondly energetic preferred for dislocation slipping in {1 1 0} plane.

As shown in Fig. 2c, the metal and nonmetal atom layers stack alternately for {1 1 1} planes, resulting in that the calculations of GSF energies for {1 1 1} planes are more complex than for other planes [37]. The slips between the neighboring Ti – Ti layers and Ti – C layers were considered to calculate the GSF energies for

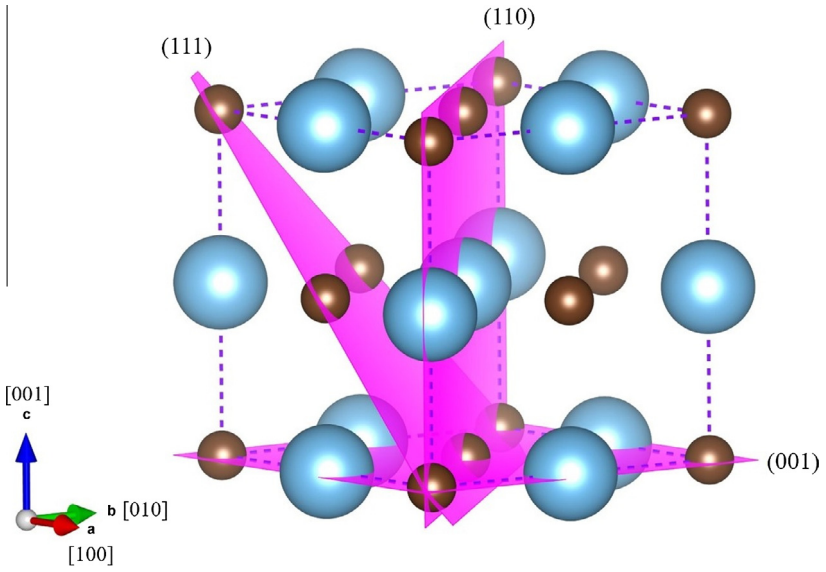

Fig. 1. The crystal structure of TiC with the indicated low index planes of {1 0 0}, {1 1 0} and {1 1 1}.