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Can twins enhance the elastic stiffness of face-centered-cubic metals?

Dejiu Shen [a], Jinglian Du [a], Roderick Melnik [b], Bin Wen [a,*]

[a] State Key Laboratory of Metastable Materials Science and Technology, Yanshan University, Qinhuangdao 066004, China
[b] M^{2}NeT Lab, Wilfrid Laurier University, Waterloo, 75 University Ave. West, Ontario N2L 3C5, Canada

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ABSTRACT

It has usually been reported that the elastic stiffness of polycrystals is lower than that of the corresponding monocrystals. Recent experimental results made by Tanigaki et al. (2013) indicate that twin boundaries can improve the elastic stiffness of synthesized nano-polycrystalline diamonds. These researches imply that it may be a universal law for the twin boundary enhancing elastic stiffness. To verify this hypothesis, the elastic properties of ten face-centered-cubic (FCC) structure metals' perfect crystals and twin crystals have been studied by using first-principles calculations. Our research findings indicated that twins cannot always enhance the elastic stiffness of FCC structure metals. These results further clarify the fact that twin boundary enhancing elastic stiffness is not a universal law.

1. Introduction

As one of the most important mechanical properties of materials, elastic stiffness reflects the ability to resist elastic deformation of crystal lattice [1]. Polycrystalline materials are composed of grain intragranular and grain boundaries [2]; since their elastic properties are totally different, the grain boundaries play a crucial role in the elastic stiffness of polycrystals [3]. Usually, the elastic stiffness of grain boundary is lower than that of grain intragranular [4], hence the elastic stiffness of polycrystals should be less than that of the corresponding monocrystals; and the elastic stiffness of polycrystals is decreasing with the decrease of grain size [4,5]. This trend has been experimentally verified for many nanosized materials [6–8].

Twin boundary is a special grain boundary of materials, its effect on yield strength and flow stress is reported to be the same as that of general grain boundary by fulfilling the Hall-Pitch and reverse Hall-Pitch relationships [9]. In this context, the effect of twin boundary on the elastic stiffness may be the same as that of the general grain boundary. Very recently, some experimental results indicate that twin boundary cannot decrease the elastic stiffness of materials; instead, it can increase the elastic stiffness of materials. For example, Tian's experimental results indicated that the Young's modulus of nanotwin cubic boron nitride is larger than that of monocrystal boron nitride [10]. Meanwhile, Tanigaki's investigations also indicate that the nanopolycrystal diamond synthesized by a direct-conversion method from graphite is stiffer than its monocrystal counterparts. The authors attributed the improvement of elastic stiffness to the twin structures in the synthesized nano-polycrystalline diamond [11]. All these experimental results imply that it seems to be a universal law for the twin boundary enhancing elastic stiffness of materials. To verify this assumption and further study the twin boundary's effect on elastic stiffness, the elastic properties of ten FCC metals' perfect crystals and twin crystals have been investigated by performing first-principles calculations. The research findings indicated that twins cannot always enhance the elastic stiffness of FCC metals studied here. And these results further clarify the fact that the twin boundary induced enhancement of elastic modulus is not a universal law.

2. Computational methods

In this work, ten FCC structure metals (i.e. Ag, Au, Co, Cu, Ni, Pd, Pt, Rh, Al and Ca) have been selected to study the twin crystal induced elastic properties' variation. The typical structures for perfect Cu and twin Cu are shown in Fig. 1(a) and (b), respectively. First-principles calculations have been performed within the framework of electronic density functional theory (DFT), as implemented in the Vienna Ab-initio Simulation Package (VASP) [12]. The exchange and correlation interaction was described in both the generalized gradient approximation (GGA) [13] and the local density approximation (LDA) [14,15]. The interactions between the ions and valence electrons were modeled by both the projector-augmented wave (PAW) potentials [16] and the ultra-soft pseudo-potentials (USPP) [17]. A plain wave cutoff energy of 320 eV has been used for Cu, 330 eV for Ag, Co, Ni and Pd, 280 eV for Pt, 310 eV for Ca and Rh, 160 eV for Al and 360 eV for Au.

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* Corresponding author. Tel.: +86 335 8568761.
E-mail addresses: sdj217@ysu.edu.cn (D. Shen), wenbin@ysu.edu.cn (B. Wen).

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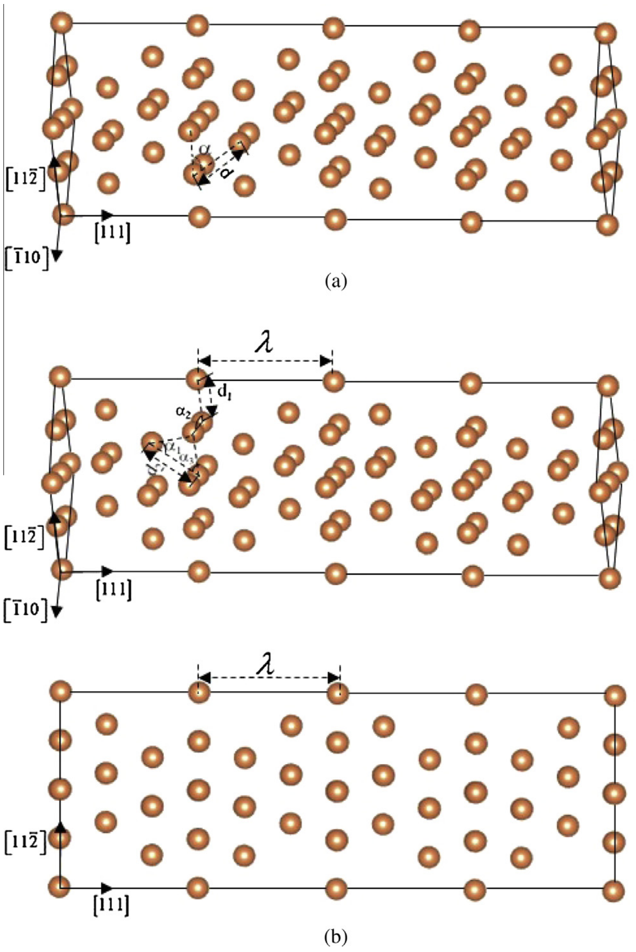

Fig. 1. The structures of (a) perfect Cu, and (b) twin Cu.

Brillouin zone integrations were performed by using the Monkhorst–Pack *k*-point mesh [18], and the *k*-point mesh of each cell has been sampled by $5 \times 5 \times 3$ for perfect Ag and Au, $4 \times 4 \times 3$ for perfect Ca, $6 \times 6 \times 4$ for perfect Co, Cu and Ni, $5 \times 5 \times 4$ for perfect Al, Pt, Pd and Rh, while $10 \times 10 \times 2$ for twin Al, Ag, Au, Pt, Pd and Rh, $7 \times 7 \times 2$ for twin Ca, $12 \times 12 \times 2$ for twin Co and Ni, and $11 \times 11 \times 2$ for twin Cu, respectively. The total energy was converged numerically to 5×10^{-7} eV/atom with respect to electronic, ionic and unit cell degrees of freedom. To verify computational accuracy, benchmark calculations have been performed for perfect Cu. The optimized lattice parameter of 0.3636 nm agrees well with the available experimental value of 0.3608 nm [19,20] and previously calculated value of 0.3643 nm [21], which confirmed that the computational scheme used in this work is reliable.

3. Results and discussion

The elastic moduli of polycrystals were deduced from the corresponding single-crystal elastic constants by using Voigt, Reuss and Hill (VRH) approximations [22,23]. In this study, the single-crystal elastic constants were obtained by computing the total energy density as a function of suitable strains [24,25]. Based on the crystal systems and various imposed deformations, the quadratic coefficient of the total energy density versus strain corresponds to either a particular elastic constant or a linear combination of elastic constants [26,27]. The total energies were calculated by imposing appropriate strains up to ±2.5% at 0.5% interval. To better compare the elastic properties, the structures of these FCC metals' perfect crystals have been transformed into hexagonal crystal system, the same as their corresponding twin crystal counterparts [28,29]. The calculated single-crystal elastic constants (C_{ij}) of perfect crystals and twin crystals for these ten FCC metals were listed in Table 1. The results indicated that for Ag, Au, Co, Cu, Ni, Pd, Pt and Rh, the elastic constants C_{11} and C_{33} of twin crystals are higher than that of their perfect counterparts, while C_{12}, C_{13} and C_{44} of twin crystals are lower than that of their perfect counterparts; whereas for Al and Ca, the elastic constants C_{11} and C_{33} of twin crystals are lower than that of their perfect counterparts, while C_{12}, C_{13} and C_{44} have no congruent change. And this variation trend does not change with different potential functions (i.e. PAW–GGA, PAW–LDA, USPP–GGA and USPP–LDA).

Accordingly, the elastic moduli of the ten FCC metals' perfect polycrystals and twin polycrystals, including shear modulus (G), bulk modulus (B), Young's modulus (E) and longitudinal modulus (M) were deduced from their respective single-crystal elastic constants (C_{ij}) via VRH approximations. The results of elastic moduli were listed in Table 2, also compared and visualized in Fig. 2. As can be seen that for Ag, Au, Co, Cu, Ni, Pd, Pt and Rh, the calculated G, E and M of twin crystals are higher than those of their corresponding perfect crystals; while for Al and Ca, the calculated G, E and M of twin crystals are lower than those of their corresponding perfect crystals. Besides, the calculated B of twin crystals almost equal to that of their perfect counterparts for the ten FCC metals studied here. Furthermore, this variation trend does not change with different potential functions (PAW–GGA, PAW–LDA, USPP–GGA and USPP–LDA), which suggests that twin crystals can indeed influence the elastic stiffness of FCC metals, but the effect does not follow the same mode.

The twin concentration can be well reflected by the twin thickness (hereafter denoted as λ) which refers to be the spacing between adjacent twin boundaries, as is shown in Fig. 1(b); and a smaller twin thickness usually signifies a higher twin concentration [30–32]. Given that twin crystals indeed can enhance the elastic modulus for most of the FCC metals studied here, thus the elastic moduli of twin Cu with four different twin thickness (i.e. $\lambda_1 = 6.355$ Å, $\lambda_2 = 12.671$ Å, $\lambda_3 = 19.006$ Å, $\lambda_4 = 25.341$ Å) have been investigated as an example to further explore the influence extent of this variation. The calculated results are summarized in Table 3 and also visualized in Fig. 3. As is shown, the twin Cu represented by λ_1 corresponds to the highest twin concentrations, and hence it possesses the largest elastic modulus G, E and M. Furthermore, with the decrease of twin concentrations, the corresponding elastic modulus G, E and M of twin Cu decreases, while the bulk modulus B is almost unaffected. And this variation trend also does not change with different potential functions (PAW–GGA and PAW–LDA). Particularly, the twin crystal with the smallest twin thickness λ_1 represents the highest twin concentrations; hence the twin induced variation of elastic modulus for FCC metals is limited.

Subsequently, the mass density which is considered as an important parameter affecting the properties of materials [33–35], was explored to understand the twin crystal induced elastic properties' variation of the ten FCC structure metals. The results were reflected in Table 4. As is shown in Table 4, the mass densities of these ten FCC metals' corresponding perfect crystals and their twin counterparts are almost equal to each other. Indeed, researches have revealed that there are close relationships between the mass density and bulk modulus of metallic materials [36–38]. Hence, the unchanged bulk modulus (B) for twin crystals and their perfect counterparts can be attributed to the unchanged mass density. According to VRH approximations, the elastic modulus G, E and M can be obtained through the following Formulas (1)–(3).