

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



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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.

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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-Petch and reverse Hall-Petch 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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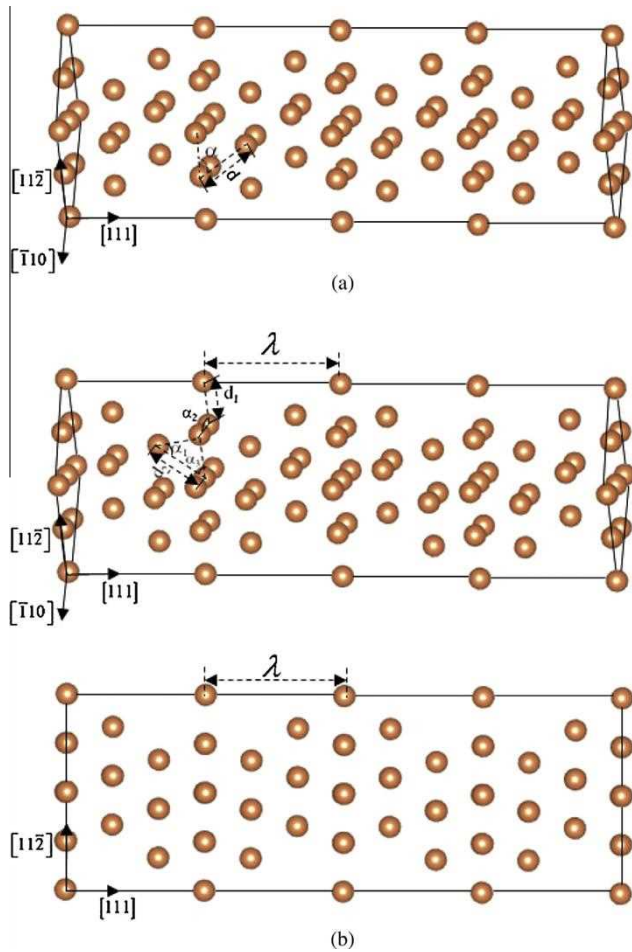


Fig. 1. The structures of (a) perfect Cu, and (b) twin Cu.

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 $\pm 2.5\%$ 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).

Table 1

The single-crystal elastic constants (C_{ij}) of the ten FCC metals' perfect crystals and their twin counterparts with PAW–GGA, PAW–LDA, USPP–GGA and USPP–LDA potential functions.

C_{ij}	C_{11} (GPa)				C_{12} (GPa)				C_{13} (GPa)				C_{33} (GPa)				C_{44} (GPa)			
Potential	PAW–GGA	PAW–LDA	USPP–GGA	USPP–LDA	PAW–GGA	PAW–LDA	USPP–GGA	USPP–LDA	PAW–GGA	PAW–LDA	USPP–GGA	USPP–LDA	PAW–GGA	PAW–LDA	USPP–GGA	USPP–LDA	PAW–GGA	PAW–LDA	USPP–GGA	USPP–LDA
Perfect Ag	136	185	120	180	76	120	67	111	78	120	71	112	137	188	128	180	48	69	37	66
Twin Ag	164	234	152	213	72	114	64	103	58	93	54	85	166	246	154	227	28	37	27	35
Perfect Au	158	215	209	155	131	186	177	123	131	187	177	124	161	217	211	156	32	40	39	34
Twin Au	192	261	250	188	113	159	151	108	120	169	159	113	178	243	237	172	22	30	29	21
Perfect Co	401	489	395	483	183	229	177	221	183	231	179	223	397	488	394	480	199	240	192	234
Twin Co	469	576	449	547	154	195	149	186	134	169	133	166	505	615	491	601	125	150	123	150
Perfect Cu	183	249	185	254	113	158	114	162	119	158	123	161	175	241	191	247	84	113	82	114
Twin Cu	242	314	242	316	103	140	106	140	77	108	84	111	246	316	253	342	53	63	48	71
Perfect Ni	251	327	260	327	173	228	176	223	172	223	170	222	254	331	259	328	111	143	112	138
Twin Ni	324	402	306	388	147	191	148	189	129	166	133	169	350	434	331	442	61	73	62	78
Perfect Pd	205	274	191	261	158	210	147	200	158	210	150	200	206	275	195	262	68	91	61	85
Twin Pd	235	312	212	289	141	187	133	178	133	178	128	171	266	359	254	345	39	52	38	51
Perfect Pt	293	367	286	359	221	274	216	268	221	275	216	268	293	368	286	360	62	82	60	81
Twin Pt	314	404	296	381	200	249	200	246	208	257	205	251	335	423	339	420	41	55	45	58
Perfect Rh	405	499	389	479	186	233	178	221	187	233	178	221	407	500	390	480	177	219	166	206
Twin Rh	455	564	428	529	157	197	150	186	154	193	151	186	471	580	451	560	121	149	117	144
Perfect Al	181	209	194	212	18	26	21	25	22	37	22	34	141	121	143	129	8	6	10	6
Twin Al	95	113	95	112	57	65	56	64	66	71	64	69	98	102	96	103	29	32	30	34
Perfect Ca	33	33	32	35	15	18	14	18	7	6	8	5	42	49	48	51	7	7	7	7
Twin Ca	32	32	31	33	11	13	10	13	10	11	9	11	36	36	34	34	4	5	4	5

Table 2

The shear moduli (G), bulk moduli (B), Young's moduli (E) and longitudinal moduli (M) of the ten FCC metals' perfect crystals and twin crystals with PAW–GGA, PAW–LDA, USPP–GGA and USPP–LDA potential functions.

Modulus	Shear modulus (GPa)				Bulk modulus (GPa)				Young's modulus (GPa)				Longitudinal modulus (GPa)			
Potential	PAW–GGA	PAW–LDA	USPP–GGA	USPP–LDA	PAW–GGA	PAW–LDA	USPP–GGA	USPP–LDA	PAW–GGA	PAW–LDA	USPP–GGA	USPP–LDA	PAW–GGA	PAW–LDA	USPP–GGA	USPP–LDA
Perfect Ag	34.3	45.2	30.8	44.3	96.9	143.5	88.5	135.9	92.1	122.8	82.8	119.9	142.6	203.8	129.6	195.1
Twin Ag	39.7	52.7	38.1	48.9	96.8	144.8	91.4	134.1	104.7	141.0	100.3	130.9	149.7	215.1	142.2	199.3
Perfect Au	19.7	22.1	21.8	23.3	140.5	196.6	133.9	188.1	56.5	63.9	61.9	67.0	166.8	226.1	162.9	219.2
Twin Au	29.5	38.7	29.7	38.2	141.0	195.4	134.8	186.2	82.7	109.0	82.9	107.3	180.5	247.1	174.4	237.1
Perfect Co	138.5	166.2	136.3	165.0	255.4	316.5	250.5	308.7	351.9	424.4	346.3	420.2	440.1	538.1	432.3	528.8
Twin Co	148.2	178.2	143.0	173.2	254.1	314.9	246.5	303.2	372.2	449.9	359.6	436.6	451.7	552.6	437.2	534.2
Perfect Cu	47.9	65.4	48.8	66.3	138.0	187.7	142.3	191.6	128.9	175.8	131.4	178.3	201.9	274.9	207.4	279.9
Twin Cu	65.4	79.9	62.2	85.5	137.9	184.0	142.9	188.7	169.4	209.3	162.8	222.8	225.1	290.5	225.8	302.6
Perfect Ni	60.7	78.3	63.7	76.9	198.7	259.1	201.3	256.4	165.2	213.3	172.8	209.7	279.6	363.5	286.2	358.9
Twin Ni	79.6	95.3	74.9	95.3	200.9	253.6	196.6	252.3	211.1	254.1	199.6	253.9	307.1	380.7	296.5	379.4
Perfect Pd	36.8	49.3	33.4	46.9	174.0	231.7	163.5	220.6	103.2	138.1	93.7	131.4	223.1	297.4	208.0	283.2
Twin Pd	46.1	61.6	42.1	57.6	172.1	229.4	161.1	217.5	127.1	169.6	116.2	158.8	233.6	311.5	217.2	294.3
Perfect Pt	44.7	58.5	43.5	57.5	244.9	305.5	239.3	298.7	126.4	164.9	123.1	162.1	304.6	383.5	297.4	375.4
Twin Pt	50.5	67.6	48.9	65.3	243.8	305.8	238.2	297.0	141.6	189.0	137.3	182.4	311.1	396.0	303.4	384.0
Perfect Rh	132.8	162.7	126.6	155.7	259.6	322.1	248.4	307.1	340.3	417.9	324.7	399.6	436.6	539.1	417.3	514.7
Twin Rh	138.6	170.1	131.3	161.9	256.8	319.1	245.5	304.1	352.2	433.3	334.3	412.6	441.5	545.8	420.6	520.0
Perfect Al	33.1	31.4	36.7	32.3	69.3	80.2	72.6	80.1	85.6	83.3	94.2	85.4	113.4	122.0	121.5	123.1
Twin Al	21.4	25.0	21.7	25.8	73.9	82.5	72.8	81.2	58.5	68.1	59.3	70.0	102.5	115.9	101.8	115.6
Perfect Ca	9.6	9.2	9.5	10.1	18.2	19.3	19.5	19.6	24.5	23.7	24.6	25.8	31.0	31.5	32.2	33.0
Twin Ca	7.3	7.9	7.3	8.3	17.9	19.3	17.1	19.0	19.3	20.9	19.1	21.6	27.7	29.9	26.8	30.0

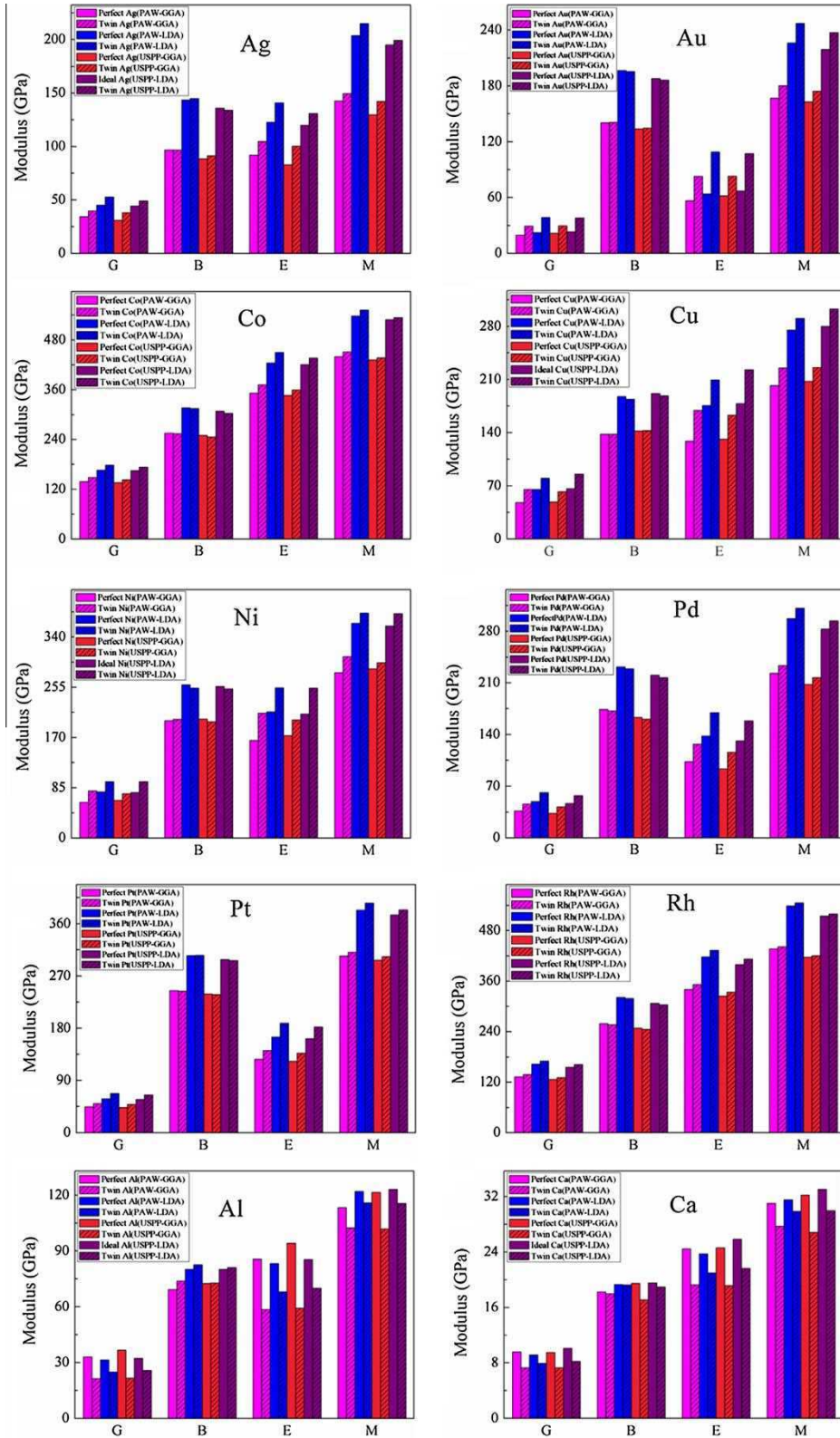


Fig. 2. The comparison of shear modulus (G), bulk modulus (B), Young's modulus (E) and longitudinal modulus (M) for the ten FCC metals' perfect crystals and twin crystals with PAW-GGA, PAW-LDA, USPP-GGA, USPP-LDA potential functions.

$$G = (\bar{C}_{11} - \bar{C}_{12} + 3\bar{C}_{44})/5 \quad (1)$$

$$E = 9BG/(G + 3B) \quad (2)$$

$$M = B + 4G/3 \quad (3)$$

In Formula (1), $\bar{C}_{11} = (C_{11} + C_{22} + C_{33})/3$, $\bar{C}_{12} = (C_{12} + C_{13} + C_{23})/3$, $\bar{C}_{44} = (C_{44} + C_{55} + C_{66})/3$. Considering the above variation trend of elastic constants C_{ij} and hence their combination \bar{C}_{11} , \bar{C}_{12}

Table 3

The shear modulus (G), bulk modulus (B), Young's modulus (E) and longitudinal modulus (M) of twin Cu with four different twin thickness (i.e. $\lambda_1 = 6.355 \text{ \AA}$, $\lambda_2 = 12.671 \text{ \AA}$, $\lambda_3 = 19.006 \text{ \AA}$, $\lambda_4 = 25.341 \text{ \AA}$) by using PAW-GGA and PAW-LDA potential functions.

Modulus Potential	Shear modulus (GPa)		Bulk modulus (GPa)		Young's modulus (GPa)		Longitudinal modulus (GPa)	
	PAW-GGA	PAW-LDA	PAW-GGA	PAW-LDA	PAW-GGA	PAW-LDA	PAW-GGA	PAW-LDA
Twin Cu ($\lambda_1 = 6.355 \text{ \AA}$)	65.39	79.86	137.95	183.99	169.40	209.29	225.13	290.47
Twin Cu ($\lambda_2 = 12.671 \text{ \AA}$)	63.01	76.12	138.94	186.50	164.21	201.00	222.95	287.99
Twin Cu ($\lambda_3 = 19.006 \text{ \AA}$)	55.00	73.37	137.04	185.99	145.53	194.57	210.38	283.85
Twin Cu ($\lambda_4 = 25.341 \text{ \AA}$)	48.84	71.94	137.74	188.14	131.04	191.41	202.87	282.06

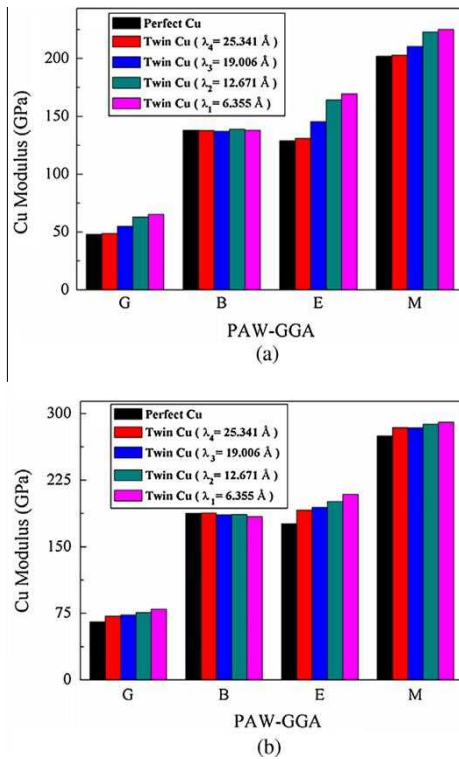


Fig. 3. The comparison of shear modulus (G), bulk modulus (B), Young's modulus (E) and longitudinal modulus (M) for perfect and twin Cu with different twin thickness; (a) PAW-GGA and (b) PAW-LDA.

and \bar{C}_{44} , it is no wonder that the shear modulus (G) of twin crystals is increased (decreased) compared to their perfect counterparts for Ag, Au, Co, Cu, Ni, Pd, Pt and Rh (for Al and Ca). Based on Formulas (2) and (3), the Young's modulus (E) and longitudinal modulus (M) have the same variation trend with the shear modulus (G), since the bulk modulus (B) is almost unchanged. Therefore, although these metals belong to the same FCC structures, the influences of their twin crystals on the elastic properties are still different.

To further understand the mechanisms of the twin induced elastic stiffness' variation, the structural properties of the ten FCC metals' corresponding perfect crystals and twin crystals have been analyzed. The near-neighbor atomic spacing and bond angle for the ten FCC metals' perfect crystals and twin crystals are summarized in Table 4. Here we also take Cu as an example to explore this issue, as can be seen that the near-neighbor atomic spacing for perfect Cu is only one type (hereafter denoted as d), while for twin Cu it can be classified into two categories (hereafter denoted as d_1 and d_2), as it is reflected in Fig. 1; one is smaller than that in perfect Cu, and the other is larger than that in perfect Cu (i.e. $d_1 < d$ and $d_2 > d$). Furthermore, the bond angles in twin Cu are classified into three categories (hereafter denoted as α_1 , α_2 and α_3), while it is only one type in perfect Cu (hereafter denoted as α); it is noteworthy that in twin Cu, these angles are either larger, smaller or equal to those in perfect Cu (namely, $\alpha_3 > \alpha$, $\alpha_1 < \alpha$ and $\alpha_2 = \alpha$). And this variation trend does not change with different potential functions (PAW-GGA, PAW-LDA, USPP-GGA and USPP-LDA). These research findings indicated that the structure's variation accompanied by the changes in near-neighbor atomic spacing and bond angle. Indeed, the elastic stiffness of a material can be reflected through its structural properties [33,39]. Therefore, the influences of twin

Table 4

The nearest neighbor atomic distance (d), bond angle (α) and mass density (ρ) of the ten FCC metals' perfect crystal and twin crystal with PAW-GGA, PAW-LDA, USPP-GGA, USPP-LDA potential functions.

	d (Å)				α (°)				ρ (g/cm ³)			
	PAW-GGA	PAW-LDA	USPP-GGA	USPP-LDA	PAW-GGA	PAW-LDA	USPP-GGA	USPP-LDA	PAW-GGA	PAW-LDA	USPP-GGA	USPP-LDA
Perfect Ag	$d = 2.9358$	$d = 2.8359$	$d = 2.9518$	$d = 2.8492$	$\alpha = 60.000$	$\alpha = 60.000$	$\alpha = 60.000$	$\alpha = 60.000$	10.011	11.107	9.849	10.952
Twin Ag	$d_1 = 2.9357$ $d_2 = 2.9388$	$d_1 = 2.8326$ $d_2 = 2.8368$	$d_1 = 2.9502$ $d_2 = 2.9526$	$d_1 = 2.8439$ $d_2 = 2.8478$	$\alpha_1 = 59.741$ $\alpha_2 = 60.000$ $\alpha_3 = 60.130$	$\alpha_1 = 59.884$ $\alpha_2 = 60.000$ $\alpha_3 = 60.058$	$\alpha_1 = 59.838$ $\alpha_2 = 60.000$ $\alpha_3 = 60.081$	$\alpha_1 = 59.963$ $\alpha_2 = 60.000$ $\alpha_3 = 60.019$	10.045	11.134	9.881	10.984
Perfect Au	$d = 2.9520$	$d = 2.8711$	$d = 2.9634$	$d = 2.8789$	$\alpha = 60.000$	$\alpha = 60.000$	$\alpha = 60.000$	$\alpha = 60.000$	17.98	19.545	17.774	19.385
Twin Au	$d_1 = 2.9445$ $d_2 = 2.9528$	$d_1 = 2.8651$ $d_2 = 2.8747$	$d_1 = 2.9549$ $d_2 = 2.9615$	$d_1 = 2.8701$ $d_2 = 2.8797$	$\alpha_1 = 59.900$ $\alpha_2 = 60.000$ $\alpha_3 = 60.050$	$\alpha_1 = 59.876$ $\alpha_2 = 60.000$ $\alpha_3 = 60.062$	$\alpha_1 = 59.997$ $\alpha_2 = 60.000$ $\alpha_3 = 60.012$	$\alpha_1 = 59.992$ $\alpha_2 = 60.000$ $\alpha_3 = 60.004$	18.033	19.559	17.838	19.406
Perfect Co	$d = 2.4439$	$d = 2.3864$	$d = 2.4584$	$d = 2.3975$	$\alpha = 60.000$	$\alpha = 60.000$	$\alpha = 60.000$	$\alpha = 60.000$	9.481	10.184	9.314	10.042
Twin Co	$d_1 = 2.4378$ $d_2 = 2.4430$	$d_1 = 2.3799$ $d_2 = 2.3853$	$d_1 = 2.4475$ $d_2 = 2.4488$	$d_1 = 2.3860$ $d_2 = 2.3882$	$\alpha_1 = 59.943$ $\alpha_2 = 60.000$ $\alpha_3 = 60.114$	$\alpha_1 = 59.939$ $\alpha_2 = 60.000$ $\alpha_3 = 60.123$	$\alpha_1 = 59.790$ $\alpha_2 = 60.000$ $\alpha_3 = 60.419$	$\alpha_1 = 59.786$ $\alpha_2 = 60.000$ $\alpha_3 = 60.428$	9.477	10.181	9.349	10.068
Perfect Cu	$d = 2.5706$	$d = 2.4901$	$d = 2.5754$	$d = 2.4949$	$\alpha = 60.000$	$\alpha = 60.000$	$\alpha = 60.000$	$\alpha = 60.000$	8.785	9.665	8.736	9.609
Twin Cu	$d_1 = 2.5764$ $d_2 = 2.5809$	$d_1 = 2.4894$ $d_2 = 2.4942$	$d_1 = 2.5749$ $d_2 = 2.5776$	$d_1 = 2.4900$ $d_2 = 2.4940$	$\alpha_1 = 59.499$ $\alpha_2 = 60.000$ $\alpha_3 = 60.251$	$\alpha_1 = 59.922$ $\alpha_2 = 60.000$ $\alpha_3 = 60.039$	$\alpha_1 = 59.963$ $\alpha_2 = 60.000$ $\alpha_3 = 60.018$	$\alpha_1 = 59.912$ $\alpha_2 = 60.000$ $\alpha_3 = 60.176$	8.788	9.644	8.726	9.589
Perfect Ni	$d = 2.4859$	$d = 2.4192$	$d = 2.4944$	$d = 2.4268$	$\alpha = 60.000$	$\alpha = 60.000$	$\alpha = 60.000$	$\alpha = 60.000$	8.975	9.738	8.883	9.646

(continued on next page)

Table 4 (continued)

	d (Å)				a (°)				ρ (g/cm ³)			
	PAW-GGA	PAW-LDA	USPP-GGA	USPP-LDA	PAW-GGA	PAW-LDA	USPP-GGA	USPP-LDA	PAW-GGA	PAW-LDA	USPP-GGA	USPP-LDA
Twin Ni	$d_1 = 2.4812$ $d_2 = 2.4888$	$d_1 = 2.4133$ $d_2 = 2.4214$	$d_1 = 2.4861$ $d_2 = 2.4872$	$d_1 = 2.4150$ $d_2 = 2.4220$	$a_1 = 59.988$ $a_2 = 60.000$ $a_3 = 60.006$	$a_1 = 59.974$ $a_2 = 60.000$ $a_3 = 60.053$	$a_1 = 59.768$ $a_2 = 60.000$ $a_3 = 60.464$	$a_1 = 59.801$ $a_2 = 60.000$ $a_3 = 60.399$	8.96	9.716	8.87	9.632
Perfect Pd	$d = 2.7511$	$d = 2.7222$	$d = 2.8049$	$d = 2.7310$	$a = 60.000$	$a = 60.000$	$a = 60.000$	$a = 60.000$	11.999	12.386	11.323	12.267
Twin Pd	$d_1 = 2.7511$ $d_2 = 2.7512$	$d_1 = 2.7060$ $d_2 = 2.7188$	$d_1 = 2.7804$ $d_2 = 2.7912$	$d_1 = 2.7081$ $d_2 = 2.7206$	$a_1 = 59.999$ $a_2 = 60.000$ $a_3 = 60.001$	$a_1 = 59.918$ $a_2 = 60.000$ $a_3 = 60.362$	$a_1 = 59.602$ $a_2 = 60.000$ $a_3 = 60.796$	$a_1 = 59.679$ $a_2 = 60.000$ $a_3 = 60.642$	12	12.363	11.31	12.26
Perfect Pt	$d = 2.8181$	$d = 2.7619$	$d = 2.8223$	$d = 2.7656$	$a = 60.000$	$a = 60.000$	$a = 60.000$	$a = 60.000$	20.471	21.746	20.379	21.66
Twin Pt	$d_1 = 2.8025$ $d_2 = 2.8279$	$d_1 = 2.7477$ $d_2 = 2.7725$	$d_1 = 2.7972$ $d_2 = 2.8242$	$d_1 = 2.7444$ $d_2 = 2.7694$	$a_1 = 59.807$ $a_2 = 60.000$ $a_3 = 60.096$	$a_1 = 59.735$ $a_2 = 60.000$ $a_3 = 60.133$	$a_1 = 59.906$ $a_2 = 60.000$ $a_3 = 60.189$	$a_1 = 59.972$ $a_2 = 60.000$ $a_3 = 60.056$	20.439	21.723	20.35	21.64
Perfect Rh	$d = 2.7176$	$d = 2.6625$	$d = 2.7275$	$d = 2.6706$	$a = 60.000$	$a = 60.000$	$a = 60.000$	$a = 60.000$	12.04	12.803	11.909	12.688
Twin Rh	$d_1 = 2.7028$ $d_2 = 2.7170$	$d_1 = 2.6488$ $d_2 = 2.6621$	$d_1 = 2.7059$ $d_2 = 2.7182$	$d_1 = 2.6492$ $d_2 = 2.6616$	$a_1 = 59.921$ $a_2 = 60.000$ $a_3 = 60.158$	$a_1 = 59.917$ $a_2 = 60.000$ $a_3 = 60.166$	$a_1 = 59.808$ $a_2 = 60.000$ $a_3 = 60.384$	$a_1 = 59.809$ $a_2 = 60.000$ $a_3 = 60.383$	12.038	12.794	11.957	12.736
Perfect Al	$d = 2.8634$	$d = 2.8208$	$d = 2.8586$	$d = 2.8136$	$a = 60.000$	$a = 60.000$	$a = 60.000$	$a = 60.000$	2.699	2.823	2.713	2.845
Twin Al	$d_1 = 2.8564$ $d_2 = 2.8811$	$d_1 = 2.8122$ $d_2 = 2.8350$	$d_1 = 2.8510$ $d_2 = 2.8743$	$d_1 = 2.8049$ $d_2 = 2.8269$	$a_1 = 59.545$ $a_2 = 60.000$ $a_3 = 60.227$	$a_1 = 59.589$ $a_2 = 60.000$ $a_3 = 60.206$	$a_1 = 59.582$ $a_2 = 60.000$ $a_3 = 60.209$	$a_1 = 59.608$ $a_2 = 60.000$ $a_3 = 60.196$	2.689	2.818	2.705	2.841
Perfect Ca	$d = 3.9089$	$d = 3.7492$	$d = 3.8789$	$d = 3.7427$	$a = 60.000$	$a = 60.000$	$a = 60.000$	$a = 60.000$	1.576	1.786	1.613	1.795
Twin Ca	$d_1 = 3.9324$ $d_2 = 3.9381$	$d_1 = 3.7679$ $d_2 = 3.7737$	$d_1 = 3.9033$ $d_2 = 3.9093$	$d_1 = 3.7595$ $d_2 = 3.7656$	$a_1 = 59.480$ $a_2 = 60.000$ $a_3 = 60.260$	$a_1 = 59.659$ $a_2 = 60.000$ $a_3 = 60.171$	$a_1 = 59.470$ $a_2 = 60.000$ $a_3 = 60.265$	$a_1 = 59.736$ $a_2 = 60.000$ $a_3 = 60.132$	1.561	1.766	1.596	1.775

crystals on the elastic properties of FCC metals can be primarily attributed to the twin crystals induced structural changes. And further investigations of the microcosmic mechanism along this direction are still in progress.

4. Conclusion

In summary, the influences of twin crystals on the elastic properties of ten FCC metals have been studied by using first-principles method. The results indicated that the shear modulus, Young's modulus and longitudinal modulus of twin crystals are higher than those of the corresponding perfect crystals for most of the FCC metals studied here, including Ag, Au, Co, Cu, Ni, Pd, Pt and Rh; whereas they are lower than those of the perfect crystals for Al and Ca. Meanwhile, their bulk modulus is almost unaffected for the ten FCC metals studied here. Furthermore, in the case of twin enhanced elastic stiffness, the shear modulus, Young's modulus and longitudinal modulus of twin Cu increase with the decreasing of twin thickness; and the effect of twin crystals on FCC metals' elastic modulus is limited. The mechanism of the twin crystals induced variation on elastic stiffness is due to the twin induced structural change. Our investigations imply that twins cannot always enhance the elastic stiffness of FCC metals, and hence further clarify the fact that twin boundary enhancing elastic stiffness of materials is not a universal law.

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