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Computer simulation of symmetrical tilt grain boundaries in noble metals with MAEAM*

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This paper reports that an atomic scale study of [$\bar{1}$10] symmetrical tilt grain boundary (STGB) has been made with modified analytical embedded atom method (MAEAM) for 44 planes in three noble metals Au, Ag and Cu. For each metal, the energies of two crystals ideally joined together are unrealistically high due to very short distance between atoms near the grain boundary (GB) plane. A relative slide between grains in the GB plane results in a significant decrease in GB energy and a minimum value is obtained at specific translation distance. The minimum energy of Cu is much higher than that of Ag and Au, while the minimum energy of Ag is slightly higher than that of Au. For all the three metals, the three lowest energies correspond to identical (111), (113) and (331) boundary successively for two translations considered; from minimization of GB energy, these boundaries should be preferable in [$\bar{1}$10] STGB for noble metals. This is consistent with the experimental results. In addition, the minimum energy increases with increasing reciprocal planar coincidence density Σ, but decreases with increasing relative interplanar distance d/a.

Keywords: noble metals, STGB, grain boundary energy, translation, MAEAM
PACC: 6170N, 6848, 6170Y

1. Introduction

The structure and energy of grain boundary (GB) have always been one of the great interesting subjects,[1−5] because many phenomena, such as diffusion,[6,7] grain boundary sliding and rotation,[8,9] segregation,[10] precipitation,[11] corrosion[12,13] and fracture[14−16] are directly influenced by them.

Following density-functional theory, Daw and Baskes developed a semi-empirical means termed as embedded atom method (EAM).[17,18] In contrast to central-force potential in which only the potential energy of a system is considered, the EAM presents the energy of atom in a system as a sum of electrostatic interactions with each of its near neighbours and an energy to embed an atom in a local electron density created by its near neighbours. It is believed that a many-body effect sensitive to the local environment of atoms makes the accurate treatment of defective structures,[19] such as surfaces,[20−22] interfaces[23−25] and GB.[26−28] Thereafter, Johnson and co-workers developed analytical EAM (AEAM) for FCC, BCC and HCP metals and calculated the dilute-limit heat of solution and heat of formation for FCC alloys.[29−32] However, in both EAM and AEAM the angle dependence of the atomic electron density in crystal is not considered. Zhang *et al*[33−36] added the energy modification corresponding to the higher order term of electron density to AEAM and developed modified AEAM (MAEAM).

In this paper, the energies of [$\bar{1}$10] symmetrical tilt grain boundary (STGB) have been calculated with MAEAM for 44 (hhk) GB planes in three noble metals Au, Ag and Cu which share the similar electronic structure. For each metal, the energies of two crystals ideally joined together are unrealistically high. A relative slide in GB plane results in a significant decrease in energy for every (hhk) GB plane and a minimum value is obtained at specific translation distance. For all the three metals, the three lowest energies correspond to identical (111), (113) and (331) boundary successively for both translations considered; from energy minimization, these boundaries should be prefer-

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able in [$\bar{1}$10] STGB. This is consistent with the experimental results of the thermal grooving[37,38] and rotating-sphere-on-a-plate.[39−44] The minimum energy increases with increasing reciprocal planar coincidence density Σ but decreases with increasing relative interplanar distance d/a.

2. MAEAM and potential for noble metals

In the MAEAM, the total energy of a system $E_{\rm total}$ is expressed as[36]

$$E_{\rm total} = \sum_i F(\rho_i) + \frac{1}{2}\sum_i \sum_{j(\neq i)} \varphi(r_{ij}) + \sum_i M(P_i), \quad (1)$$

$$\rho_i = \sum_{j(\neq i)} f(r_{ij}), \quad (2)$$

$$P_i = \sum_{j(\neq i)} f^2(r_{ij}), \quad (3)$$

where $E_{\rm total}$ is the total energy of the system, $F(\rho_i)$ is the energy to embed atom i in its site with electron density ρ_i given by a linear superposition of spherical averaged atomic electron density of the other atoms $f(r_{ij})$, r_{ij} is the separation distance of atom j from atom i, $\varphi(r_{ij})$ is the interaction potential between atoms i and j, and $M(P_i)$ is the modified term, which describes the energy change due to non-spherical distribution of electrons (P_i) and deviation from the linear superposition of atomic electronic density. Embedding function $F(\rho_i)$, pair potential $\varphi(r_{ij})$, modified term $M(P_i)$, and atomic electron density $f(r_{ij})$ take the following forms:[36]

$$F(\rho_i) = -F_0[1 - n\ln(\rho_i/\rho_{\rm e})](\rho_i/\rho_{\rm e})^n, \quad (4)$$

$$\varphi(r_{ij}) = k_0 + k_1(r_{ij}/r_{1\rm e})^2 + k_2(r_{ij}/r_{1\rm e})^4 + k_3(r_{1\rm e}/r_{ij})^{12}, \quad (5)$$

$$M(P_i) = \alpha(P_i/P_{\rm e} - 1)^2 \exp[-(P_i/P_{\rm e} - 1)^2], \quad (6)$$

$$f(r_{ij}) = f_{\rm e}(r_{1\rm e}/r_{ij})^6, \quad (7)$$

where subscript e indicates equilibrium and $r_{1\rm e}$ is the first nearest neighbour distance at equilibrium. In this paper, the electron density at equilibrium $f_{\rm e}$ is chosen as[34]

$$f_{\rm e} = [(E_{\rm c} - E_{1\rm f})/\Omega]^{3/5}, \quad (8)$$

where $\Omega = a^3/4$ is the atomic volume in FCC metals, a is lattice constant.

Eight parameters F_0, n, k_0, k_1, k_2, k_3, α and $f_{\rm e}$ in the Eqs.(4–8) can be determined by fitting lattice constant a, cohesion energy $E_{\rm c}$, monovacancy formation energy $E_{1\rm f}$, and elastic constants C_{11}, C_{12} and C_{44} of specific metal. According to the principle that the energy vs separation distance curve fits the Rose equation,[45] we have

$$F_0 = E_{\rm c} - E_{1\rm f}, \quad (9)$$

$$n = \sqrt{\Omega(C_{11} + 2C_{12})(C_{11} - C_{12})/(216E_{1\rm f}C_{44})}, \quad (10)$$

$$\alpha = \Omega(C_{12} - C_{44})/32 - n^2F_0/8. \quad (11)$$

The potential parameters of FCC structures can be calculated with the following formulae:[36]

$$k_0 = -E_{1\rm f}/9 - \Omega(5481C_{44} + 2989C_{12} - 2989C_{11})/42840, \quad (12)$$

$$k_1 = \Omega(1311C_{44} + 939C_{12} - 939C_{11})/9520, \quad (13)$$

$$k_2 = \Omega(32C_{11} - 32C_{12} - 33C_{44})/1020, \quad (14)$$

$$k_3 = 8\Omega(9C_{44} - C_{11} + C_{12})/5355. \quad (15)$$

The cut-off function is taken from Ref.[33] and the potential terminates at $r_{\rm c} = r_{2\rm e} + \frac{3}{4}(r_{3\rm e} - r_{2\rm e})$, where $r_{2\rm e}$ and $r_{3\rm e}$ is the second and the third nearest neighbour distance at equilibrium respectively.

Substituting lattice constant a, cohesion energy $E_{\rm c}$, mono-vacancy formation energy $E_{1\rm f}$, and elastic constants C_{11}, C_{12} and C_{44} of the metals[36] listed in Table 1 into Eqs.(9)–(15), we obtain the parameters needed for energy calculation and list in Table 2. Substituting the values of $k_i (i = 0-3)$ into Eq.(5), we can obtain the interatomic potentials for the three metals and plot in Fig.1.

Table 1. Physical parameters of Au, Ag and Cu.[46,47]

Metals	a/Å	$E_{\rm c}$/eV	$E_{1\rm f}$/eV	C_{11}/GPa	C_{12}/GPa	C_{44}/GPa
Au	4.0788	3.93	0.90	186	157	42.0
Ag	4.0857	2.85	1.02	124	93.4	46.1
Cu	3.6147	3.54	1.14	168	121	75.4

Table 2. Calculated parameters of Au, Ag and Cu for MAEAM.

Metals	F_0/eV	f_e	n	α	k_0/eV	k_1/eV	k_2/eV	k_3/eV
Au	3.03	0.355750	0.433930	0.309718	−0.455208	0.309962	−0.047608	0.055280
Ag	1.83	0.262080	0.315890	0.134690	−0.514350	0.354890	−0.056640	0.061180
Cu	2.40	0.384444	0.276754	0.082182	−0.596568	0.424147	−0.071207	0.069632

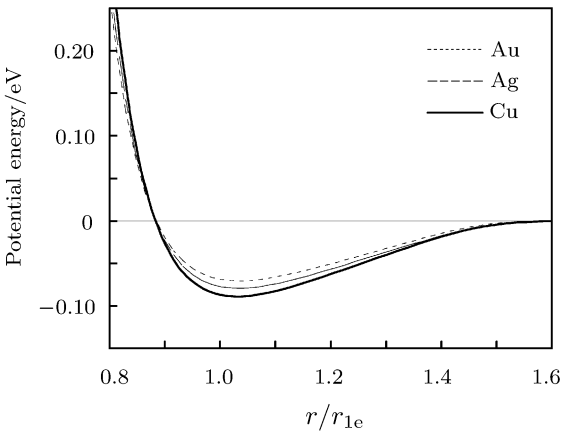


Fig.1. The interatomic potential of Au, Ag and Cu, r_{1e} is the first-nearest-neighbour distance at equilibrium.

To calculate GB energy, Eq.(1) can be rewritten simply as

$$E_{\text{total}} = \sum_i E_i, \tag{16}$$

in which

$$E_i = F(\rho_i) + \frac{1}{2}\sum_{j(\neq i)} \varphi(r_{ij}) + M(P_i)$$

is the energy contributed from atom i. GB energy is the superabundance relative to bulk material due to the existence of GB. Thus a contribution to the GB energy by atom i can be shown as $E_i - E_s$, here E_s is the sublimation energy for each atom in perfect crystal and equals to the negative value of cohesion energy E_c. Summing contributions of all atoms in GB and then dividing it by the area of GB plane A, we can get the GB energy density

$$E_{GB} = \frac{1}{A}\sum_{l=1}^{N}\sum_i (E_i^l - E_s), \tag{17}$$

where E_i^l is the energy of atom i on the lth lattice plane parallel to GB plane and N is the number of lattice planes in the boundary region.

3. GB structure

The structure of GB is a function of five macroscopic geometrical degrees of freedom, they can be defined as the rotation axis $\hat{n}_r$, the rotation angle θ and the GB plane normal $\hat{n}_p$. If $\hat{n}_r$ is perpendicular to $\hat{n}_p$, the GB is called a tilt boundary, in addition, if $\hat{n}_p$ is the same in both crystals, then the GB is a symmetrical tilt boundary. Thus only two macroscopic degrees of freedom are needed for STGB. As an example, Fig.2 shows a projection of the (221) STGB onto the $(\bar{1}10)$ plane, which can be regarded as crystal 2 (accompany with two basis vectors $[110]^{(2)}$ and $[001]^{(2)}$ in $(\bar{1}10)$ plane) rotating an angle $\theta = 2\tan^{-1}(\sqrt{2}/4) = 38.94°$ about common $\hat{n}_r = [\bar{1}10]$ axis with respect to crystal 1 (accompany with two basis vectors $[110]^{(1)}$ and $[001]^{(1)}$ in $(\bar{1}10)$ plane), where the atoms on two adjacent planes perpendicular to the tilt axis $\hat{n}_r = [\bar{1}10]$ are represented by open and solid symbols while the atoms in different crystals are distinguished by squares and circles respectively. The unit length is taken as $\sqrt{2}\,a/4$ and $a/2$ along the [110] and [001] direction respectively in both of the two coordinate systems.

Since a periodic boundary exists in the two directions parallel to the GB plane, two equivalent rectangular boxes could be selected with the GB plane as a bisector. For (221) STGB as shown in Fig.2, the periodic lengths in the GB plane are $\sqrt{2}\,a/2$ along the tilt axis and $L_{(221)} = 3\sqrt{2}\,a/2$ is perpendicular to the tilt axis, the shortest length of each box along the normal of GB plane could be chosen as r_c mentioned above, that is $r_c = r_{2e} + 3(r_{3e} - r_{2e})/4 = (2 + 3\sqrt{6}\,a)/8$, therefore each box has a volume of

$$\Big(\frac{\sqrt{2}}{2}a \times \frac{3\sqrt{2}}{2}a \times \frac{2+3\sqrt{6}}{8}a\Big).$$

This analysis could be extended to any arbitrary (hhk) STGB and the volume of each box is

$$\left(\frac{\sqrt{2}}{2}a \times \sqrt{h^2 + \Big(\frac{\sqrt{2}}{2}k\Big)^2}\,a \times \frac{2+3\sqrt{6}}{8}a\right).$$

For each (hhk) GB, the rotation angle θ is calculated by $\theta = 2\tan^{-1}(\sqrt{2}k/(2h))$, and reciprocal density of coincidence-site Σ (defined as the ratio of the primitive unit cell of the coincidence site lattice for the bicrystal to that of a single crystal lattice) by $(2h^2 + k^2)$, if $(2h^2 + k^2)$ is an even number, it should be divided by 2 until an odd number is reached. Calculated rotation angle θ, reciprocal density of coincidence-site Σ and relative interplanar spacing d/a are listed in Table 3 for 44 GB planes.

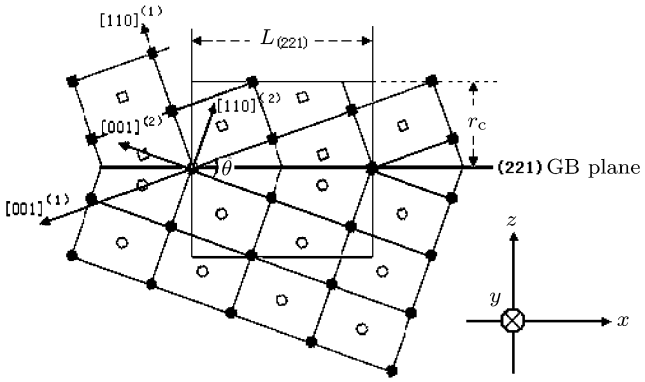


Fig.2. Projection plot of the (221) STGB onto ($\bar{1}10$) plane.

Table 3. Parameters and energies for noble metals in [$\bar{1}10$] STGB.

GB plane	$\theta/(^\circ)$	Σ	d/a	$l_{x\,\min}/L_x$	$E^x_{\min}/(\mathrm{J}\cdot\mathrm{m}^{-2})$			$E^y_{\min}/(\mathrm{J}\cdot\mathrm{m}^{-2})$		
					Au	Ag	Cu	Au	Ag	Cu
(111)	70.53	3	0.5774	0	0	0	0	0	0	0
(112)	109.47	3	0.2041	0.175	0.9938	1.0755	1.5629	2.3843	2.4819	3.5839
(113)	129.52	11	0.3015	0.475	0.2531	0.241	0.3342	0.3507	0.3376	0.4663
(114)	141.06	9	0.1179	0.775	2.6285	2.7634	4.0032	23.8381	25.5500	37.0631
(115)	148.41	27	0.1925	0.55	1.3020	1.2474	1.7619	3.2376	3.4059	4.9346
(116)	153.47	19	0.0811	0.50	3.2581	3.3822	4.8913	49.8959	53.9031	78.2717
(117)	157.16	51	0.1400	0.30	2.2199	2.2229	3.1857	13.7063	14.6146	21.2088
(118)	159.95	33	0.0615	0.50	3.4013	3.4768	5.0185	66.7447	72.2696	104.967
(119)	162.14	83	0.1098	0.50	2.8927	2.8908	4.1392	28.4949	30.6101	44.4413
(221)	38.94	9	0.1667	0.85	1.0744	0.9994	1.3819	6.7392	7.1076	10.2963
(223)	93.37	17	0.1213	0.80	1.3102	1.3061	1.8566	22.0214	23.4933	34.0648
(225)	121.01	33	0.0870	0.50	2.0775	2.135	3.063	45.0104	48.6318	70.6220
(227)	136.00	57	0.0662	0.625	3.0385	3.1437	4.5222	62.6338	67.8626	98.5755
(229)	145.11	89	0.0530	0.80	2.9979	3.1069	4.4816	74.2539	80.5255	116.977
(331)	26.53	19	0.2294	0.875	0.8631	0.8764	1.2484	1.3274	1.3045	1.8423
(332)	50.48	11	0.1066	0.50	2.5709	2.6512	3.8233	30.5741	32.8363	47.6693
(334)	86.63	17	0.0857	0.50	4.1851	4.2891	6.172	46.1781	49.7591	72.2398
(335)	99.37	43	0.1525	0.625	1.2534	1.2617	1.8032	9.8679	10.4577	15.1664
(337)	117.56	67	0.1222	0.175	1.6793	1.704	2.443	21.5521	23.0640	33.4484
(338)	124.12	41	0.0552	0.50	2.6438	2.7297	3.9286	72.3273	78.4283	113.926
(441)	20.05	33	0.0870	0.725	1.9880	2.0927	3.0337	45.0465	48.6694	70.6753
(443)	55.88	41	0.0781	0.70	1.8534	1.8872	2.7077	52.4838	56.6327	82.2305
(445)	82.95	57	0.0662	0.50	2.2483	2.3041	3.3149	62.6826	67.7632	98.4151
(447)	102.12	81	0.0556	0.275	2.7774	2.9143	4.2102	72.0398	78.0674	113.397
(449)	115.70	113	0.0470	0.375	3.6748	3.824	5.5129	79.5766	86.3054	125.362
(551)	16.10	51	0.1400	0.50	1.9468	1.9629	2.8068	13.7883	14.7323	21.3737
(552)	31.59	27	0.0680	0.50	2.4713	2.5391	3.6517	61.1065	66.1608	96.0931
(553)	45.98	59	0.1302	0.30	1.5635	1.6314	2.3582	17.7153	18.8675	27.3573
(554)	58.99	33	0.0615	0.85	2.1996	2.2356	3.2117	66.8280	72.2582	104.937
(556)	80.63	43	0.0539	0.50	2.1730	2.2129	3.1831	73.5031	79.5558	115.554
(557)	89.42	99	0.1005	0.925	2.1302	2.2163	3.202	34.7923	37.4111	54.3139
(558)	97.05	57	0.0468	0.15	2.3169	2.3702	3.4033	79.7666	86.4575	125.582
(559)	103.69	131	0.0874	0.50	1.8639	1.9546	2.8305	44.7665	48.3160	70.1544
(661)	13.44	73	0.0585	0.675	3.7807	3.9631	5.7317	69.4963	75.3155	109.392
(665)	61.02	97	0.0508	0.775	3.0004	3.1183	4.5029	76.3080	82.5979	119.968
(667)	79.04	121	0.0455	0.575	2.1034	2.149	3.0935	80.9807	87.6954	127.379

Table 3. (continued)

GB plane	$\theta/(^\circ)$	Σ	d/a	$l_{x\,\min}/L_x$	$E^x_{\min}/(\mathrm{J\cdot m^{-2}})$			$E^y_{\min}/(\mathrm{J\cdot m^{-2}})$		
					Au	Ag	Cu	Au	Ag	Cu
(771)	11.54	99	0.1005	0.70	2.6821	2.7564	3.9735	34.7761	37.5032	54.4585
(772)	22.84	51	0.0495	0.925	2.6377	2.7172	3.9096	77.4293	83.9671	121.965
(773)	33.72	107	0.0967	0.65	1.8620	1.9361	2.7915	37.5425	40.4842	58.7853
(774)	44.00	57	0.0468	0.875	2.2957	2.3726	3.417	79.7849	86.4772	125.610
(775)	53.59	123	0.0902	0.425	2.8599	2.9763	4.2917	42.5780	45.8669	66.5946
(776)	62.44	67	0.0432	0.80	2.2151	2.2372	3.2102	82.9831	89.8763	130.548
(778)	77.88	81	0.0393	0.10	2.1975	2.2371	3.2206	86.4433	93.6367	136.008
(779)	84.55	179	0.0747	0.225	2.2524	2.28	3.2639	55.2873	59.7124	86.7179

4. The minimum GB energy during translation parallel to GB plane

Initial calculations show that the energies corresponding to the STGB constructed directly by two crystals are unrealistically high, therefore such ideally joined configurations are unstable. As we know, relative slide between two adjacent grains plays an important role in deformation especially in nano-crystalline materials, so it is necessary to investigate the variation of GB energy during translation. For the convenience of description, as shown in Fig.2, another coordination system is chosen and taking the x-axis in GB plane and perpendicular to tilt axis, y-axis along tilt axis and z-axis along $[hhk]$ direction. Suppose crystal 1 translates along x- or y-axis (T_x or T_y) with respect to crystal 2, variations of GB energy with relative translation distances l_x/L_x and l_y/L_y ($L_x = \sqrt{h^2 + (\sqrt{2}k/2)^2}\,a$ and $L_y = \sqrt{2}\,a/2$ are the period length of the box along x- and y-axis respectively) have been investigated for all 44 STGB planes. The results show that, although GB energy changes with translation distance for each (hhk) GB plane, a minimum value of energy $E^x_{\min}$ and $E^y_{\min}$ respectively could be obtained at certain relative translation distance $l_{x\min}/L_x$ and $l_{y\,\min}/L_y$. It is interesting to note that, except for (111) and (113), the other 42 GB planes have the same $l_{y\,\min}/L_y$ value of 50% for translation along y-axis, so we only give their corresponding minimum energies $E^y_{\min}$ in the last three columns of Table 3 for Au, Ag and Cu respectively. As for translation along x-axis, the minimum energies $E^x_{\min}$ correspond to different values of $l_{x\min}/L_x$ for each metal, so the minimum energies $E^x_{\min}$ for Au, Ag, Cu and corresponding $l_{x\min}/L_x$ which is the same for three metals having the same FCC structure are listed in Table 3. In order to compare the effects of both translations on GB energy, Figs.3(a) and 3(b) plot the minimum GB energy versus rotation angle θ for translation along x- and y-axis respectively.

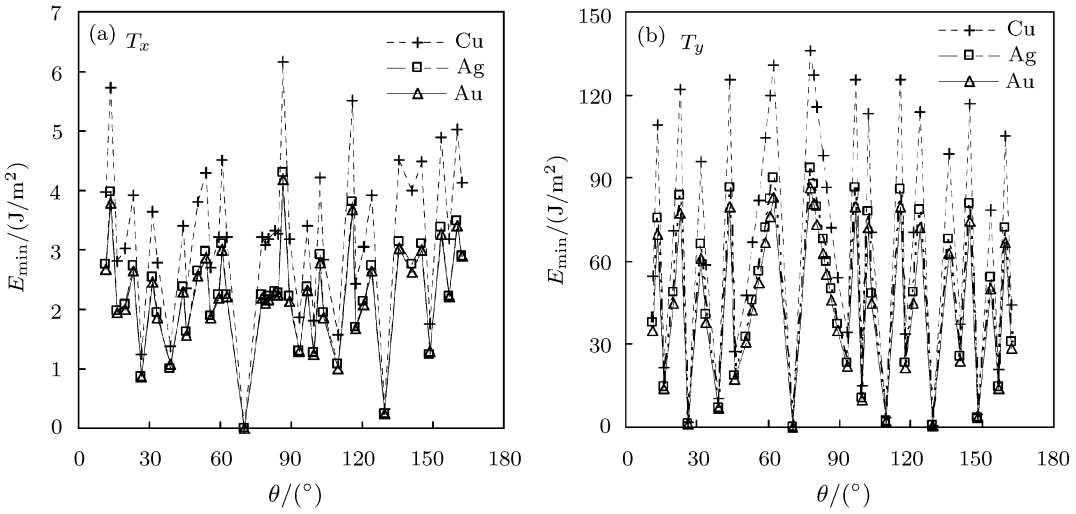


Fig.3. The minimum GB energy versus rotation angle θ.

It is noted that, firstly for various GB planes, the minimum energy of Cu is much higher than that of Ag and Au, while the minimum energy of Ag is slightly higher than that of Au. This is consistent with the calculated results of surface energy[22] and twist GB energy.[48] Secondly, for both translations in three metals, the three lowest energies correspond to identical (111), (113) and (331) boundary successively, and the minimum GB energies obtained from translation along the x-axis are much lower than that along the y-axis so we conclude that the main translation direction should be along the x-axis that is in the GB plane and perpendicular to tilt axis. The correlation between the minimum GB energy and reciprocal density of coincidence-site Σ is shown in Figs.4(a) and 4(b) respectively for translation along x- and y-axis in three metals, we can see that the energy increases oscillatorily with increasing Σ especially for small Σ. In addition, for GB planes with the same Σ in each metal, the minimum GB energy decreases with increasing relative interplanar distance d/a. This relation also exists in the other GB planes as shown in Figs.5(a) and 5(b) for translation along x- and y- axis respectively. This correlation was also obtained in our previous papers for Ag/Ni and Ag/Si interfaces[24,25] and [001] STGB in BCC metal Fe.[49]

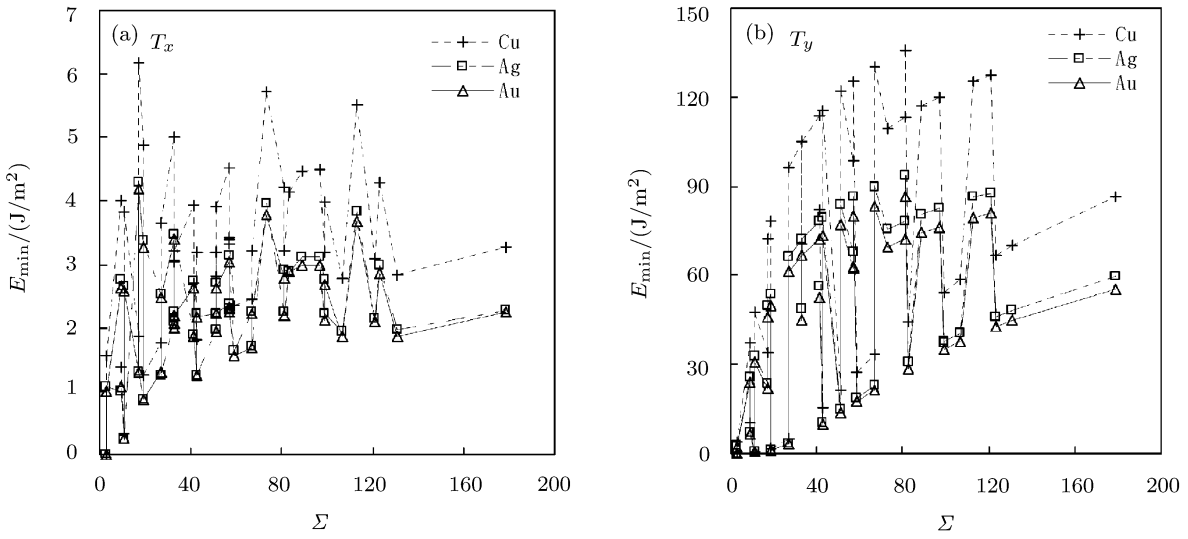


Fig.4. Correlation of GB energy with Σ.

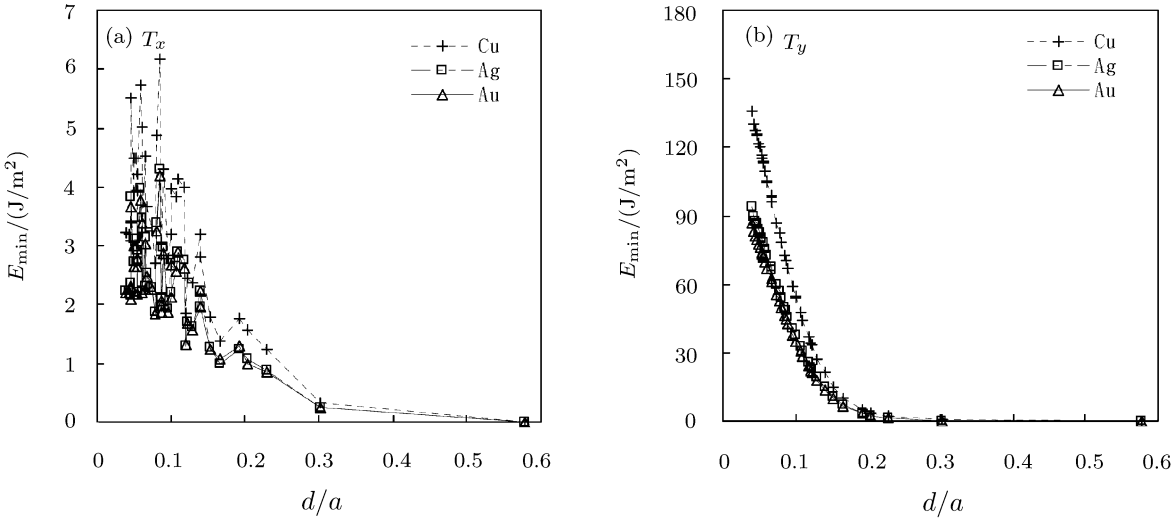


Fig.5. Variation of GB energy with interplanar distance d/a.

5. Conclusions

With MAEAM, the energies of [$\bar{1}$10] STGB have been calculated for 44 (hhk) GB planes in three noble metals Au, Ag and Cu. For each metal the energies of two crystals ideally joined together are unrealistically high, a relative slide between grains results in a significant decrease in GB energy especially for translation in GB plane and perpendicular to tilt axis. For various GB planes, the minimum energy of Cu is much higher than that of Ag and Au, while the minimum energy of Ag is slightly higher than that of Au. This is consistent with the calculated results of surface energy and twist GB energy. For both translations the three lowest energies correspond to identical (111), (113) and (331) boundary successively for all of the three metals, from minimization of GB energy, these boundaries (especially for translation along the x-axis) should be preferable in [$\bar{1}$10] STGB. This is consistent with the experimental results. In addition, the minimum energy increases with increasing reciprocal planar coincidence density Σ, but decreases with increase of interplanar spacing d/a. The latter correlation was also obtained in our previous papers for Ag/Ni and Ag/Si interfaces.

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