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First-principles Study on the Properties of GPBII (Al2CuMg) (001) and S (Al2CuMg) (001) Surfaces

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Abstract. Surface structure and electronic properties of (001) surfaces of GPBII and Sphase were studied by using first-principles calculations. The calculations are performed within the density functional framework using the projector augmented plane wave (PAW) method. For different terminations of GPBII and S, the results in the GGA-PW91 and GGA-PBE almost give the same description for relaxation of different layers, and the relaxation results in GGA-PW91 and GGA-PBE are more reliable in this calculation as compared with LDA.As compared the Total DOS of GPBII-Al(Cu)(001) termination surface and S-Al(Al)(001) termination surface, there are apparent differences on the height of main peak and the band district of the peak of density of states. The interaction of atoms in S-Al(Al)(001) termination surface is stronger than that of GPBII-Al(Cu)(001) termination surface.

Introduction

The high strength Al-Cu-Mg alloys with improved toughness and fatigue resistance properties are primary structural materials used in the aircraft industry. Surface stress and surface energy have been identified as the decisive factors for the understanding of a wide variety of surface phenomena [1].The surface energy can supply an additional driving force for abnormal grain growth change after thermal treatments, therefore, the relaxation of the surfaces determine the equilibrium crystal shape of the crystals [2]. Therefore, a theoretical determination of the surface atomic structures and electronic properties is very significant. First-principles calculations are widely used in the study of surfaces and interfaces [3], providing much information that cannot be obtained by experiments. The purpose of the present work is to study the surface structure and electronic properties of (001) surfaces of GPBII and S phase, aiming to get information about surface structure relaxation and electronic density of states for different termination of these two phases.

Methodology

The calculations presented in this study were carried out using the Vienna ab initio simulation package (VASP) based on density functional theory with projector-augmented wave (PAW) pseudo potential method[4,5].The Perdew-Wang[6](GGA-PW91), Perdew-Burke-Ernzerh of [7](PBE) and the local-density approximations[8](LDA) are used for the exchange-correlation functions. A conjugate-gradient algorithm was used to relax the ions into their ground states, the energies and the forces on each ion were converged within 1.0 ×10-5eV/atom and 0.02eV/Å respectively. The kinetic energy cutoff of 350eV was used throughout, and the surfaces were described in the framework of the slab model and a 6×6×1 grid in the Brillouin zone as proposed by Monk horst and Pack [9] was used for the slab structure. A Gaussian broadening of 0.05eV was chosen and all values were obtained at 0 K. During the surface structure optimization, the outermost three layer atoms of both sides are relaxed and the central layer atoms are fixed.

To assess the accuracy of our computation method, in particular, of the pseudo potentials used, we performed a series of calculations on the bulk properties of Ω phase. A6×6×6 grid was adopted for optimization of the bulk Ω phase, and the obtained lattice constants are in good agreement with

experimental value. The lattice parameters, cohesive energies and formation enthalpy are listed in Table 1.Overall, the methods of simulation and the calculation parameters are reliable.

Table 1 Lattice parameters (in Å), cohesive energy Ecoh (in eV atom^{-1}) and bond length (in A °) of GPBII and S phase

		Lattice constant(nm)	Cohesive energy(eV)	Formation enthalpy(eV)
GP BII	Exp.	a=0.405nm, c=0.810nm	4.26	0.1564
	LDA	a=0.398nm, c=0.775nm	4.38	-0.1064
	GGA	a=0.406nm, c=0.791nm	4.15	0.0433
	PBE	a=0.406nm, c=0.791nm	4.05	- 0.3468
S	Exp.	a=0.400nm, b=0.923nm,c=0.714nm	8.35	0.3535
	LDA	a=0.392nm, b=0.908nm,c=0.702nm	8.53	0.3190
	GGA	a=0.402nm, b=0.926nm,c=0.714nm	8.22	0.4907
	PBE	a=0.402nm, b=0.926nm,c=0.714nm	8.00	0.0526

Surface Properties

Surface Structure Relaxations

The results of surface relaxation as a function of slab thickness for GPBII-Mg(Al)(001) termination and S-Al(Al)(001) termination are listed in Table 2 and Table 3, respectively. From these results, it can be seen that when the slab thickness is increased, the interlayer distance is gradually converged. It appears that 13 and 14 layers for GPBII-Mg(Al)(001) termination and S-Al(Al)(001) termination are thick enough to make interlayer thickness converge, which implies that the two slabs with more than 13 and 14 layers posses the bulk-like characteristic interiors and guarantee the reliability of the surface investigation.

Table 2 GPBII-Mg(Al)(001) termination surface relaxation as a function of slab thickness (Δij represents the change of the interlayer spacing as a percentage of the bulk spacing)

Interlayer	Slab thickness, n				
	5	9	13	17	21
Δ12	16.20%	17.29%	16.91%	18.00%	20.80%
Δ23	-14.57%	-15.20%	-14.59%	-14.20%	-14.94%
Δ34	——	-12.74%	-12.19%	-10.73%	-9.38%

Table 3 S-Al(Al)(001) termination surface relaxation as a function of slab thickness (Δij represents the change of the interlayer spacing as a percentage of the bulk spacing)

Interlayer	Slab thickness, n			
	8	11	14	17
Δ12	-22.75%	-20.39%	-19.51%	-21.52%
Δ23	11.57%	12.13%	12.12%	11.31%
Δ34	-0.80%	0.13%	-0.48%	1.41%

The relaxation of the outermost three layer atoms of GPBII(001) and S(001) surfaces for different terminations in GGA-PW91, GGA-PBE and LDA are shown in Table 4. It can be seen that there are apparent variations in the surface structures caused by relaxation. It can also be seen that for different terminations of GPBII and S, the results in the GGA-PW91 and GGA-PBE almost give the same description for relaxation of different layers.

Table 4 Surface relaxation for different terminations of GPBII and S calculated by different pseudo potential (ΔZm is a measurement of the distance of the mth layer moves as a percentage of the interlayer spacing, and Δij is a measurement of the relaxation of the distance between the ith and jth layers).

Surface		Δz1	Δz2	Δz3	Δ12	Δ23	Δ34
GPBII	PBE	0.1436	-0.5767	-0.2705	-36.42%	15.48%	13.68%
Cu(Al)	GGA	0.1568	-0.5961	-0.2821	-38.07%	15.88%	14.27%
(001)	LDA	0.1945	-0.3660	-0.1556	-28.35%	10.64%	7.87%
GPBII	PBE	0.2195	-0.0496	-0.3896	-13.61%	-17.19%	19.70%
Al(Cu)	GGA	0.2357	-0.0229	-0.3706	-13.08%	-17.58%	18.74%
(001)	LDA	0.3045	-0.0220	-0.3990	-16.51%	-19.06%	20.18%
GPBII	PBE	0.1952	0.5295	0.2410	16.91%	-14.59%	-12.19%
Mg(Al)	GGA	0.1889	0.5448	0.2633	18.00%	-14.24%	-13.31%
(001)	LDA	0.3326	0.6565	0.3155	16.38%	-17.25%	-15.95%
GPBII	PBE	0.2533	0.0492	0.3553	-10.32%	15.48%	-17.97%
Al(Mg)	GGA	0.2674	0.0465	0.3599	-11.17%	15.85%	-18.20%
(001)	LDA	0.4154	-0.0465	0.3204	-23.84%	18.93%	-16.54%
S	PBE	0.0400	-0.1858	-0.0217	-17.71%	11.84%	2.62%
Al(CuMg)	GGA	0.0403	-0.2016	-0.0267	-19.71%	12.62%	3.34%
(001)	LDA	0.0195	-0.1128	0.0251	-9.55%	9.95%	-3.14%
S	PBE	0.0734	-0.1014	0.0155	-18.70%	14.61%	-1.17%
CuMg(Al)	GGA	0.0825	-0.1081	0.0167	-20.50%	15.61%	-1.21%
(001)	LDA	0.0294	-0.0647	0.0580	-6.79%	15.33%	-4.19%
S	PBE	0.0209	-0.1613	0.0066	-16.51%	12.12%	-0.48%
Al(Al)	GGA	0.0229	-0.1762	-0.0115	-18.90%	11.89%	0.83%
(001)	LDA	0.0430	-0.1065	0.0227	-18.69%	9.33%	-1.64%

Electronic Structure of the Surface

Analysis of total density of states (TDOS) and partial density of states (PDOS) of GPBII-Al(Cu)(001) termination surface and S-Al(Al)(001) termination surface are performed to understand their respective bonding characteristics, as shown in Fig.1 and Fig.2.

It can be seen from the Total DOS of Fig.1 that there is no band gap between the conduction bands and the valence bands, so that pure GPBII and S phase have metallic properties. As compared the Total DOS of GPBII-Al(Cu)(001) termination surface and S-Al(Al)(001) termination surface, there are apparent differences on the height of main peak and the band district of the peak of density of states. From Fig. 2 we can see that there is a stronger hybridization of the Al(p),Cu(s),Cu(d)and Mg(s)states at the main peak in S-Al(Al)(001) termination surface, compared with that of the

GPBII-Al(Cu)(001) termination surface. So the interaction of atoms in S-Al(Al)(001) termination surface is stronger than that of GPBII-Al(Cu)(001) termination surface.

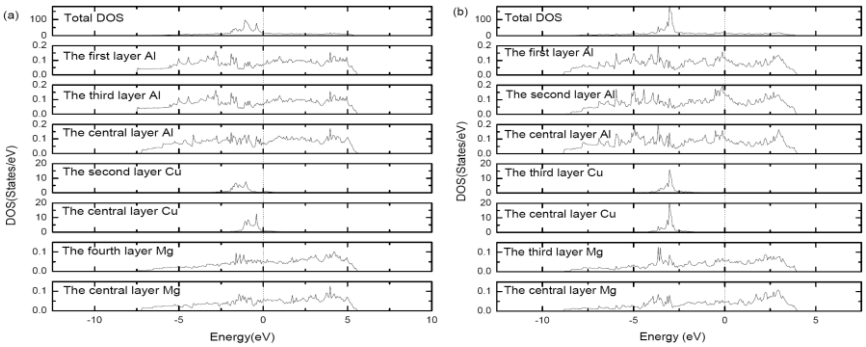

Fig.1. Total DOSs for surfaces and atoms: (a) GPBII-Al(Cu)(001) termination surface; (b) S-Al(Al)(001) termination surface

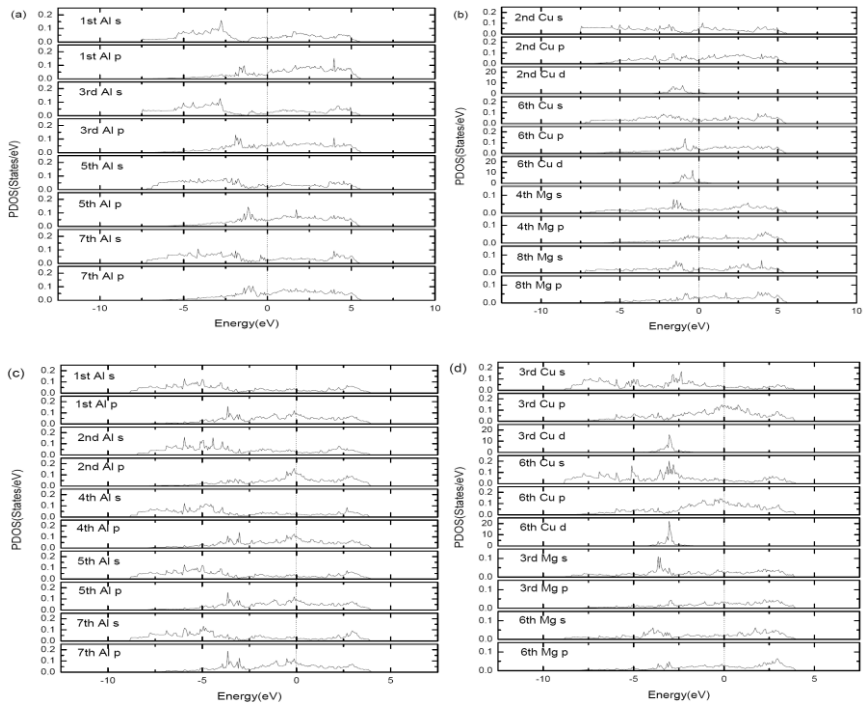

Fig.2. Partial DOSs for each layer of (a) Al atoms in GPBII-Al(Cu)(001) termination surface; (b) Cu and Mg atoms in GPB-Al(Cu)(001) termination surface;(c) Al atoms in S-Al(Al)(001) termination; (d) Cu and Mg atoms in S-Al(Al)(001) termination.

It can be seen from Fig.1(a) and Fig.2(a)(b) that the main bonding peak focus on the energy between -3eV and -1eV.The bonding peak mainly originate from the contribution of valence electrons of Al(p), Cu(p), Cu(d) and Mg(s) orbits. The PDOS of Cu(d) is localized and forms the greatest contribution to the TDOS of GPBII-Al(Cu)(001) termination surface. It can also be seen from Fig.1(b) and Fig.2(c)(d) that the main bonding peak focus on the energy between -4eV and -2eV.The bonding peak mainly originate from the contribution of valence electrons of Al(p), Cu(s), Cu(d) and Mg(s) orbits.

Conclusions

In summary, the geometric structure and electronic properties of the different terminated (001) surfaces of GPBII and S phase have been studied by using the first-principles calculations. The results are:

For different terminations of GPBII and S, the results in the GGA-PW91 and GGA-PBE almost give the same description for relaxation of different layers, and the relaxation results in GGA-PW91 and GGA-PBE are more reliable in this calculation as compared with LDA.

As compared the Total DOS of GPBII-Al(Cu)(001) termination surface and S-Al(Al)(001) termination surface, there are apparent differences on the height of main peak and the band district of the peak of density of states. The interaction of atoms in S-Al(Al)(001) termination surface is stronger than that of GPBII-Al(Cu)(001) termination surface.

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