

# On the First-principles Density Functional Theory Calculation of Electromigration Resistance Ability for Sn-based Intermetallic Compounds

Wen-Hwa Chen<sup>1,2</sup>, Ching-Feng Yu<sup>1</sup> and Hsien-Chie Cheng<sup>2,3</sup>

**Abstract:** The aim of the study is to investigate the interactions between Sn adatoms in a solder bump and three typical Sn-based intermetallic compounds (IMCs) surface, i.e.,  $\text{Cu}_3\text{Sn}$ ,  $\text{Cu}_6\text{Sn}_5$ , and  $\text{Ni}_3\text{Sn}_4$ , at the atomistic scale. The adsorption energy, average bond length, and bond population of the Sn/ $\text{Cu}_3\text{Sn}$ , Sn/ $\text{Cu}_6\text{Sn}_5$ , and Sn/ $\text{Ni}_3\text{Sn}_4$  systems are calculated through the first-principles density functional theory (DFT) calculation to investigate how the Sn adatoms influence the IMC surface. The calculated results show that the Sn atoms on the  $\text{Cu}_3\text{Sn}$  (0 0 1) surface hold the largest adsorption energy, average bond length and bond population, implying that the  $\text{Cu}_3\text{Sn}$  (0 0 1) surface is the most stable surface for Sn adatoms. Moreover, the electromigration resistance ability of three typical Sn-based IMCs can be further identified according to the nominal the adsorption energy, average bond length, and bond population, which are estimated through averaging the adsorption energy, average bond length, and bond population for the  $\text{Cu}_3\text{Sn}$ ,  $\text{Cu}_6\text{Sn}_5$  and  $\text{Ni}_3\text{Sn}_4$  IMCs at seven crystal surfaces, i.e., (1 0 0), (0 1 0), (0 0 1), (1 1 0), (1 0 1), (0 1 1) and (1 1 1). The results reveal that  $\text{Cu}_3\text{Sn}$  holds the best electromigration resistance ability, followed by  $\text{Ni}_3\text{Sn}_4$  and  $\text{Cu}_6\text{Sn}_5$ .

**Keywords:** Intermetallic compound, Density functional theory, Electromigration.

## 1 Introduction

The electromigration is a mass transport phenomenon, in which, metal atoms migrate along the direction of electron flux [Iwasaki and Miura (2003); Gerstle, Silling, Read, Tewary, and Lehoucq (2008)]. This directional diffusion would lead to the

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<sup>1</sup> Department of Power Mechanical Engineering, National Tsing Hua University, Hsinchu, Taiwan, ROC.

<sup>2</sup> Corresponding author.

<sup>3</sup> Department of Aerospace and Systems Engineering Feng Chia University, Taichung, Taiwan, ROC.

formation of hillocks at the anode side and voids at the cathode side of the solder. This phenomenon can induce the signal delay, distortion or even short-circuit failure for electronic component under long-firing operation, thereby leading to a decrease of the electronic component reliability. In addition, the current density can be significantly increased as dimension of the solder becomes smaller, thus resulting in a significant current crowding effect. The current effect is a nonhomogeneous distribution of current density, which can remarkably enhance the electromigration phenomenon of the solder.

The electromigration issue on the solder joints through experimental approach has been investigated. For example, Gan and Tu (2005) investigated the polarity effect of electromigration on kinetics of IMC formation at the anode and the cathode in solder. In the study, V-groove solder line samples, with width of 100  $\mu\text{m}$  and length of 500-700  $\mu\text{m}$ , were applied to study interfacial IMC growth between Cu electrodes and Sn-3.8Ag-0.7Cu solder under different current density and temperature settings. The result exhibited that growth of the IMC layer would be enhanced by electric current at the anode and inhibited at the cathode, and showed that the growth of IMC at the anode had a parabolic dependence on time and the growth rate increased with current density. Zhang, Ou, Huang, Tu, Gee, and Nguyen (2006) present that the Cu-Sn IMCs might have better electromigration resistance ability than the solder since electromigration voids generally form at the interface of solder and IMCs. Chae, Chao, Zhang, Im, and Ho (2007) proposed a numerical method based on simulated annealing to deduce diffusivities and effective charge numbers of Cu and Sn components in  $\text{Cu}_3\text{Sn}$  and  $\text{Cu}_6\text{Sn}_5$ . Chen and Huang (2008) pointed that  $\text{Ag}_3\text{Sn}$  phase could intercept the Bi migration from the cathode side to the anode side after Ag was doped into Sn-58Bi solder. Zhang, Guo, and Shang (2008) presented that an abnormal polarity effect would be observed after direct current was applied to the Cu/Sn-9Zn/Cu interconnect. The results further showed that IMC at the cathode side was thicker than that at the anode side, which was in contrast to the Cu/In/Cu and Cu/Sn-Pb/Cu interconnects [Yamanaka, Tsukada, and Suganuma (2007)]. Kumar, Yang, Wong, Kripesh, and Chen (2009) evaluated the effect of moderate electric current density on mechanical properties of Ni-P/Sn-3.5Ag/Ni-P and Ni/Sn-3.5Ag/Ni solder joints, and it was found that the electromigration induced brittle failure of the solder joints and this tendency for brittle failure increased with increasing current density. Chen, Huang, and Lin (2009) investigated the electromigration behavior of Cu/Sn-8Zn-3Bi/Cu interconnects. They found that Bi was the dominant migrating species but Sn and Zn were relatively immobile under EM at 80 °C. Wu, Chung, Chen, and Ho (2009) put their focus on evaluating the electromigration effect on the Cu-Ni cross-interaction in Cu/Sn/Ni diffusion couples and showed that the Cu-Ni crossinteraction strongly depended on

the direction of electron flow. Lin, Lin, and Chuang (2009) studied the electromigration behavior of Sn-3Ag-0.5Cu and Sn-3Ag-0.5Cu-0.5Ce-0.2Zn solder joints at room temperature with a current density of  $3.1 \times 10^4$  A/cm<sup>2</sup>. The evaluated results demonstrated that after doping with Zn and Ce, the electromigration process of Sn-Ag-Cu solder joints was accelerated due to the refinement of the solder matrix. Chen, Huang, and Zhou (2010) adopted the line-type Cu/Sn/Cu interconnections to determine the growth kinetics of interfacial IMCs under current densities ranging from  $5.0 \times 10^3$ - $1.0 \times 10^4$  A/cm<sup>2</sup> at 100 °C and 150 °C, respectively. The results showed that interfacial IMCs at the anode side were thicker than those at the cathode side. To further enhance the electromigration resistance ability, many elements, such as Cr [Cabral, Harper, Holloway, Smith, and Schad (1992); Sandberg and Holmestad (2006)], Al [Ding, Lanford, Hymes, and Murarka (1994)], Zr [Hu and Luther (1995)] and Ag [Menzel, Strehle, Wendrock, and Wetzig (2005)], had been added into Cu interconnection to increase the diffusion activation energy, thereby improving the electromigration resistance ability. Lee, Hu, and Tu (1995) found that the electromigration activation energy for Cu was 0.73 eV at temperature of 250-450 °C and current density of  $5.0 \times 10^5$ - $2.1 \times 10^6$  A/cm<sup>2</sup>. Nevertheless, the activation energy would increase to 0.95 eV, 1.25 eV and 1.14 eV after alloying Sn with concentrations of 0.5 wt%, 1.0 wt% and 2.0 wt%, respectively. Yan, Suh, Ren, Tu, Vairagar, Mhaisalkar, and Krishnamoorthy (2005) proposed that a 20 nm thick Cu<sub>3</sub>Sn IMC on the Cu surface would block the surface diffusion paths, thus resulting in an improvement of electromigration lifetime. Yu, Liu, Lu, and Chen (2007) performed first-principles calculation on evaluating Sn or Cu adatom/Cu (0 0 1), (0 1 0) and (1 1 1) surface systems within local density approximation. They found that the Sn/Cu system was more stable than Cu/Cu system based on the calculated adsorption energy, density of states and electron population analysis.

In literature, the electromigration behaviors of solder joints were well addressed by numerous studies, and the electromigration lifetime would be improved by doping metal elements, such as Cr, Al, Zr, and Ag, in the Cu interconnection. However, it is found that only few studies were made on quantifying the electromigration resistance ability of IMC. In other words, the IMC influence on the electromigration resistance ability of solder bump is not fully understood. Therefore, the alternation goal of the study is to investigate the interactions between Sn adatoms in a solder bump and three typical Sn-based IMCs surface, i.e., Cu<sub>3</sub>Sn, Cu<sub>6</sub>Sn<sub>5</sub>, and Ni<sub>3</sub>Sn<sub>4</sub>, at the atomistic scale. The adsorption energy, average bond length, and bond population of the Sn/Cu<sub>3</sub>Sn, Sn/Cu<sub>6</sub>Sn<sub>5</sub>, and Sn/Ni<sub>3</sub>Sn<sub>4</sub> systems are calculated through the first-principles DFT calculation to investigate how the Sn adatoms influence the IMC surface. These calculations could give guideline for interconnect materials design for an enhanced electromigration resistance ability.

## 2 Computational details

Seven crystal surfaces, namely (1 0 0), (0 1 0), (0 0 1), (1 1 0), (1 0 1), (0 1 1) and (1 1 1), are studied for each IMC (i.e.,  $\text{Cu}_3\text{Sn}$ ,  $\text{Cu}_6\text{Sn}_5$  and  $\text{Ni}_3\text{Sn}_4$ ). The surface slab size for  $\text{Cu}_3\text{Sn}$ ,  $\text{Cu}_6\text{Sn}_5$  and  $\text{Ni}_3\text{Sn}_4$  is  $2 \times 2 \times 1.5$ ,  $2 \times 2 \times 1$  and  $3 \times 3 \times 1.5$ , respectively, and vacuum region is 15 Å, as shown in Figs. 1-3. In specific, a  $2 \times 2$  surface unit cell with 1.5 slab unit cell thickness is chosen to model the adsorbed surface of  $\text{Cu}_3\text{Sn}$ . For  $\text{Cu}_6\text{Sn}_5$  and  $\text{Ni}_3\text{Sn}_4$ , the  $2 \times 2$  surface unit cell with 1 slab unit cell thickness and  $3 \times 3$  surface unit cell with 1 slab unit cell thickness are adopted, respectively. The periodic boundary condition is further imposed to the all IMC surface slab. The dimension of these models could ensure that the adatoms can fully relax on the IMC surface but at the same time the computational cost would also be effectively reduced.

In the study, all the simulations are carried out using the first-principles DFT calculation through Cambridge Serial Total Energy Package (CASTEP) code [Payne, Teter, Allan, Arias, and Joannopoulos (1992)]. The Vanderbilt's ultrasoft pseudopotential scheme [Vanderbilt (1990)] is further utilized to model the interactions of valence electrons with ion cores. The exchange-correlation potential is calculated within the GGA using the PBE correlation functional, which depends on both the electron density and its gradient at each space point. The well-known Broyden-Fletcher-Goldfarb-Shanno (BFGS) variable-metric minimization algorithm [Head (1985)] is then utilized to seek the ground state or geometry optimization. It has been demonstrated that the technique is very efficient and robust to explore the optimal minimal energy crystalline structure. The plane wave basis set is truncated using a cutoff energy of 440 eV. To sample the Brillouin zone [Cheng, Yu, and Cheng (2013)], the Monkhorst-Pack kpoint mesh is employed [Monkhorst and Pack (1976)]. It is selected based on the convergence of the k-point mesh, where the change of total energy becomes less than 1 meV/atom [Boukhvalov and Son (2012)]. In the study, the selected  $k$ -point mesh is  $3 \times 3 \times 1$ . The convergence conditions considered in the geometry optimization include an energy tolerance of  $2 \times 10^{-5}$  eV/atom, maximum ionic Hellmann-Feynman force within 0.01 eV/Å, maximum stress within 0.02 GPa and maximum ionic displacement within  $5 \times 10^{-4}$  Å.

## 3 Results and discussion

### 3.1 Adsorption energy for Sn adatoms on IMC surface

Adsorption energies are extracted by subtracting the energy of the adsorption system from the energies of Sn adatoms and IMCs surface, as shown in following

equation,

$$E_{ad} = E_{IMC\ surface/Sn} - (E_{IMC\ surface} + E_{Sn}), \quad (1)$$

where  $E_{IMC\ surface/Sn}$  is the total energy of Sn adatoms on the IMC surface,  $E_{IMC\ surface}$  the total energy of the IMC surface and  $E_{Sn}$  the total energy of Sn adatoms. According to the definition, it is noted that a stable adsorption site on a IMC surface can be recognized as the  $E_{ads}$  is negative.

Table 1: The adsorption energies (eV) and average bond length,  $d_{average}$  (Å), of Sn adatoms on IMC surface versus crystal surface.

IMC type	Crystal surface	$E_{IMC\ surface/Sn}$	$E_{IMC\ surface}$	$E_{Sn}$	$E_{ad}$	$d_{average}$
Cu <sub>3</sub> Sn	(1 0 0)	$-1.6417 \times 10^5$	$-1.6250 \times 10^5$	$-1.7119 \times 10^3$	-4.821	2.920
	(0 1 0)	$-7.3739 \times 10^4$	$-7.2022 \times 10^4$	$-1.7119 \times 10^3$	-5.589	2.825
	(0 0 1)	$-7.3732 \times 10^4$	$-7.2010 \times 10^4$	$-1.7119 \times 10^3$	-10.580	2.721
	(1 1 0)	$-7.3999 \times 10^4$	$-7.2278 \times 10^4$	$-1.7119 \times 10^3$	-8.460	2.779
	(1 0 1)	$-9.7448 \times 10^4$	$-9.5731 \times 10^4$	$-1.7119 \times 10^3$	-5.067	2.879
	(0 1 1)	$-1.2803 \times 10^5$	$-1.2631 \times 10^5$	$-1.7119 \times 10^3$	-5.174	2.856
	(1 1 1)	$-9.8146 \times 10^4$	$-9.6429 \times 10^4$	$-1.7119 \times 10^3$	-4.516	2.964
Cu <sub>6</sub> Sn <sub>5</sub>	(1 0 0)	$-1.5108 \times 10^5$	$-1.4937 \times 10^5$	$-1.7119 \times 10^3$	-3.645	2.979
	(0 1 0)	$-1.5106 \times 10^5$	$-1.4934 \times 10^5$	$-1.7119 \times 10^3$	-4.869	2.856
	(0 0 1)	$-6.2103 \times 10^4$	$-6.0389 \times 10^4$	$-1.7119 \times 10^3$	-2.604	3.078
	(1 1 0)	$-9.7010 \times 10^4$	$-9.5295 \times 10^4$	$-1.7119 \times 10^3$	-2.817	3.015
	(1 0 1)	$-1.8803 \times 10^5$	$-1.8631 \times 10^5$	$-1.7119 \times 10^3$	-7.052	2.799
	(0 1 1)	$-1.8802 \times 10^5$	$-1.8630 \times 10^5$	$-1.7119 \times 10^3$	-3.666	2.892
	(1 1 1)	$-1.1373 \times 10^5$	$-1.1201 \times 10^5$	$-1.7119 \times 10^3$	-5.218	2.827
Ni <sub>3</sub> Sn <sub>4</sub>	(1 0 0)	$-8.1749 \times 10^4$	$-8.0029 \times 10^4$	$-1.7119 \times 10^3$	-7.927	2.767
	(0 1 0)	$-1.6180 \times 10^5$	$-1.6009 \times 10^5$	$-1.7119 \times 10^3$	-4.000	2.884
	(0 0 1)	$-6.3198 \times 10^4$	$-6.1484 \times 10^4$	$-1.7119 \times 10^3$	-2.762	3.001
	(1 1 0)	$-1.6024 \times 10^5$	$-1.5853 \times 10^5$	$-1.7119 \times 10^3$	-4.521	2.864
	(1 0 1)	$-7.6825 \times 10^4$	$-7.5107 \times 10^4$	$-1.7119 \times 10^3$	-5.866	2.825
	(0 1 1)	$-6.3960 \times 10^4$	$-6.2244 \times 10^4$	$-1.7119 \times 10^3$	-5.003	2.842
	(1 1 1)	$-7.2089 \times 10^4$	$-7.0377 \times 10^4$	$-1.7119 \times 10^3$	-2.597	3.110

The results obtained for Sn adatoms on IMC surface as a function of crystal surface are shown in Table 1, and their corresponding configurations are demonstrated in Figs. 1-3. From Table 1, it is evident that Sn adatoms on the Cu<sub>3</sub>Sn (0 0 1) surface holds the largest adsorption energy, -10.580 eV, followed by the Cu<sub>3</sub>Sn (1 1 0), Cu<sub>3</sub>Sn (0 1 0), Cu<sub>3</sub>Sn (0 1 1), Cu<sub>3</sub>Sn (1 0 1), Cu<sub>3</sub>Sn (1 0 0) and Cu<sub>3</sub>Sn (1 1 1). This

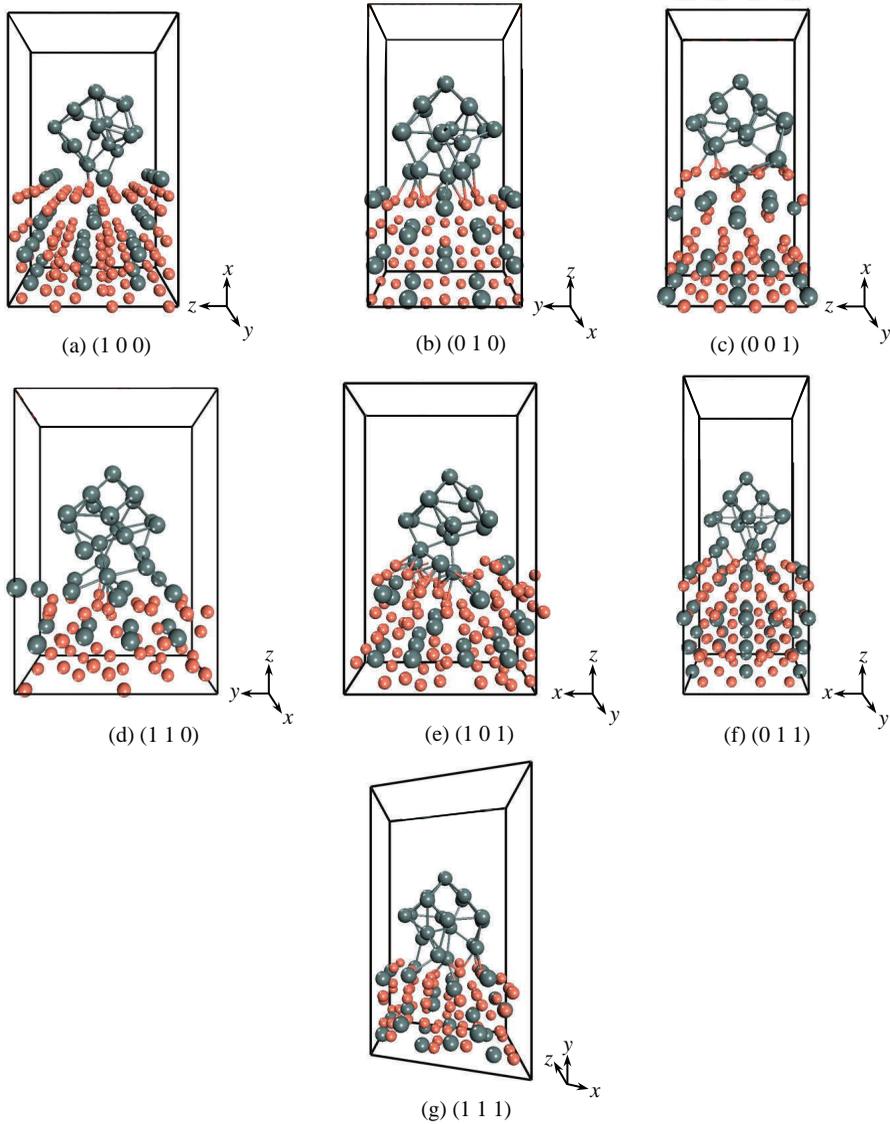


Figure 1: The atomic models of Sn adatoms on  $\text{Cu}_3\text{Sn}$  IMC slab versus crystal surface.

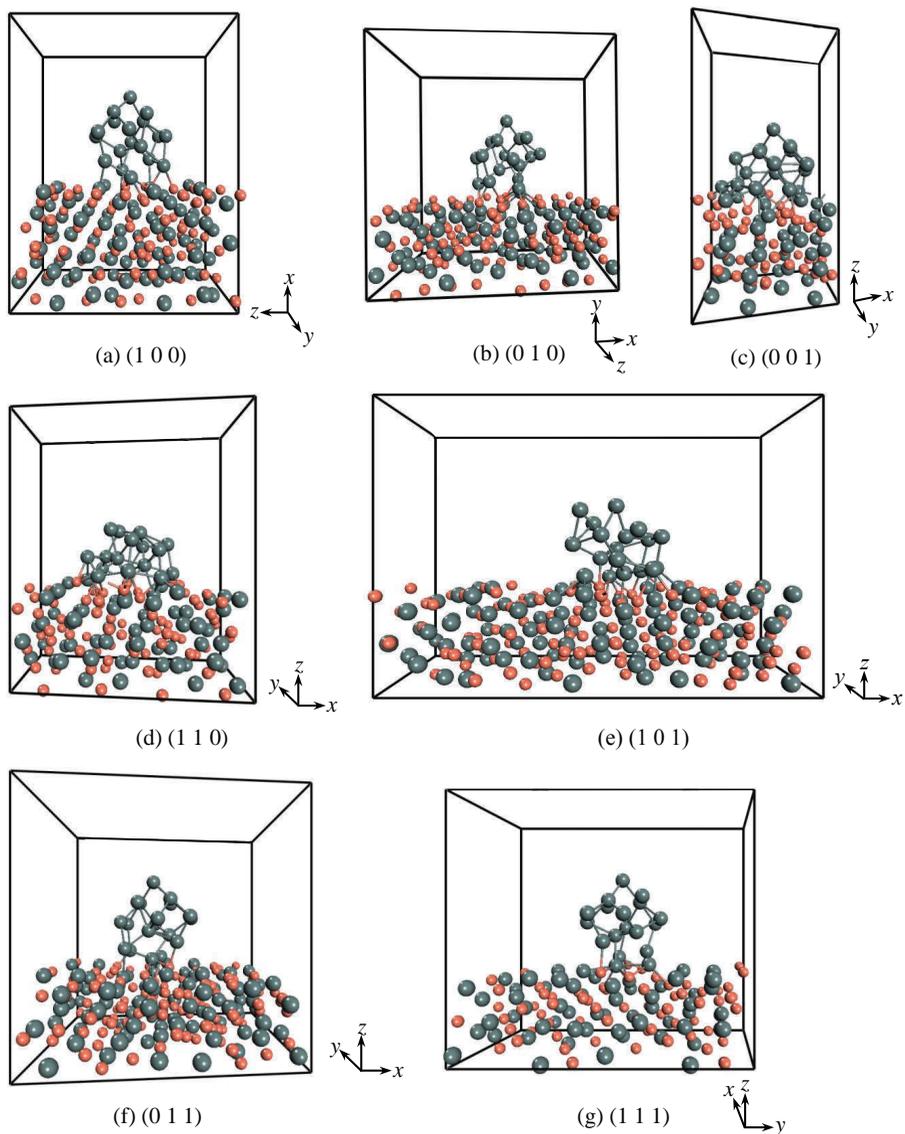


Figure 2: The atomic models of Sn adatoms on  $\text{Cu}_6\text{Sn}_5$  IMC slab versus crystal surface.

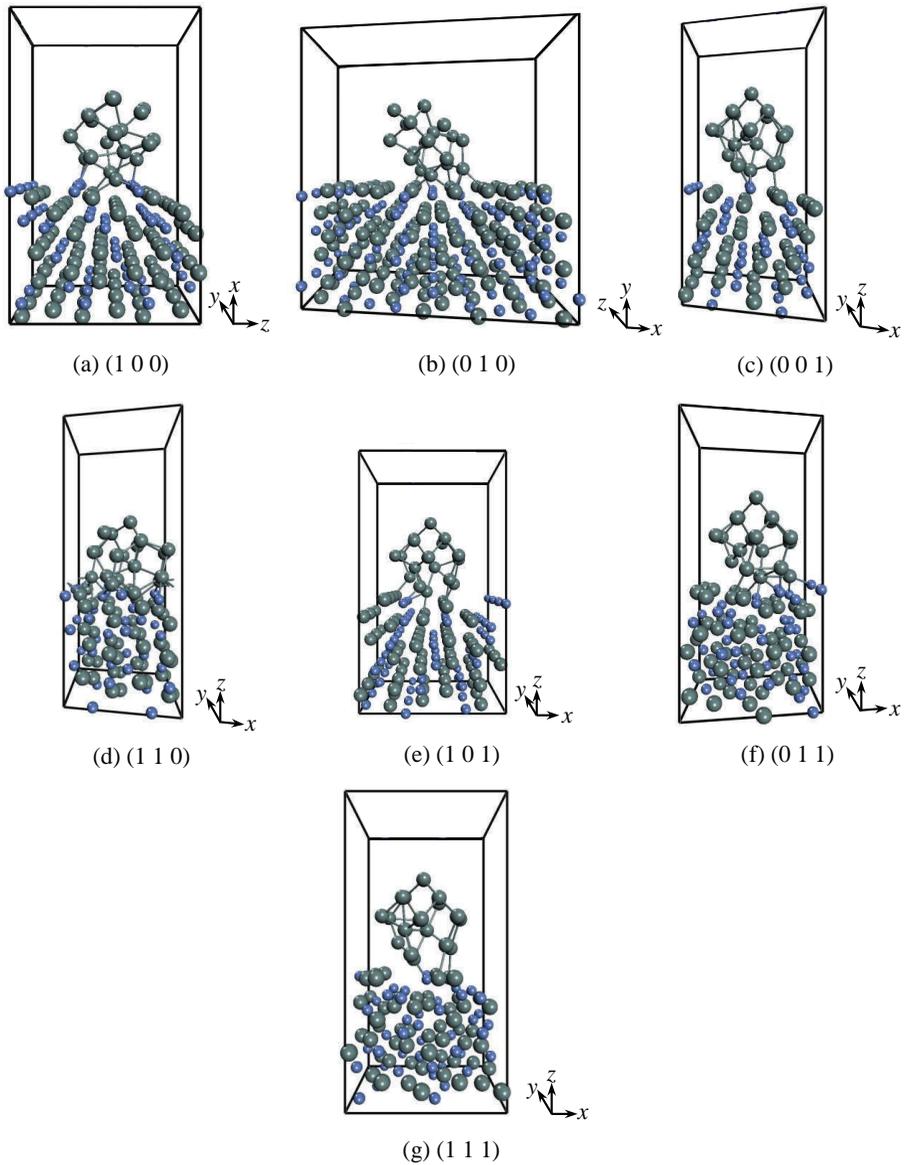


Figure 3: The atomic models of Sn adatoms on  $\text{Ni}_3\text{Sn}_4$  IMC slab versus crystal surface.

indicates that the  $\text{Cu}_3\text{Sn}$  (0 0 1) surface is the most stable surface for Sn adatoms. For the  $\text{Cu}_6\text{Sn}$  IMC, the (1 0 1) surface is the most stable one for Sn adatoms. Besides, Table 1 also exhibits that Sn adatoms on the  $\text{Ni}_3\text{Sn}_4$  (1 0 0) surface possesses the largest adsorption energy as compared to that of other crystal surfaces of  $\text{Ni}_3\text{Sn}_4$  IMC, suggesting that Sn adatoms on the  $\text{Ni}_3\text{Sn}_4$  (1 0 0) surface can dwell in the most stable state. Consequently, by averaging the adsorption energies of seven crystal surfaces of each IMC (i.e.,  $\text{Cu}_3\text{Sn}$ ,  $\text{Cu}_6\text{Sn}_5$  and  $\text{Ni}_3\text{Sn}_4$ ), it appears that the average adsorption energies of the  $\text{Cu}_3\text{Sn}$ ,  $\text{Cu}_6\text{Sn}_5$  and  $\text{Ni}_3\text{Sn}_4$  IMCs are around -6.315 eV, -4.267 eV and -4.668 eV. Notably, the adsorption energies of  $\text{Cu}_3\text{Sn}$ ,  $\text{Cu}_6\text{Sn}_5$  and  $\text{Ni}_3\text{Sn}_4$  IMCs are all larger than -0.400 eV [Lou, Zhang, Liang, Li, and Zhu (2010); Wang, Han, Hao, Zhang, and Xu (2012)], indicating that the Sn adatoms on the all IMCs surface are categorized as chemical adsorption. Moreover, that the  $\text{Cu}_3\text{Sn}$  IMC has the best electromigration resistance ability among the Sn-based IMC phases. In other words, the  $\text{Cu}_6\text{Sn}_5$  IMC are more susceptible to electromigration than the  $\text{Cu}_3\text{Sn}$  and  $\text{Ni}_3\text{Sn}_4$  IMCs. Most importantly, the ranking of the electromigration resistance ability of Sn-based IMCs (i.e.,  $\text{Cu}_3\text{Sn} > \text{Ni}_3\text{Sn}_4 > \text{Cu}_6\text{Sn}_5$ ) is also in excellent agreement with the literature experimental results [Chae, Chao, Zhang, Im and Ho (2007); Wang, Shen and Lai (2010)].

### 3.2 Average bond length for Sn adatoms on IMC surface

As the Sn adatoms are placed on the IMC surface, several Sn-Sn, Sn-Cu and Sn-Ni bonds are developed, and the calculated average bond lengths are listed in Table 1. It is found that the average bond length for  $\text{Cu}_3\text{Sn}$  at the seven crystal surfaces (i.e., (1 0 0), (0 1 0), (0 0 1), (1 1 0), (1 0 1), (0 1 1) and (0 1 1)) is about 2.920 Å, 2.825 Å, 2.721 Å, 2.779 Å, 2.879 Å, 2.856 Å and 2.964 Å. The predicted results are confirmed with the calculated adsorption energy, thereby implying that much higher adsorption energy would induce a much shorter average bond length, resulting in a stronger bonding force. This fact can be also observed in the  $\text{Cu}_6\text{Sn}_5$  and  $\text{Ni}_3\text{Sn}_4$  IMCs.

### 3.3 Bond population analysis for Sn adatoms on IMC surface

Bond population analysis is extensively applied in the electronic structure calculations carried out with linear combination of atomic orbitals (LCAO) basis sets [29]. The total overlap population may be used to provide an objective criterion for bonding between atoms, and also, assess the covalent or ionic nature of a bond. A high value of the bond population indicates a covalent bond, while a low value denotes an ionic interaction. The total overlap populations for all the IMC systems are listed in Table 2. It can be seen that the Sn adatoms on the  $\text{Cu}_3\text{Sn}$  (0 0 1) surface possesses the largest total bond population, which suggests that the bonding abil-

ity of Sn adatoms on the  $\text{Cu}_3\text{Sn}$  (0 0 1) surface is the best among the other  $\text{Cu}_3\text{Sn}$  surfaces. The finding is in agreement with the results for the adsorption energy and average bond length versus crystal surface shown in Table 1. Likewise, the Sn adatoms on the  $\text{Cu}_6\text{Sn}_5$  (0 0 1) and  $\text{Ni}_3\text{Sn}_4$  (1 0 0) surfaces would also hold a much larger total bond population as compared to Sn adatoms on the other surfaces, which are also consistent with the calculations for the adsorption energy and average bond length versus crystal surface.

Table 2: The total overlap population of Sn adatoms on IMCs surface as a function of crystal surface.

IMC type	Crystal surface	Total overlap population
$\text{Cu}_3\text{Sn}$	(1 0 0)	0.61
	(0 1 0)	1.65
	(0 0 1)	2.74
	(1 1 0)	1.78
	(1 0 1)	0.77
	(0 1 1)	1.34
	(1 1 1)	0.55
$\text{Cu}_6\text{Sn}_5$	(1 0 0)	0.60
	(0 1 0)	1.09
	(0 0 1)	0.38
	(1 1 0)	0.51
	(1 0 1)	2.43
	(0 1 1)	0.72
	(1 1 1)	1.54
$\text{Ni}_3\text{Sn}_4$	(1 0 0)	2.58
	(0 1 0)	0.95
	(0 0 1)	0.68
	(1 1 0)	1.33
	(1 0 1)	1.58
	(0 1 1)	1.46
	(1 1 1)	0.56

#### 4 Conclusions

In summary, by evaluating the adsorption energy, average bond length and bond population for the Sn atoms in the solder on the crystal surface of the Sn-based

IMCs at different crystal surfaces, the IMCs with better electromigration resistance ability can be characterized. The calculations exhibit that the Sn atoms on the Cu<sub>3</sub>Sn (0 0 1) surface possess the largest adsorption energy, average bond length and bond population, suggesting that the Cu<sub>3</sub>Sn (0 0 1) surface is the most stable surface for Sn adatoms. Additionally, based on the averaging adsorption energy, average bond length, and bond population for the Cu<sub>3</sub>Sn, Cu<sub>6</sub>Sn<sub>5</sub> and Ni<sub>3</sub>Sn<sub>4</sub> IMCs at seven crystal surfaces, their electromigration resistance ability is further identified. The results reveal that Cu<sub>3</sub>Sn holds the best electromigration resistance ability, followed by Ni<sub>3</sub>Sn<sub>4</sub> and Cu<sub>6</sub>Sn<sub>5</sub>, which is consistent with the literature experimental results.

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