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Investigation of surface alloy formed with coadsorption of Pb and Bi/Sb/Sn on Cu(001) by low energy electron diffraction

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Abstract
Surface alloy obtained by the coadsorption of Pb and Bi/Sb/Sn on Cu(001) substrate has been determined by tensor low energy electron diffraction (LEED). The best-fit structure of all of combinations can be described as a ternary alloy having 1D chain arrangement of Pb and Bi/Sb/Sn atoms in the [110] direction between the Cu rows in the same direction. This type of 1D arrangement is previously obtained by sole Pb adsorption on the same substrate with c(4×4) periodicity. In all of the coadsorption cases, creation of a vacancy causes a large displacement of the Pb atoms from the fourfold-hollow site and the atoms having smaller atomic radius, Bi or Sb or Sn, located in the exact fourfold-hollow site. The structure of the Pb-Bi, Pb-Sb and Pb-Sn coadsorption on Cu(001) that we have obtained in our previous works are compared and described here.

1. Introduction

Coadsorption of more than one element on the substrate is a familiar method to produce surface new materials. The surface phases produced by coadsorption and the determination of this phases may be used to realize the properties of the newly formed materials. [1] It would be a good study of coadsorption of two materials of which one is Pb, and other is one of the Bi/Sb/Sn materials on the substrate Cu(001). In this study, we investigated the coadsorption of these materials in the combination of (Pb, Bi), (Pb, Sb), and (Pb, Sn) on Cu(001). We considered Pb, because it is individually used as surfactant in the thin film growth. [1] On the other hand, Bi/Sb/Sn are materials having large magnetic moment and promising material for the magnetic applications. [2] Interestingly, these three combinations have also bulk alloy. Individually, Pb, Bi, Sn on Cu(001) makes different alloy and overlayer structures at the different coverages except the Sb atoms. [3-4] Only p(2x2) alloy structure is possible for Sb on Cu(001). [5]

After coadsorption of these three systems, we got a c(4x4) phase for (Pb, Bi) [6] and p(4×4) phase for (Pb, Sb/Sn) systems all of which were obtained at the coverage of Pb of ~0.25 and Bi/Sb/Sn of ~0.125. For all the three systems, we got 1D chain arrangement Pb and Bi/Sb/Sn atoms between Cu rows in the [110] direction.

2. EXPERIMENTAL

The experiments were done in an ultrahigh vacuum (UHV) chamber equipped with four grid low energy electron diffraction (LEED) system. The base pressure of the chamber was always maintained better than 3×10^{-8} Pa during the whole experiment. The Cu(001) substrate was cleaned by several cycles of Ar^+ ion sputtering (1 kV, 6.5 μA, 15 min) and subsequent annealing at 800 K until a sharp (1×1) LEED pattern was obtained. The best-fit model was obtained through best agreement between the experimental and theoretical I(E) curves, which was decided by minimizing Pendry's reliability factor (R_p). [7] The error bars on the structural parameters were calculated by variance of R_p, $\Delta R = R_{min}(8|V_{oi}|/\Delta E)^{1/2}$, where R_{min} is the minimum R_p value and ΔE is the total energy range of the experimental I(E) curves. [8]

3. Results and Discussion

3.1 c(4x4)-Pb,Bi coadsorption

The room temperature coadsorption of Pb and Bi was carried out by starting the deposition of Pb atoms on Cu(001) at a certain coverage. After that, Bi atoms were deposited on the Pb pre-adsorbed surface. The coverage of Bi atoms was increased gradually and we checked the LEED patterns. When we reversed the deposition order, the same LEED patterns were obtained. In this way, the c(4×4) structure was obtained at the coverage of Pb at ~0.25 and Bi at

~0.125. According to the coverage calculation of the c(4×4) unit cell, 0.375 corresponds to the three adsorbate atoms. Thus, there are two Pb atoms and one Bi atom in the unit cell, and the coverages of Pb and Bi are 2/8 and 1/8, respectively. Considering this 3 adsorbates, the best-fit structure of this phase is given in the following figure 1.

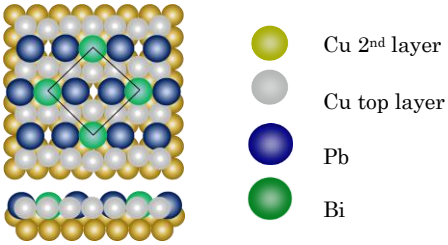

Figure 1: The best-fit structure of the c(4x4)-(Pb, Bi) coadsorption system. Upper one is top view and the lower one is the side view.

We confirmed this structure by the lower Rp factor of 0.21. This structure can be defined as 1D chain arrangement of –Bi-Pb-Pb-Bi- in the [110] direction. [6]

3.2 p(4x4)-Pb Sb coadsorption

In case of Pb and Sb coadsorption, we got p(4x4) phase at the coverage of Pb at ~0.25 and Sb at ~0.125. This coverage combination is the very similar to the above Pb and Bi coadsorption system. Moreover, the LEED pattern of the p(4×4) phase was very clear up to ~220 eV of the beam energy. Above this energy, only c(4×4) points were visible and other points of p(4×4) points are totally invisible. According to the coverage calculation of the p(4×4) unit cell, 0.375 corresponds to the six adsorbate atoms. Thus, there are four Pb atoms and two Sb atoms in the unit cell. Considering this 6 adsorbates, the best-fit structure of this phase is given in the figure 2(a). We confirmed this structure by the lower Rp factor of 0.23. This structure also can be defined as 1D chain arrangement of –Sb-Pb-Pb-Sb- in the [110] direction.

3.3 p(4x4)-Pb Sn coadsorption

In case of Pb and Sn coadsorption, we also got p(4x4) phase at the coverage of Pb at ~0.25 and Sb at ~0.125. And the p(4x4) fraction points becoming weaker in this case also. Considering these similarities with the Pb and Sb coadosorption system, we got similar best-fit structure having 1D chain arrangement of –Sn-Pb-Pb-Sn- in the [110] direction. The best-fit structure of this phase is shown in figure 2(b). We confirmed this structure by the Rp 0.21

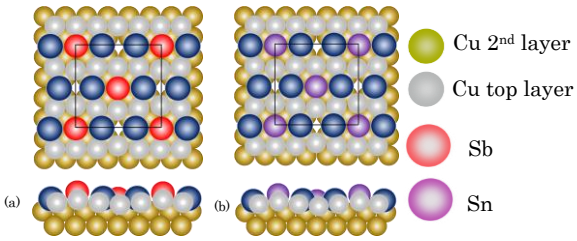

Figure 2: The best-fit structure of the (a) p(4x4)-(Pb, Sb) coadsorption system and (b) the p(4x4)-(Pb, Sn) coadsorption system. Upper one is top view and the lower one is the side view.

4. CONCLUSION

In summary, it is possible to obtain the surface alloy of heavy and larger atomic radius metals on the lighter and smaller atomic radius of Cu(001). Although the different phases are obtained for these three combinations but the structure are similar. The structures are defined as the 1D arrangement of –Bi/Sb/Sn-Pb-Pb-Bi/Sb/Sn- between the Cu rows in the direction of [110]. Also, it can be predicted that Pb may have significant effect to make such type of chain arrangement as individually Pb makes this type of structure and the theoretical investigation is needed for this purpose.

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