LEED structural analysis of ordered mixed surface structures formed by coadsorption of Bi and Mg, and Bi and Li on Cu(001)

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Recently, we studied surface structures formed by the coadsorption of Mg and alkali metal (AM) on Cu(001) at room temperature. $(2\sqrt{2}\times\sqrt{2})R45^\circ$ and $(\sqrt{5}\times\sqrt{5})R26.7^\circ$ structures are formed for Mg and Li, and Mg and K (Cs), respectively, and all the structures were determined by LEED *I-V* analysis [1]. The adsorbates are mixed on reconstructed Cu(001) surfaces instead of separation into individual phases. Mg and Li form no bulk compound as shown in Fig. 1. The $(2\sqrt{2}\times\sqrt{2})R45^\circ$ structure formed by Mg and Li is denoted as $(2\sqrt{2}\times\sqrt{2})R45^\circ$-Mg,Li and depicted in Fig. 2. From obtained structural parameters, it is suggested that the ordered mixed surface structure is stabilized by a cooperative interaction between Mg and Li atoms through substrate Cu surface atoms [1]. That is, Mg atoms attain a deeper vertical position owing to a lateral displacement of surface Cu atoms as shown by arrows in Fig. 2, resulting in larger adsorption energy than in the individual adsorption. This suggestion is confirmed theoretically [2], and the same scenario can be applied to the $(\sqrt{5}\times\sqrt{5})R26.7^\circ$-Mg, K(Cs) structures.

In this paper, we performed contrastive coadsorptions of Mg and Bi, and Bi and Li on Cu(001): both coadsorbetes form stable bulk compounds as shown in Fig. 1. We have determined many ordered mixed surface structures by LEED I-V analysis [3], and the (4x4)-Mg,Bi structure is depicted in Fig. 3. Structural parameters clearly indicate the presence of a direct bonding between Mg and Bi atoms, as apparently seen in the atomic arrangement in Fig. 3. Other determined structures also indicate the presence of attractive interactions between Mg and Bi, and also between Bi and Li. The results are in accordance with the presence of stable bulk compounds of Mg_3Bi_2 and LiBi (Li_3Bi). We will show details of other determined structures, and will describe the difference in the interaction with substrate Cu surface atoms between Mg and Bi. We will discuss the formation reason for ordered mixed surface structures.

References

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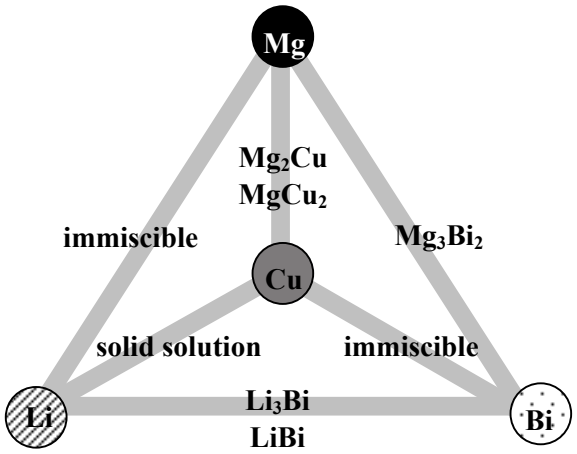

Fig. 1 Relationships of bulk compounds formation between the coadsorbates, and between the adsorbates and Cu in equilibrium condition.

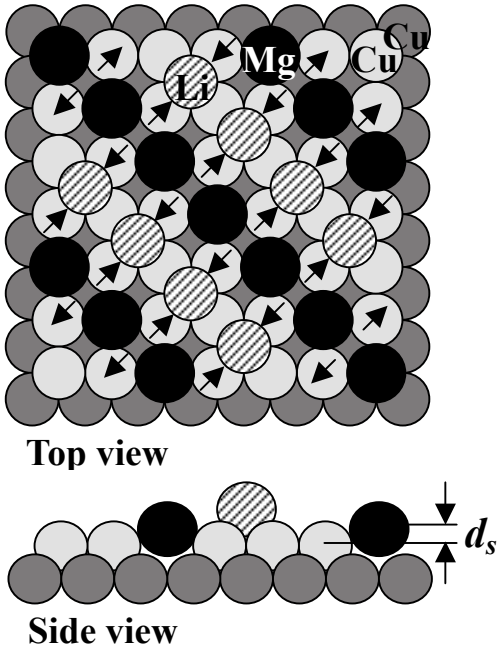

Fig. 2 Top and side views of Cu(001)-(2 $\sqrt{2} \times \sqrt{2}$)R45°-Mg,Li. Arrows indicate directions of the lateral displacements of Cu atoms in the first layer.

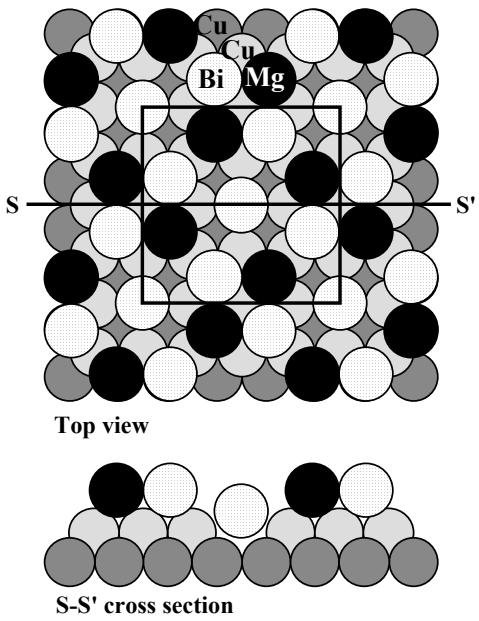

Fig. 3 Top and cross sectional views of Cu(001)-(4x4)-Mg, Bi. Primitive unit cell is outlined.