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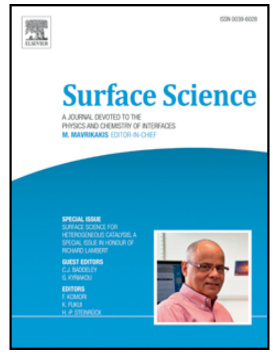

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Bismuth–Indium Two-Dimensional Compounds on Si(111) Surface

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Scanning tunneling microscopy; DFT calculations

Abstract

Using scanning tunneling microscopy (STM) observations, it has been found that codeposition of Bi and In onto Si(111)7×7 surface, followed by 250-550°C annealing, induces formation of a set of the ordered (Bi, In)/Si(111) stable structures, including 2√3×3, 5×5, √7×√7 and 2×2. Under appropriate conditions, the structures can occupy almost the entire surface, except for 2√3×3 which are formed only locally. Scanning tunneling spectroscopy has demonstrated that the 5×5 and √7×√7 structures are semiconducting, while the 2×2 is metallic. The 5×5, √7×√7, and 2×2 structural models have been proposed on the basis of DFT calculations and comparison of simulated and experimental STM images.

1. Introduction

Present work has been done in the frame of searching surface alloys on silicon with spin-split bands due to Rashba effect as promising materials for spintronics. The choice of the Bi–In couple was dictated by the following reasons. Bismuth forms one-layer structure on the Si(111) surface, β-√3×√3 reconstruction [1] with a giant spin splitting of surface-state bands [2,3,4]. However, the split bands are located in the valence band without crossing the Fermi level [2,3,4]. Meanwhile, for spintronic applications, materials with metallic properties having spin-splitting near Fermi level and which can be grown on a semiconductor are actually required. Thus, thin Bi film on Si(111) has to be modified by another metal to get required properties. Two alloys of this kind, Si(111)√3×√3-(Bi, Na) [5] and Si(111)4×4-(Bi, Ag) [6], have already been discovered, but both have certain drawbacks. The first alloy, Si(111)√3×√3-(Bi, Na), has a giant spin splitting of metallic surface-state bands, but it is unstable against even low-temperature heating. The second one, Si(111)4×4-(Bi, Ag), is stable up to ~250°C, but it has a modest spin-splitting and it cannot be formed as well-ordered array in a simple way, because formation of other (Bi, Ag)/Si(111) structures occurs locally at any local lack or excess of Bi [6]. Indium is thought to be a promising candidate to complete the metal pair. Bismuth and indium hypothetically could form the III–V semiconductor, but there has been no report on synthesis of this compound. On the other hand, alloys of these metals in a wide range of compositions are metallic and are usually used as a solder or, much rare, in ultra-reliable accumulators. Thus, one can expect that possible low-dimensional Bi–In alloys on Si(111) might be thermally stable and metallic. An additional interest to the growth of the atom-layer Bi–In compounds is associated with very recent theoretical predictions that two-dimensional III–V compounds might possess