Surface Stability of Reconstructions on BAs (001) Surface: An Ab Initio-Based Approach

○(DC)Cai Peiyang[1], Toru Akiyama[2], Shunta Harada[1, 3], Miho Tagawa[1, 3], Toru Ujihara[1, 3]
E-mail: caipeiy@unno.material.nagoya-u.ac.jp
1 Grad. School of Eng. Nagoya Univ., Japan
2 Grad. School of Eng. Mie Univ., Japan
3 IMaSS Nagoya Univ., Japan

III-V semiconductor BAs has become a material of great interest in recent years due to the extremely high thermal conductivity of 1300 W/ m·K [1]. However, epitaxial growth of BAs has not been reported, and the research on the 2-dimensions form of BAs is still at the stage of calculation. Kangawa et al. proposed that first-principles surface reconstruction calculations can provide guidance for the growth conditions of epitaxy methods such as MBE and MOVPE [2]. Calculating the stability of various reconstructed surfaces that may be formed under different experimental conditions will help us to select appropriate conditions to control the epitaxy growth process.

In the present study, we calculated the formation energy of various reconstructed BAs (001) surfaces, which illustrates the most stable surface reconstructions. Then we compared the adsorption energy of As with the chemical potential of As vapor. Through this method, we can get a state diagram of the relationship between the decomposition of each structure of BAs and the BEP (Beam equivalent pressure) or growth temperature conditions. Our calculations are based on density-functional theory (DFT) using generalized gradient approximation (GGA) and norm-conserving pseudopotentials. In addition, since the supply sources of As during the growth of BAs can be divided into As_4 and As_2, in this study we will also compare the effects of As_2 and As_4 on the growth of two different As sources.

As shown in Figure 1., the critical conditions for As desorption from BAs under As_2 and As_4 conditions were obtained, respectively. It can be concluded that the decomposition temperature of BAs grown under As_2 source at high temperature is much higher than that of As_4 source. And for the reconstructions under the condition of As_2 source, the figure shows that above the temperature of 886 K ~ 1087 K, the 3As-dimer structure under the C44 period is the most stable structure, while in the interval below this temperature, the As dimer under the (1x2) period becomes the most stable structure. In the case of As_4 as the As source, only a stable surface reconstruction of 3As-dimer exists. From the results, we can find that, as the temperature increases, the adsorption of As tends to decrease. Comparing the calculation results of As_4 and As_2, we can find that in the case of As_2, the surface can allow more As to stay on the surface. Through this calculation, we predict the stable structure models during the growth of BAs, which lays the foundation for the calculation of adsorption and surface diffusion. We also narrowed the range of growth conditions of BAs and provided a crucial basis for judging the reason for the loss of As during the growth.

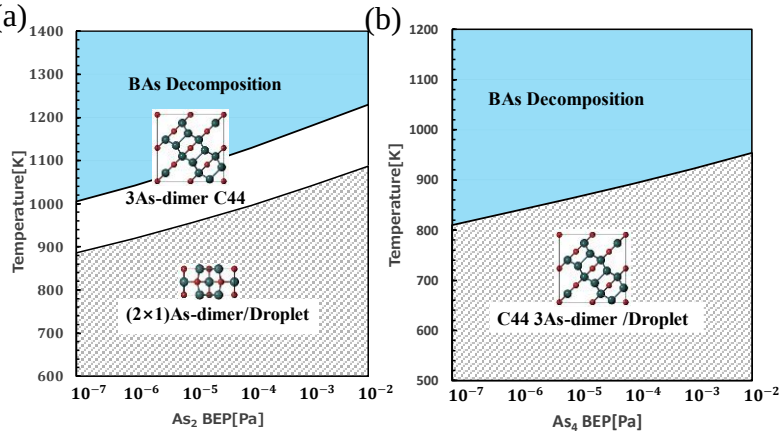

Fig.1. Pressure-temperature phase diagram for the BAs (001) surface under the condition that As source is (a)As_2 (b)As_4

[1] Kang *et al.*, Science 361 2018, 575–578
[2] Kangawa *et a*l., Materials 6 2013, 3309-3360