Poster 01

Surface structure and surface energies of InAs

In Won Yeu[1,2], Cheol Seong Hwang[2], and Jung-Hae Choi[1*]

[1]*Center for Electronic Materials, Korea Institute of Science and Technology, Seoul 136-791, Korea*

[2]*Department of Materials Science and Engineering, Seoul National University, Seoul 151-744, Korea*

The Ⅲ-Ⅴ compounds are one of the most promising semiconductors for high speed and low power switching devices due to their superior electron transport properties. A key restriction to the use of Ⅲ-Ⅴ semiconductor is the lack of the high quality surface and interface states compared to the Si/SiO_2 system. Therefore, the low index surfaces of the Ⅲ-Ⅴ semiconductors have been studied and it is well known that the surfaces exhibit various reconstruction structures depending on the preparation conditions such as cleavage, epitaxial growth and annealing [1]. Among them, surface structures of GaAs (001) reconstruction have been one of the most intensively studied due to its importance as a substrate for epitaxial growth [2]. Even though the importance of other surfaces becomes significant with the epitaxial growth of the nanostructures including nanowires, (111) surfaces of Ⅲ-Ⅴ semiconductor have been less investigated due to the difficulty to separate the (111) surface from the $(\bar{1}\ \bar{1}\ \bar{1})$ surface. To determine the individual surface energies of the (111) and $(\bar{1}\ \bar{1}\ \bar{1})$ in the zinc blende structure, it is essential the separate them but it is impossible in the standard slab geometry. Chetty *et al.* [3] solved this problem and calculated the surface energy of the (111) in the zinc-blende structure by introducing the local energy density approach. However, the method suffered from the approximation of the local energy density. Later, Zhang *et al.* [4] suggested an infinite triangular prism geometry in order to separate the (111) surface from the $(\bar{1}\ \bar{1}\ \bar{1})$ surface and calculated the {111} surface energies of Ge, GaAs, and ZnSe directly. The prism geometry made it possible to calculate other polar surfaces and there have been some revised results on the surface energies in the wurtzite and zinc-blende GaAs but not about those for InAs. In this study, the accurate surface energies and the structures of InAs surfaces were studied by density-functional theory in the slab and the triangular prism geometries.

[1] Srivastava GP. Theory of semiconductor surface reconstruction. Reports on Progress in Physics. 1997;60(5):561-613.

[2] Ohtake A. Surface reconstructions on GaAs (001). Surf Sci Rep. 2008;63(7):295-327.

[3] Chetty N, Martin RM. First-principles energy density and its applications to selected polar surfaces. Physical Review B. 1992;45(11):6074.

[4] Zhang S, Wei S-H. Surface energy and the common dangling bond rule for semiconductors. Physical Review Letters. 2004;92(8):086102.