[WA1-C-3]

Surface reconstruction and equilibrium shape of Ⅲ-Ⅴ compound semiconductors as a function of pressure and temperature by *ab-initio* thermodynamics

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The properties of the III - V compound semiconductors vary depending on the orientation and reconstruction of the surface as well the shape and orientation of the crystal, which are highly dependent on the thermodynamic conditions such as pressure and temperature. Therefore, the prediction of the surface structure is important in order to control the characteristics of these materials. In this presentation, we show the systematic way to investigate the thermodynamic effects on the surface reconstruction of the III-V compound semiconductors, such as GaAs, InAs, GaSb, and InSb by *ab-initio* thermodynamic calculations. To the authors' knowledge, this is the first report which provides the fraction of the surface reconstruction as a function of T and P[1]. Then, we determine the equilibrium shapes of these materials as a function of T and P in the range relevant to the experimental growth condition and compare with the experimental growth shapes. This methodology is powerful to directly compare with the experimental results and applicable to various materials.

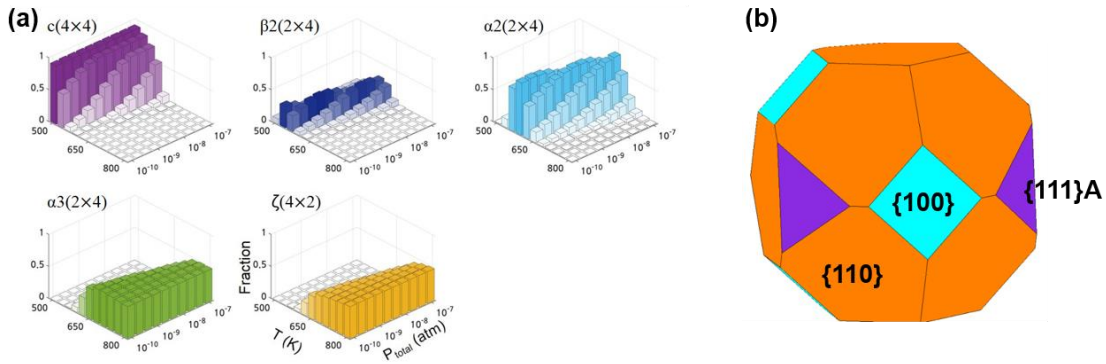

Fig 1. (a) Fraction of the dominant reconstructions of InAs (001) as a function of T and P (b) equilibrium shape of InAs at 750 K and 4e-09 atm.

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References [1] In Won Yeu, et al., *Scientific Reports* 7, 10691 (2017).