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조직위원

손영우 (KIAS)
김세중 (UST, KIAS)
지승훈 (POSTECH, KIAS)

담 당 자 : 김혜미 (KIAS)
전　　화 : 02-958-2638
이 메 일 : hmkim@kias.re.kr
홈페이지 : http://events.kias.re.kr/h/ESCW2019/

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Poster 23

Theoretical understanding on the growth and stacking-fault mechanism of GaAs nanowires grown by catalyst-free method

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

[1]*Center for Electronic Materials, Korea Institute of Science and Technology, Seoul 02792, Korea*

[2]*Department of Materials Science and Engineering, and Inter-University Semiconductor Research Center, Seoul National University, Seoul 08826, Korea*

The precise control in the growth of GaAs nanowire on commercial Si substrate has been developed to integrate the novel functionalities originated from the one dimensional geometry as well as intrinsic properties. Dislocation and crack caused by the mismatch in lattice constant and thermal expansion coefficient have been effectively reduced by the small contact area between the nanowire and Si substrate. The last remaining difficulty to grow perfect nanowires is the stacking-fault, which is shown to be abundant and randomly distributed to date. In this study, the growth and stacking-fault mechanism in GaAs nanowire is theoretically explained using the nucleation model during the growth of GaAs nanowire using catalyst-free methods. The changes in adsorption behavior and interface energy during the growth are calculated as a function of temperature and pressure using ab-initio thermodynamics [1]. By considering the variation in Gibbs energy of nucleation depending on growth conditions, the reason why the GaAs crystal grows preferentially in one direction is confirmed to be the preferential adsorption on the growing surface. In addition, the origin of experimental observations about stacking-fault behavior depending on growth conditions and direction is thoroughly explained.

[1] In Won Yeu *et al.*, Sci. Rep. 9, 1127 (2019).