Poster Session | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[PO-F2]Poster Session 2

Symposium F

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-53]Multiscale Modelling of Indirect-to-Direct Band Gap Transition in Silicon Nanosheets

○Byung-Hyun Kim[1], Chan-Woo Lee[1], Mina Park[2], Gyubong Kim[2], Kersti Hermansson[3], Peter Broqvist[3], Heon-Jin Choi[4], Kwang-Ryeol Lee[2] (1.R&D Platform Center, Korea Institute of Energy Research, Korea, 2.Computational Science Research Center, Korea Institute of Science and Technology, Korea, 3.Dept. of Chemistry-Ångström Laboratory, Uppsala University, Sweden, 4.Dept. of Materials Science and Engineering, Yonsei University, Korea)

Two-dimensional (2D) nanomaterials such as graphene, boron nitride (BN), and MoS_2 have attracted great attention owing to their exceptional and tuneable properties, which are distinguishable from those of their bulk phases. Recently, Si nanosheets (Si NSs) have been synthesized by various experimental techniques. Compared to other materials, Si-based nanostructures have great advantages when it comes to commercialization, as Si is compatible with the conventional device manufacturing processes in the microelectronics industry.

In experiments, (111) Si NSs showed thickness-dependent light emissions in the visible wavelength regime, originating from quantum confinement effects. This observation indicates that thin (111) Si NSs have a direct band gap, whereas bulk Si normally has an indirect band gap. However, the question of the physical origin behind this nano-effect of Si left unanswered.

The effect of biaxial strain on the band structure of 2D Si NSs with (111), (110), and (001) exposed surfaces was investigated by means of a multiscale modelling approach combining molecular dynamics simulations with a reactie force field and the density functional theory. For all the considered Si NSs, an indirect-to-direct band gap transition occurs as the lateral dimensions of Si NSs increase, i.e. increasing lateral biaxial strain from compressive to tensile always enhances the direct band gap characteristics. Further analysis revealed the mechanism of the transition which is caused by preferential shifts of the conduction band edge at a specific *k*-point due to their bond characteristics. Our results explain a photoluminescence result of the (111) Si NSs [U. Kim *et al.*, *ACS Nano* **2011**, *5*, 2176-2181] in terms of the plausible tensile strain imposed in the unoxidized inner layer by the surface oxidation.