

Stability of wurtzite semipolar surfaces: Algorithms and practices

Title

Yiou Zhang, Jingzhao Zhang and Junyi Zhu

Department of Physics, The Chinese University of Hong Kong, China

Authors and institutions (underline the presenting author)

A complete knowledge of absolute surface energies with any arbitrary crystal orientation is important for the improvements of semiconductor devices because it determines the equilibrium and nonequilibrium crystal shapes of thin films and nanostructures. It is also crucial in the control of thin film crystal growth and surface effect studies in broad research fields. However, obtaining accurate absolute formation energies is still a huge challenge for the semipolar surfaces of compound semiconductors. It mainly results from the asymmetry nature of crystal structures and the complicated step morphologies and related reconstructions of these surface configurations. Here we propose a general approach to calculate the absolute formation energies of wurtzite semipolar surfaces by first-principles calculations, taking GaN as an example. We mainly focused on two commonly seen sets of semipolar surfaces: a-family (11 (2) over \bar{X}) and m-family (10 (1) over \bar{X}). For all the semipolar surfaces that we have calculated 2 in this paper, the self-consistent accuracy is within 1.5 meV/angstrom(2). Our work fills the last technical gap to fully investigate and understand the shape and morphology of compound semiconductors.

Abstract (max. 500 words)