

Atomic Design of Polarity of GaN Films Grown on SiC(0001)

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(Received: 2003-7-8; Revised:)

Abstract: Ab initio total energy calculations are used to determine the interface structure of GaN films grown on 6H-SiC(0001) with different substrate reconstructions. The results indicate that GaN films grown on bare SiC(0001) are of the Ga-polarity, while GaN films grown on SiC(0001) with Si adlayer are of the N-polarity if there is no N-Si interchange at the interface. With the interchange, the GaN films are of the Ga-polarity.

PACS: 68.35.Ct, 61.72.Nn, 68.55.-a, 81.15.Aa

Key words: polarity, total energy calculation, adlayer, interface

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