The nonpolar- semipolar boundaries in III-nitrides: Atomic structure and influence on defect introduction

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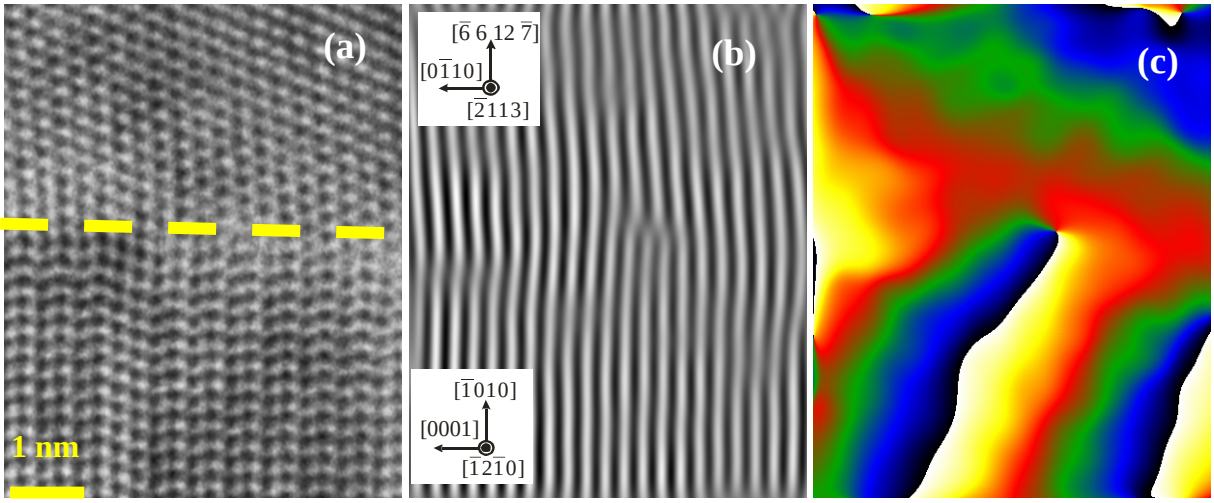
In III-Nitride compound semiconductor nanotechnology, a lot of emphasis has been placed recently on achieving good quality epilayers grown along nonpolar and semipolar orientations. This is done in order to reduce the polarization-induced internal electrostatic fields and the quantum-confined Stark effect that hamper the quantum efficiency of optoelectronic device active regions. During the growths of both nonpolar or semipolar nitrides on *r*-plane or *m*-plane sapphire respectively, parasitic misoriented nanocrystals are often observed at the epilayer/substrate interface causing introduction of threading dislocations (TDs) [1,2]. This phenomenon is facilitated by the high order of common symmetry conserved by the $90^{o}[11\bar{2}0]$ rotation which characterizes the misorientation between the parasitic nanocrystals and the matrix epilayers. In the present work we characterize by atomistic simulations combined with high resolution transmission electron microscopy (HRTEM) observations the $(10\bar{1}0)/(2\bar{1}\bar{1}2)$ grain boundary (GB) which was found to be important in *a*-plane GaN epilayers grown on *r*-plane sapphire, and to lead to TD introduction. For the atomistic simulations the modified Stillinger –Weber and Tersoff empirical interatomic potentials were employed. Two principal structural configurations were compared, in particular a GB comprising interfacial dislocations and a GB with interfacial disconnections i.e. dislocations exhibiting also step character. It was found that, the dislocated GB exhibits curvature at the points where the interfacial dislocations are located. On the other hand the disconnected GB exhibits no curvature and moreover, appears to explain the HRTEM observations. The Burgers vector of the disconnections is of the $1/6[2\bar{2}03]$ type and was verified on the HRTEM image by using circuit mapping. In agreement with nodal balance requirements, such defects can give rise to TDs emanating into the epilayer. This nanomechanism of defect introduction is in agreement with the experimental observations.



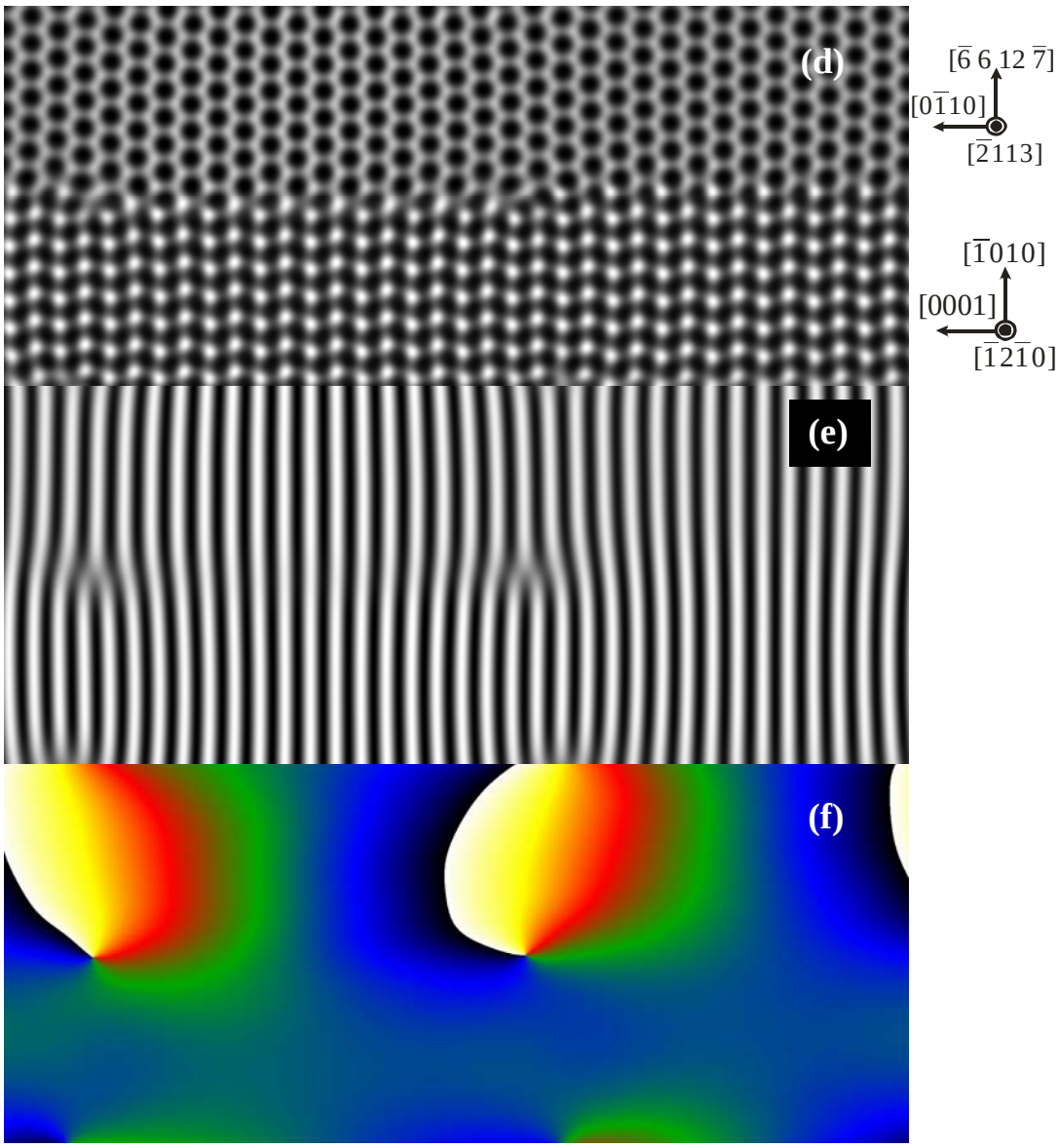


Figure 1. (a)HRTEM image of the $(10\bar{1}0)/(2\bar{1}\bar{1}2)$ GB viewed along the $[\bar{1}2\bar{1}0]/[\bar{2}113]$ directions of the two adjacent GaN domains respectively.(b) the Bragg filtered image and (c) the geometric phase image.
(d) The corresponding HRTEM image simulation of the relaxed atomistic configuration of the GB. (e) the Bragg filtered image and (f) the geometric phase image.

[1] J. Smalc-Koziorowska, Ph. Komninou, S.-L. Sahonta, J. Kioseoglou, G. Tsiakatouras, and A. Georgakilas, *phys. stat. sol. (c)* **5**, 3748 (2008).
[2] J. Smalc-Koziorowska, G. P. Dimitrakopulos, S.-L. Sahonta, G. Tsiakatouras, A. Georgakilas, and Ph. Komninou, *Appl. Phys. Lett.* **89**, 021910 (2008)

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