Simulation supported analysis of the effect of SiN_x interlayers in AlGaN on the dislocation density reduction

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In the last few years aluminium nitride (AlN) has attracted much attention due to its extremely large direct band gap of approximately 6.0 eV and its impressive chemical and thermal stability. Thus AlN and $Al_xGa_{1-x}N$ ternary alloys are promising materials for high-power high temperature electronic applications and optoelectronic devices in UV range. For group-III nitride wafers are still not available in sufficient amount and quality, AlN has to be grown on foreign substrates such as Al_2O_3 (Sapphire). Unfortunately the large lattice mismatch between the AlGaN/Al_2O_3 interface of up to -14% leads to the formation of threading dislocations (TD), inducing a high dislocation density in the range of $10^{10}cm^{-2}$ and decreasing the crystal quality [1, 2]. Thus it is still a big challenge to grow AlGaN directly on foreign substrates with small dislocation density. As is already known, SiN interlayers can act as anti-surfactants and drastically reduce the dislocation density in pure GaN layers [3, 4]. In our work we could observe a very efficient dislocation annihilation of the **a**-type TDs at the SiN interlayer even in $Al_xGa_{1-x}N$ layers with relatively high Al content of x=0.2.

In this work we investigated $Al_xGa_{1-x}N$ layers (x=0.2) with an intermediate SiN layer, placed at a distance of 150 nm to the AlN:O nucleation layer. The AlGaN was grown on c-plane sapphire by MOVPE. The investigations were focused on the effect of the SiN interlayer on the dislocation density reduction of the **a**-type TDs. The investigations were carried out directly at the SiN interlayer by exploiting the 3g weak beam dark field (WBDF) method and high resolution (HR) TEM, using a Philips CM20 microscope (figure 1). In addition an appropriate dislocation model was developed for the **a**-type TD in AlGaN and its bending due to lateral overgrowth of the SiN nano-mask by AlGaN to compare the experimental images with multislice simulations and explain the annihilation process of the **a**-type TDs at the SiN interlayer (figure 2).

It is shown by our simulation supported HRTEM and WBDF analyses, that the most frequently occuring effect for the reduction of the **a**-type TDs is the conversion of an **a**-type TD into an **a**-type basal dislocation at the SiN interface due to lateral overgrowth of the SiN by AlGaN. After the bending the basal dislocation can be annihilated by interacting with another **a**-type dislocation. The consistence of the calculated images with our experimental investigations confirms the applicability of the developed atomic dislocation model to the propagation of the **a**-type TDs at the SiN interface in the investigated crystal system.

1. Kuwano N, Tsuruda T, Kida Y, Miyake H, Hiramatsu K and Shibata T 2003 *Physica Status Solidi (c)* **0** 2444-7
2. Thapa S B, Kirchner C, Scholz F, Prinz G M, Thonke K, Sauer R, Chuvilin A, Biskupek J, Kaiser U and Hofstetter D 2007 *Journal of Crystal Growth* **298** 383
3. Engl K, *et al.* 2006 *Journal of Crystal Growth* **289** 6
4. Tanaka S, Takeuchi M and Aoyagi Y 2000 *Jpn. J. Appl. Phys.* **39**

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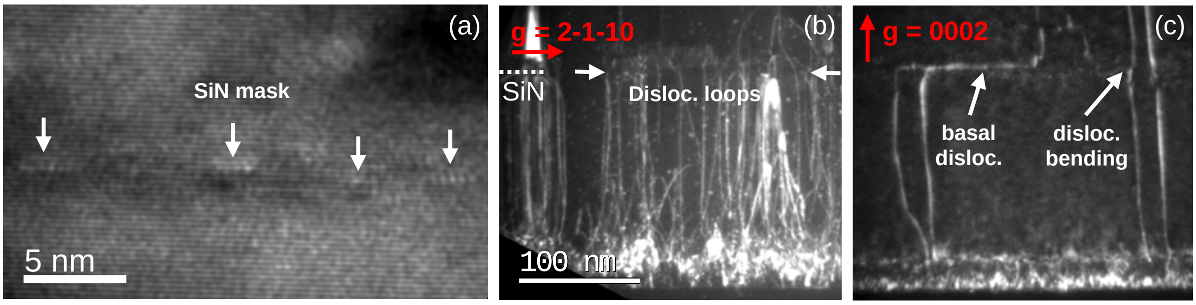

Figure 1. HRTEM (a) and WBDF micrographs in the area of the SiN interface at a zone of high annihilation grade. Image (a) illustrates the fractional coverage of AlGaN with SiN (Si deposition indicated by arrows). The bending of the **a**-type TDs and the annihilation by the formation of dislocation loops is clearly visible in image (b). Image (c) shows the propagation of the TDs with screw component. Even there, the conversion of the TDs into basal dislocations leads to an interaction of the TDs.

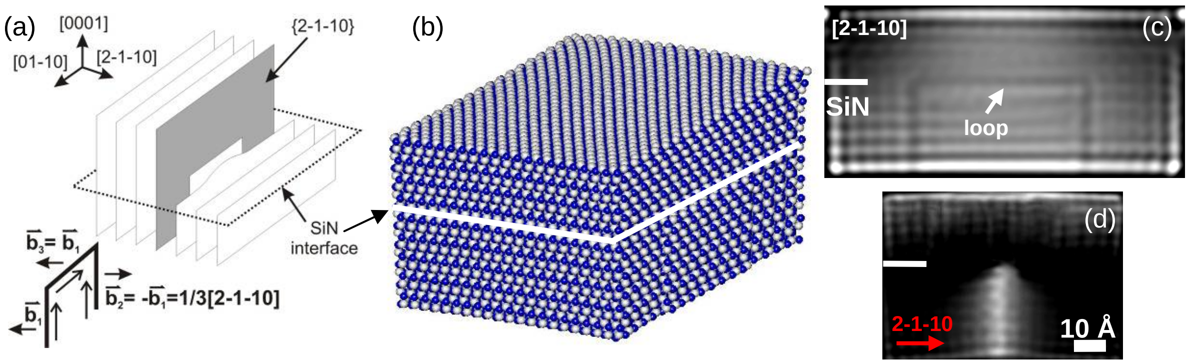

Figure 2. Extended atomic model for the annhilation process of the **a**-type TDs in Al(Ga)N at the SiN interface by the formation of a dislocation loop (a, b). The BF calculation at the [2-1-10] zone clearly shows the dislocation loop created by an **a**-type basal dislocation (c). In the WBDF calculation close to the [01-10] zone the propagation of the dislocation line seems to end at the SiN interface as it was observed in figure 1b (d).