Atomistic scale investigation of dislocations in III-nitride materials.

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Abstract:

III-nitride compounds semiconductors, constituted by gallium nitride (GaN), aluminium nitride (AlN), indium nitride (InN) and their ternary and quaternary alloys are key materials for electronic and optoelectronic devices including light emitters such as LEDs and lasers, as well as high frequency and high-power electronic devices [1,2]. For optoelectronics, they offer the potential of bandgap engineering from near infrared to deep ultraviolet wavelengths, by tuning their alloy compositions [1,3]. Heteroepitaxial growth on structurally and thermally mismatched substrates is at the origin of the introduction of high densities of extended defects, mainly threading dislocations in III-nitride epilayers. Threading dislocations typical densities range from 10^8 to $10^{10}cm^{-2}$.

Dislocations have been proven to have detrimental impact on the performance of GaN-based devices [4]. By introducing gap states, they were found to give rise to parasitic luminescence. They were also demonstrated to behave as strong non-radiative recombination centers, degrading light emission efficiency. By providing pathways to leakage currents, screw TDs were identified to be responsible for electrical shorts in electronic devices. When getting charged, dislocations act as scattering centers, limiting the mobility of charge carriers. Despite their harmful impact, GaN was found to be more tolerant to dislocations than conventional semiconductors. For instance, in the case of GaAs, a TD density as low as 10^4cm^{-2} is usually sufficient to prevent optical device operation.

In this conference, investigations on the impact of dislocations on different properties of III-nitride materials will be presented. These investigations were conducted in the framework of atomistic simulations based on Density Functional Theory (DFT) or empirical potentials. The presented results concern the prediction and the impact of the growth conditions or the growth direction on the atomic core configurations of dislocations in GaN, AlN and InN [5,6]. They concern also, the impact of dislocations on leakage currents in GaN [7,8], and the role of dislocations in the bulk n-type conductivity in InN [9]. Some results concerning the mobility of dislocations under electron beam irradiation [10] and the impact of dislocations on thermal conductivity of GaN [11] will be presented as well.

Key words: Dislocations, core configurations, mobility, thermal conductivity, GaN, AlN, InN, DFT, empirical potentials.

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