Nanocomposites and nanomaterials

Simulation of X-ray Diffraction Profiles for Compositionally Graded $Al_xGa_{1-x}N$ Layers and Nanowires

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The demonstration of *p*-type doping through the so-called polarization doping technique for graded $Al_xGa_{1-x}N$ alloys is finding more practical applications in modern optoelectronic devices. The Al depth profile is the key factor in modifying the properties of $Al_xGa_{1-x}N$ graded layers (GLs) and nanowires (NWs). The different in- and out-of-plane strain profiles resulting from the free surface of NWs leads to the difference in: (i) the polarization-induced doping carrier densities and (ii) the strain-related defects density. Also, there is a difference between the strain profiles of catalyst-free and top-down fabricated NWs obtained by dry etching. Therefore, tuning the properties of $Al_xGa_{1-x}N$ GLs and NWs requires a rapid and reliable characterization of the chemical composition and strain depth profiles.

High resolution X-ray diffraction (HRXRD) is a nondestructive technique that permits rapid determination of the chemical composition, strain state, and thickness of epitaxial GLs. In this study we extend the HRXRD method to the case of graded $Al_xGa_{1-x}N$ NWs produced either by catalyst-free MBE growth or by dry etching of planar structures. The symmetrical *2Theta/omega - scans* for GLs and NWs are calculated through the kinematical theory of X-ray diffraction. The influence of $Al_xGa_{1-x}N$ thickness, Al(%), and deformation distribution on the shape of the intensity profile is studied theoretically. Particular attention is paid to the in-plane lattice parameter relaxation in $Al_xGa_{1-x}N$ NWs due to the free sidewalls and how this compares with continuous coherently grown $Al_xGa_{1-x}N$ GLs. In addition, as opposed to homogeneous dry etched structures, NW inhomogeneity must be considered for catalyst-free grown NWs. Thus, we calculated the XRD profiles for a whole $Al_xGa_{1-x}N$ NWs ensemble taking into account the diameter distribution resulting in a distribution of the in-plane relaxation for a given depth.