X-ray diffraction profiles from dislocations and stacking faults in a-plane AlN films

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The as-grown a-plane AlN films grown by MOVPE on r-plane sapphire contain basal stacking faults, predominantly I_1 type, bounded by partial dislocations. The plane of the basal stacking faults is perpendicular to the film plane and the dislocations bounding them are threading dislocations. After high-temperature annealing at 1680 °C, stacking faults shrink,some of partial dislocations merge into full dislocations or annihilate. This transformation of the real structure is revealed by transmission electron microscopy.

We characterise types and densities of dislocations and stacking faults before and after high-temperature annealing in more detail by combining laboratory X-ray diffraction measurements (rocking curves in skew diffraction geometry and reciprocal space maps) and Monte Carlo simulations of X-ray diffraction from these defects. The extension of our previous Monte Carlo simulations for full dislocations to stacking faults is straightforward and requires to take care of the directions of the cuts in the dislocation displacement fields: the cuts have to be directed along the line connecting the partial dislocations.

The I_1 type basal stacking faults with displacement vectors f=1/6<20-23> are visible (the scalar product g.f is not multiple of 2*pi) in reflections g=(10-10) and (20-20), and invisible in other available reflections. We observe the ~q^-2 intensity decay in these reflections due to stacking faults, and find a stacking fault density of 6x10^5 cm^-1 by Monte Carlo simulations. Further reflections, insensitive to stacking faults, reveal the q^-3 intensity decay due to partial dislocations bounding stacking faults. Monte Carlo modelling of these reflections provides the density of partial dislocations of 6x10^10 cm^-2 and shows that one third of these dislocations are a+c type dislocations dissociated into partials, while the remaining stacking faults are bounded by partials with the opposite Burgers vectors.

Measurements and simulations of the X-ray diffraction curves after high-temperature annealing reveal only full threading dislocations of a+c type with the density of 1x10^10 cm^-2. Hence, the stacking faults bounded by partial dislocations with opposite Burgers vectors shrink and vanish, while the ones bounded by the dissociated a+c dislocations shrink to full a+c dislocations. The measurement and simulations of the reciprocal space maps complement characterisation of the real structure of the as-grown samples by revealing the misfit dislocations of an effective density (taking into account their positional correlations) in the as-gown sample of 1.5x10^6 cm^-1, which reduces on annealing by a factor of 2, by developing stronger correlations.