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Multiplicity vs. Composition Study to Understand the Field Evaporation of Polar $Al_xGa_{1-x}N$ Heterostructures: A New Approach

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Polar AlGaN/GaN heterostructures have proven to be a potential material system in the advancement of high-voltage, high-power, and high-temperature microwave electron device technology [1]. Obtaining compositional and spatial data from these complex heterostructure systems requires an advanced analysis method; such as Atom Probe Tomography (APT). However, there are critical challenges to analyze them in APT; such as trajectory aberration and multi-hit events due to the dissimilar field evaporation. As a result, chemical quantification and determination of interfacial nature become uncertain. Hence a sincere effort to understand the field evaporation mechanism and how it is impacted by heterostructure chemistry is essential. Our aim is to design a protocol for measuring multiplicity and its correlation with the composition to understand the field evaporation behavior across polar heterostructure interfaces. We propose that tracking the occurrence and count of multi-hit events during atom probe analysis can elucidate interfacial chemistry characteristics related to field evaporation. This work will aid in the understanding of how the polarity of the crystals plays a role in the field evaporation.

The heterostructures were grown on GaN crystals with two potential orientations: Ga-polar and N-polar, shown in Fig. 1a and 1b, respectively. The polar heterostructures analyzed in this study consist of four individual $Al_xGa_{1-x}N$ layers with varying concentrations: x = 1.0, 0.7, 0.4, and 0.1. The thickness of these layers is 2 nm each and separated by GaN buffer layers. The heterostructures were previously grown and analyzed in APT for a published study; the details can be found in the literature by Mazumder *et al*. [2]. Figure 1c and 1d show the III-site concentration of Al and Ga, with varying Al concentration across the different layers. Following APT data collection, an EPOS file was generated to obtain 3D spatial data, mass-charge ratio, and multiplicity counts. The ratio of multi-hit events per total hits, shown in Fig. 1e and 1f, was measured sequentially along the analysis direction (z-axis). Each measurement represents the ratio of multi-hit events occurring within a specified volume. Each volume encompasses the cross-sectional area in the xy-plane with 0.5 nm thickness in z. It is observed that the occurrence of multi-hit events drops within layers with decreasing Al concentration [3]. This apparent chemical influence on multiplicity indicates a relationship with field evaporation. Layers with AlN demonstrated higher field compare to other AlGaN and GaN layers in the voltage history and higher multiplicity, marked by evaporation of molecular species ($Al\text{-}N_x$ $N\text{-}N_x$, x = 0-2) [3]. The slope in multiplicity with z-depth indicates the change in multi-hit events while transitioning across heterostructure interfaces. The variation in slope can be seen by the relative number of equidistant points. Peak edges with a visibly greater number of points, for the same height, have a broader slope. For Ga-polar samples, the magnitude of the slope in multiplicity was higher in the AlGaN/GaN interfaces than the GaN/AlGaN interfaces. This is indicated by a broader slope on the left sides (GaN/AlGaN interface) of the peaks in Fig. 1e. The trend reverses for the N-polar sample, where the right sides (GaN/AlGaN interface) of the peaks have a broader slope in Fig. 1f. These also imply that the interfacial nature is influenced by polarity and not an artifact from APT analysis. Interfaces with broader slopes have less abrupt transitions in multiplicity and therefore a less abrupt change in field evaporation.

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Our findings suggest that the polarity impacts the transition in multiplicity in heterostructures, and hence the nature of the interfaces. Our proposed protocol utilizes multiplicity as a metric for interfacial chemistry analysis and can later be applied to other polar heterostructure systems. This work will aid in our continued understanding of how crystal polarity relates to and possibly influences field evaporation.

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[4] The growth and APT analysis of heterostructures were performed at University of California, Santa Barbara in past, we acknowledge Prof. James S. Speck for all the support.

Figure 1. Schematic of (a) Ga-polar and (b) N-polar crystal orientation. III-site concentration across (c) Ga-polar and (d) N-polar heterostructures, percentage of multi-hit events out of the total number of hits along the depth in (e) Ga-polar and (f) N-polar samples. The variation in slope can be seen by the relative number of points, peak edges with a visibly greater number of points for the same height, have a broader slope.

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