Optical Visualization of Radiative Recombination at Partial Dislocations in GaAs

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Abstract—Individual dislocations in an ultra-pure GaAs epilayer are investigated with spatially and spectrally resolved photoluminescence imaging at 5 K. We find that some dislocations act as strong non-radiative recombination centers, while others are efficient radiative recombination centers. We characterize luminescence bands in GaAs due to dislocations, stacking faults, and pairs of stacking faults. These results indicate that low-temperature, spatially-resolved photoluminescence imaging can be a powerful tool for identifying luminescence bands of extended defects. This mapping could then be used to identify extended defects in other GaAs samples solely based on low-temperature photoluminescence spectra.

Index Terms — semiconductor device measurement, photoluminescence, semiconductor epitaxial layers

I. INTRODUCTION

Multijunction photovoltaics have been the leader in solar cell efficiency for over 20 years [1]. For high-efficiency multi-junction photovoltaics, the constituent semiconductor bandgaps must be precisely tuned to the solar spectrum and the resulting heterostructure must be grown with low dislocation densities. These requirements cannot be simultaneously satisfied using lattice-matched materials [2], leading to a trade-off between more-optimal band gaps and higher dislocation densities due to lattice mismatch. Currently the highest efficiency cells avoid this issue either by wafer bonding [2], or by using compositionally-graded buffer layers to minimize the presence of dislocations in specific regions [3]. Since energy devices often contain dislocations that degrade device quality, it is advantageous to develop new tools for characterizing material quality.

In this work, we use a model system to investigate the radiative and non-radiative properties of individual dislocations and stacking faults. We use photoluminescence mapping to image 10 µm-scale extended defects in an ultra-pure GaAs epilayer, finding that different types of dislocations show markedly different luminescence behaviors. This non-destructive technique can be used to characterize individual dislocations in samples where the dislocation density is low compared with the optical resolution (≤ 10⁷ cm⁻²). This work is in stark contrast to other studies of dislocations, which typically explore average material properties as a function of defect densities. Further, the knowledge gained from unambiguous studies of defects in ultra-pure samples can be used to characterize materials where single defects cannot be optically isolated.

II. EXPERIMENT

A. Sample preparation

Stacking fault (SF) structures and associated dislocations are embedded in a 10-µm-thick [001] GaAs epilayer grown by molecular beam epitaxy, see Ref. [4] for details. The stacking fault defects nucleate at the substrate-epilayer interface during epitaxial growth [5, 6]. Two kinds of defects are observed, see Fig. 1 and are depicted schematically in Fig. 2 stacking fault pyramids and stacking fault trapezoids, which are each bordered by dislocations. We will refer to the dislocations surrounding the pyramid as DP_R and DP_NR and those surrounding the trapezoid as DT_R and DT_NR, where the subscript denotes whether radiative (R) or non-radiative (NR) transitions are observed. Since we did not perform structural microscopy, we cannot confirm the identity of the dislocations observed. However, previous studies typically find stacking fault structures to be bordered by stair-rod partial dislocations [7, 8, 9, 10].

B. Photoluminescence imaging

Figure 1(a) shows a low-temperature confocal scan of the sample in which photoluminescence (PL) is excited with an above-bandgap laser. The PL arises from excitons generated in the bulk that bind to extended defects and recombine radiatively. There are four main spectral bands of interest: PL from dislocations, PL from stacking faults, band edge PL, and laser reflection from the sample surface.
Strong photoluminescence is observed at 1.480 eV from the DP_R defect in Fig. 1(a), arising from excitons bound to the dislocation at the intersection of two SFs in a pyramid defect. We also observe luminescence due to excitons bound to the trapezoid edges, which is comprised of a dislocation-SF-dislocation structure as seen in Fig. 2(a). PL at the trapezoid edges shows a large spread of ~20 meV in the center of the PL emission energy. We attribute this to the variable distance between the two edge dislocations in a trapezoid defect [11], leading to a variable binding energy of excitons to the edge. Considering that the typical distance between stacking faults in a trapezoid defect is ~14 nm [11], [12] and the typical SF-bound exciton size is >10 nm [4], the dislocations must play a role in the exciton binding potential at the trapezoid edge. In particular, strong non-radiative recombination at a dislocation would quench the PL. Therefore, we will also refer to the luminescence originating from the trapezoid edges as due to excitons bound to dislocations.

Moreover, at the low experimental temperature (~2 K) even a small excitonic potential of ~1 meV is sufficient to bind excitons. Due to the non-isotropic strain fields surrounding a dislocation, we expect nearly all dislocations to create an attractive potential either to the electron or the hole, thus leading to a bound exciton [13]. Therefore, if no radiative recombination is observed at a dislocation, we conclude that the dislocation is a strong non-radiative-recombination center.

Luminescence from stacking faults is shown in Fig. 1(c)-(d). In comparing Figs. 1(a) and 1(c) we note that the up and down stacking faults show no PL from the dislocations at their edges, while the majority of the left and right stacking faults have strong PL from the adjacent dislocations [directions explained in Fig. 2(b)]. This demonstrates that there are two types of partial dislocations, DT_R and DT_NR, with markedly different effects on charge carriers. These results are in contrast with the typical expectation that dislocations introduce strong non-radiative recombination centers [14], [15], but in line with related experiments where the type of dislocation changes the strength of non-radiative recombination observed [16], [17], [18], [19]. Further, we observe pyramid defects where the dislocations are all D_P_N or all D_P_R, see Fig. 3. In Figs. 3(d) and 3(f), the stacking fault and band-edge PL appear quenched near the D_P_N defects.

The band-edge PL, Figs. 1(e),(f) quenches wherever the stacking faults intersect the surface. Surprisingly, this quenching seems unrelated to the surface oval defects, visible in Fig. 1(g)-(h), which only occur on the left and right stacking faults [20]. Thus surface oval defects do not significantly affect the strength of non-radiative recombination occurring at the intersection of a stacking fault and the sample surface.

Lastly, we found the center-of-mass of the dislocation and stacking-fault PL for each trapezoid defect visible in Fig. 1 and performed a cross-correlation of these two emission energies (Fig. 3). The PL center energy from the dislocation and the nearby stacking fault have a strong inverse correlation. This emission energy is related to the exciton binding energy, which is a function of the inter-stacking-fault distance in the trapezoid defect. Future work incorporating the full solution of the exciton effective-mass wavefunction could elucidate the physical mechanism behind this inverse correlation.

Fig. 1. (a) Confocal scan of dislocations bordering stacking faults. The image is formed by coloring emission in different wavelength bands as red, blue or green, as depicted in b. Both radiative and non-radiative dislocations are observed. (b) Spectra of the sample at colored dots in a. PL is observed at the dislocations bordering the stacking faults. (c-d) Same as a-b except with integration bands centered on the stacking fault bound exciton PL. (e-f) Same as a-b except with integration bands centered on the band edge PL. Dark lines are observed where the stacking faults intersect the sample surface. (f-h) Laser reflection image of sample. The vertical lines are oval defects. Scale bar 10 µm.
These defects may be useful for identifying stacking faults and dislocations in materials with high defect densities where individual defects cannot be optically isolated. For example, stacking fault densities could be estimated by comparing PL intensity to a reference sample. Lastly, we note that stacking faults and dislocations are present in a wide variety of zinc-blende and wurtzite materials, and that the same PL imaging techniques can be used to study other materials.

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