Microsc. Microanal. 22 (Suppl 3), 2016
© Microscopy Society of America 2016

Advancement of Heteroepitaxial III-V/Si Thin Films through Defect Characterization

Julia I. Deitz,[1] David W. McComb,[1], Tyler J. Grassman[1,2]

[1] Dept. of Materials Science & Engineering, The Ohio State University, Columbus, OH, 43210, USA
[2] Dept. of Electrical & Computer Engineering, The Ohio State University, Columbus, OH, 43210, USA

III-V semiconductor materials heteroepitaxially integrated with low-cost Si substrates present a potentially disruptive solar cell technology, providing the combination of highly efficient devices at low manufacturing cost, as well as being relevant to a wide range of other (opto)electronic applications. However, for the integration of materials with significant dissimilarities (e.g. lattice constant, crystal structure, bond chemistry, etc.), various detrimental defects can form and degrade device performance. Of particular interest are misfit and threading dislocations which arise due to lattice mismatch, because they tend to act as charge carrier recombination centers. To date, the detailed mechanisms behind dislocation formation, dislocation dynamics, and dislocation electronic behavior are still not completely understood—especially within a heterovalent system, with its itinerant complexities, like that of III-V/Si—and this information will be imperative for the engineering of higher performance photovoltaics (PV). In this contribution, defect characterization is performed for the GaP/Si system via electron channeling contrast imaging (ECCI), highlighting relevant growth-dislocation relationships along with opportunities for different microscopy methods to gain insight into the nature of the dislocations.

Heteroepitaxial GaP on Si has long been seen as a route for integration of III-V materials and devices with Si substrates and microelectronics due to their relatively small lattice mismatch. Recent developments in overcoming issues related to epitaxy at this heterovalent interface (e.g. antiphase domains, stacking faults), with both molecular beam epitaxy [1] and metalorganic chemical vapor deposition [2], have opened possibilities for its use in the application of III-V/Si multi-junction solar cells. Nonetheless, control of dislocation populations in the GaP/Si system, and thus throughout subsequent III-V epitaxial layers, is still a work in progress. Minimization of dislocation density requires maximization of dislocation glide and minimization of nucleation. To achieve these interrelated goals, a significantly deeper understanding of dislocation formation, interaction, and multiplication mechanisms in such systems must be obtained. Specifically, questions regarding the impact of multiple issues—interface heterovalency, substrate vicinality, step-bunching/faceting, and growth conditions—on dislocation formation and evolution must be addressed.

ECCI performed in a scanning electron microscope has recently surfaced as an ideal technique for defect characterization in heteroepitaxial structures, as it bypasses sample preparation issues associated with transmission electron microscopy and allows for large-scale, high-throughput, nondestructive analysis [3-5]. Here, ECCI is applied to GaP/Si samples with varying GaP thickness (30 – 250 nm) for investigation of misfit dislocation networks, with particular attention to anisotropic dislocation behaviors in the $<\bar{1}10>$ and $<110>$ line directions resulting from fundamental properties of the zinc blende structure, as well as substrate orientation, preparation, and growth conditions. Examination of the onset of critical thickness, along with subsequent dislocation nucleation/evolution, will be presented. Additionally, emphasis will be placed on apparent dislocation-dislocation interactions, such as those indicated in Figure 1(a). The findings will then be related to sample growth to try to bridge the gap between structure, growth, nucleation and interaction information. Also of particular interest is the difference in contrast for dislocations, suggesting the potential of differing core structures, as highlighted in Figure 1(b). These findings demonstrate opportunity for analysis through other microscopy techniques, particularly atomic-resolution HAADF-STEM and electron energy-loss spectroscopy to further understand core structure, as well as ECCI combined with *in-situ* thermal annealing and/or mechanical straining to verify dislocation interactions and reactions. Such work will lend critical insight into dislocation dynamics in this technologically important materials system, providing a basis for the ultimate optimization of heterostructure based electronics.

[1] T. J. Grassman, M. R. Brenner, S. Rajagopalan, R. Unocic, R. Dehoff, M. J. Mills, H. Fraser, and S. A. Ringel, Appl. Phys. Lett. 94, 232106 (2009).
[2] T. J. Grassman, J. A. Carlin, B. Galiana, L. M. Yang, F. Yang, M. J. Mills, and S. A. Ringel, Appl. Phys. Lett. 102, 142102 (2013).
[3] J. I. Deitz, S. Carnevale, S. A. Ringel, D. W. McComb, and T. J. Grassman, J. Vis. Exp., 52745R2, (2015).
[4] S. D. Carnevale, J. I. Deitz, T. J. Grassman, J. A. Carlin, Y. Picard, M. De Graef, S. Ringel, Appl. Phys. Lett. 104(23), 232111, (2014).
[5] S. D. Carnevale, J. I. Deitz, T. J. Grassman, J. A. Carlin, Y. Picard, M. De Graef, and S. A. Ringel, IEEE J. PV., 5(2), 676 (2015).

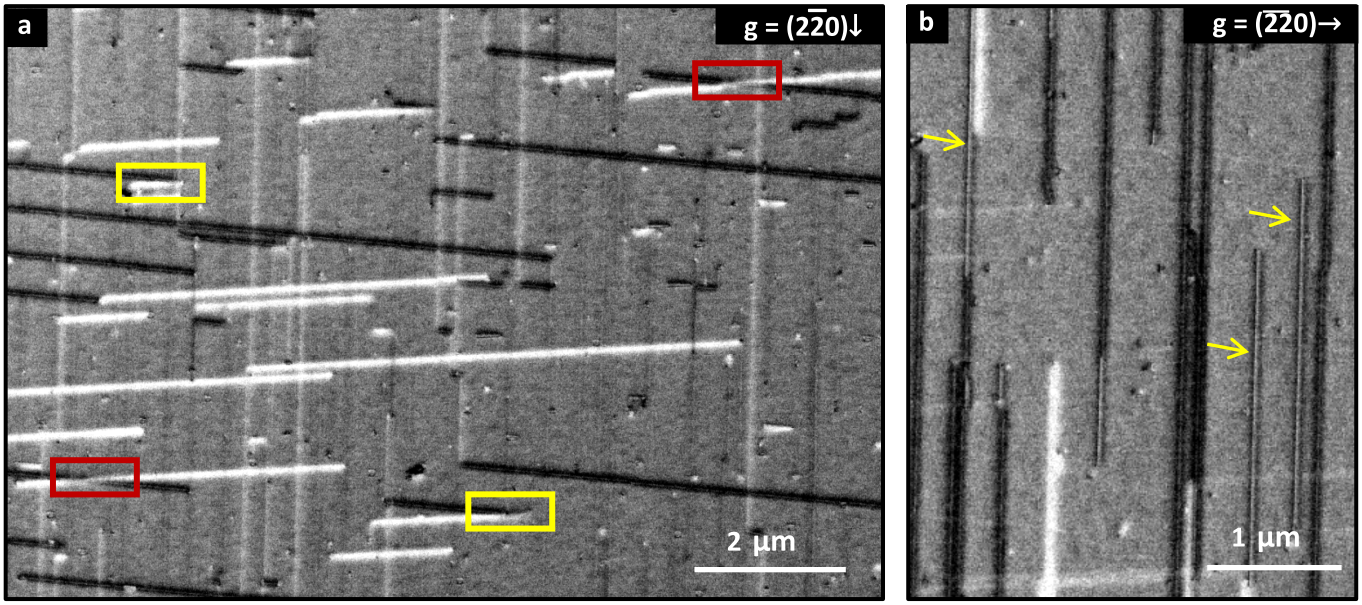

Figure 1. (a) 50nm GaP/Si misfit dislocations in the <110> direction with potential dislocation interactions marked in red and dislocations either starting or ending at the same point marked in yellow and (b) 50nm GaP/Si sample with dislocations showing both bright and dark contrast marked with yellow arrows.