

Abstract Submitted
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The Role of Interface Defects on Phase Selection in ZnO/MgO Core/Shell Nanowires¹ DOMINIC CRITCHLOW, Austin Peay State University, Vanderbilt University, ZHINENG LI, Stony Brook University, Vanderbilt University, XIAO SHEN, CLAIRE MARVINNEY, YEVGENIY PUZYREV, LIDA PAN, JAMES MCBRIDE, RICHARD HAGLUND, SOKRATES PANTELIDES, Vanderbilt University — ZnO nanowires, coated with MgO, have potential for optical devices. The optical properties of the ZnO/MgO coreshell structures depend on the properties of the interface. Both epitaxial interface with wurtzite MgO on ZnO and non-epitaxial interface with rocksalt MgO have been observed. Differences in MgO interface structure poses questions to what type of defects must be present to achieve these different crystal structures. Density functional theory calculations are carried out to explore the role of surface oxygen vacancies and the step edges. The results from DFT calculations show that oxygen vacancies have no effect on the crystal structure. On the other hand, the calculations show that the step edges make rocksalt MgO structure more favorable. TEM images taken on the ZnO nanowires that has rocksalt MgO coating revealed steps in the ZnO Nanowire, confirming the theoretical prediction.

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