Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Crystalline non-polar GaN films grown on vicinal Si: theoretical predictions[1] ALEX KUTANA, STEVEN ERWIN, Naval Research Laboratory, CENTER FOR COMPUTATIONAL MATERIALS SCIENCE TEAM — The ability to grow highly crystalline non-polar GaN films on silicon substrates would be an important advance in optoelectronic device fabrication. We propose a simple strategy to achieve this goal: tilting the Si substrate out of interface plane to provide a good lattice match between the film and substrate. We consider epitaxial interfaces between M-plane GaN and arbitrary Si(hhk) substrates. Using the model introduced in the previous talk, we downselect these substrates using two geometric criteria—low residual strain and short coincidence-lattice period. We then use density-functional theory to compute the interface formation energies of these selected candidates, which include Si(001), (112), (113), (114), and (223). We find that M-plane GaN films have the lowest interface formation energy when grown on the (113) and (112) surfaces. The formation energies are significantly lower than on Si(001) or (111), the substrates most often used for growing GaN. On this basis we predict that Si(113) and (112) substrates will enable growth of non-polar GaN films of higher crystalline quality than can be attained on Si(001) or (111).

[1]Part of this work was performed under the ASEE program at NRL.

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Date submitted: 19 Nov 2011 Electronic form version 1.4