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Crystalline Fe films grown on non-polar GaN: theory and experiment STEVEN ERWIN, Naval Research Laboratory, CUNXU GAO, CLAUDIA RODER, JONAS LAEHNEMANN, OLIVER BRANDT, Paul Drude Institute, Berlin — We report an unexpected mechanism by which single crystals of Fe grow epitaxially on M-plane GaN substrates despite having a different crystal structure and strongly mismatched lattice constant. A simple model is proposed in which one material tilts out of the interface plane to create a coincidence-site lattice that balances two competing geometrical criteria—low residual strain and short coincidence-lattice period. We apply this model, along with complementary first-principles total energy calculations, to the interface formed by molecular-beam epitaxy of cubic Fe on hexagonal GaN and find excellent agreement between theory and experiment. The success of this model also suggests a strategy for growing non-polar GaN films on a substrate material with a suitably chosen Miller index. One very promising material is Si, which is already in widespread use as a flat substrate for GaN/Si epitaxy despite high dislocation densities. The next talk will present our predictions of the most promising Si(hhk) substrates for growing non-polar GaN with high crystalline quality.

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