Strain-Induced Band Gap Variation in InGaN/GaN Short Period Superlattices

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SUPPLEMENTARY MATERIAL

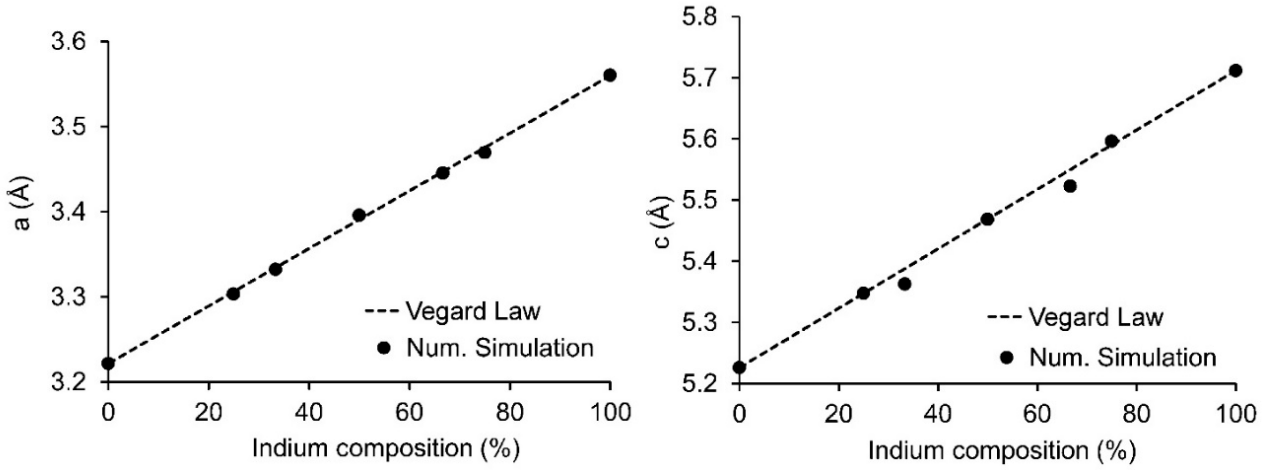

Figure S1. Calculated equilibrium lattice parameters of $In_xGa_{1-x}N$ bulk alloys, with respect to indium composition. A linear behavior is observed, in line with Vegard's law. There is a slight deviation in the *c*-parameter of $In_{33}Ga_{67}N$ and $In_{67}Ga_{33}N$ equal to ~−0.03 Å.

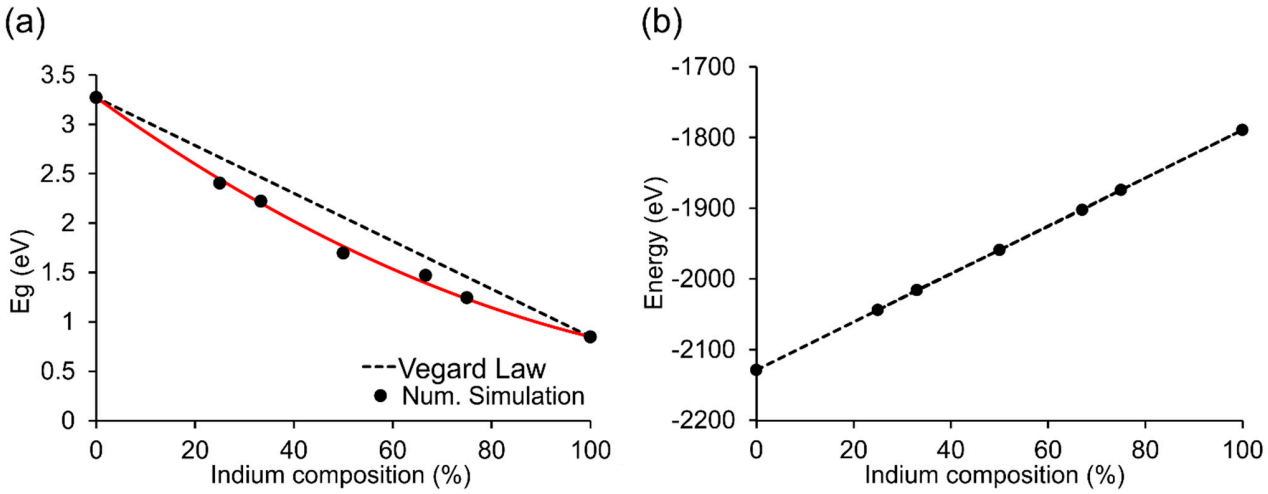

Figure S2. (a) Calculated band gap versus indium composition, of the $In_xGa_{1-x}N$ alloys showing bowing consistent with a bowing parameter of $b = 1.18 \pm 0.09$ eV. (b) Total energy of the $In_xGa_{1-x}N$ supercells per atomic column with respect to alloy composition.

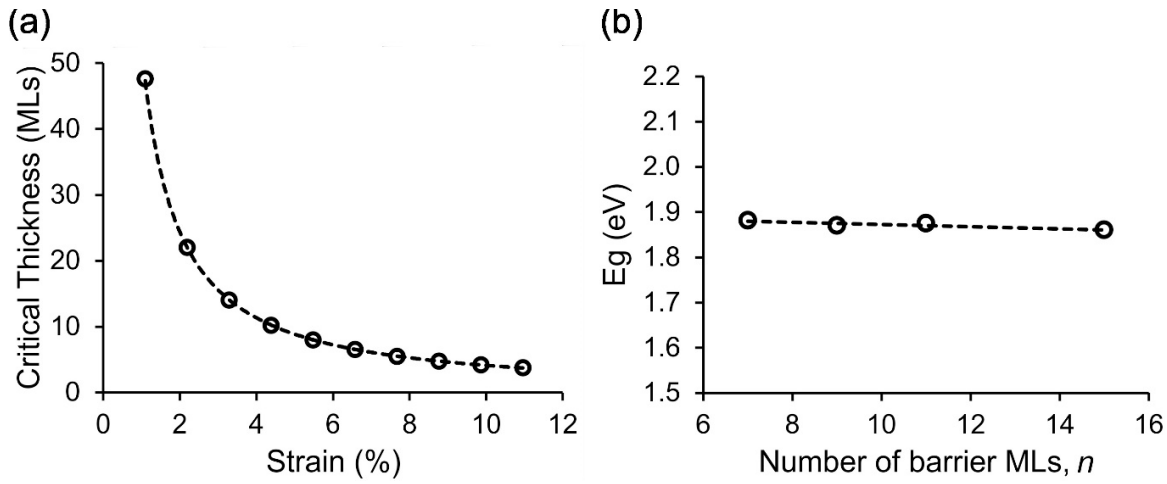

Figure S3. (a) Critical thickness of GaN with respect to the in-plane strain obtained using the model of Fischer et al. [1]. The formation of elastically strained GaN barriers with thickness at least 10 MLs is permitted for in-plane strain values up to ~4%. (b) Band gap variation of 1InN/*n*GaN short-period superlattices as a function of GaN barrier thickness n (unstrained barrier). The dependence of the band gap energy on the barrier thickness is negligible for GaN barriers thicker than 7 MLs.

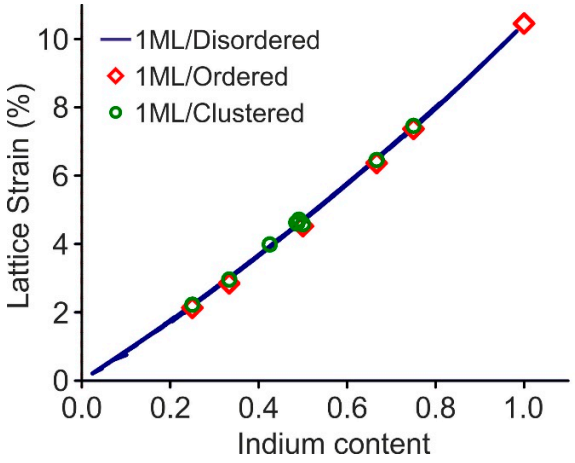

Figure S4. Calculated lattice strain with respect to the indium content for ordered, disordered and clustered $In_xGa_{1-x}N$/GaN quantum wells of one monolayer thickness. The plotted lattice strain is the reduced relative variation of the *c*-lattice constant along [0001] having as reference the *c*-lattice constant of GaN. The disordered quantum wells were obtained from empirical potential calculations as described elsewhere [2]. The ordered and the clustered quantum wells were obtained by both empirical potential calculations and DFT calculations.

References

1. Fischer, A.; Kühne, H.; Richter, H. New Approach in Equilibrium Theory for Strained Layer Relaxation. *Phys. Rev. Lett.* **1994**, *73*, 2712–2715, https://doi.org/10.1103/physrevlett.73.2712.
2. Vasileiadis, I.G.; Lymperakis, L.; Adikimenakis, A.; Gkotinakos, A.; Devulapalli, V.; Liebscher, C.H.; Androulidaki, M.; Hübner, R.; Karakostas, T.; Georgakilas, A.; et al. Substitutional synthesis of sub-nanometer InGaN/GaN quantum wells with high indium content. *Sci. Rep.* **2021**, *11*, 1–13, https://doi.org/10.1038/s41598-021-99989-0.