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**Interfacial segregation and electrodiffusion of dopants in AlN/GaN superlattices** P. BOGUSLAWSKI, IF PAN, PL-02-668 Warsaw, J. BERNHOLC, N. C. State U., Raleigh, NC 27695-7518, N. GONZALEZ SZWACKI, Texas Tech U., Lubbock, TX 79409 — Properties of semiconductors and their devices entirely rely on accurate control of doping and stoichiometry, determined in turn by solubility of impurities and the presence of native defects. In fact, it has been experimentally shown that thermally activated segregation of impurities through heterointerfaces leads to concentration differences that reach two orders of magnitude. We develop a first-principles theory of interfacial segregation in heterostructures and apply it to hydrogen and typical dopants and defects in GaN/AlN superlattices [1]. We show that the equilibrium concentrations of a dopant at two sides of an interface may differ by up to a few orders of magnitude depending on its identity and charge state, and are not directly given by dopant solubilities of bulk constituents. In addition, the presence of strong electric fields in GaN/AlN systems induces field-driven electromigration and accumulation of hydrogen at the appropriate interfaces. [1] P. Boguslawski, J. Bernholc, and N. Gonzalez Szwacki, Phys. Rev. Lett. 96, 185501 (2006).

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