

## **Analysis of strain and validity of Vegard's law in the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ semiconductor thin films**

A.V. Davydov<sup>1</sup>, W.J. Boettinger<sup>1</sup>, A.J. Shapiro<sup>1</sup>, N. Sanford<sup>1</sup>, V. Soukhoveev<sup>2</sup>, V. Dmitriev<sup>2</sup>,  
and S. Keller<sup>3</sup>

<sup>1</sup> NIST, Gaithersburg, MD; <sup>2</sup> TDI, Inc., Silver Spring, MD; <sup>3</sup> University of California, Santa-Barbara, CA

$\text{Al}_x\text{Ga}_{1-x}\text{N}$  semiconductor thin films are important materials for optoelectronic and electronic applications, such as bright UV- and visible light-emitting diodes, power devices etc. For device engineering, it is essential to know the compositional dependence of band-gap,  $E_g$ , in these alloys. Evaluation of the  $E_g$  vs.  $x$  requires accurate determination of alloy composition, which is often inferred from postulated Vegard's law for  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  lattice parameters vs.  $x$ . Therefore, reliable compositional dependence of lattice parameters (both stressed and stress-free) is needed to estimate  $x$  in films of unknown composition by applying calibration curves to experimental lattice parameters determined from XRD.

This paper examines validity of Vegard's law in the GaN-AlN system by exploring relationship between measured (stressed), calculated (stress-free) wurtzite lattice parameters and independently determined composition  $x$  in HVPE and MOCVD grown  $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{c-sapphire}$  films. The  $a$  and  $c$  lattice parameters in  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  alloys were measured by XRD Bond-method on (00.6) and (20.5) reflections. The film compositions were calibrated by two independent methods, RBS and EDS, which agreed within 2 at. %.

Experimental measurements combined with strain-stress modeling revealed positive deviation from Vegard's law in this system with evident bowing remaining even for the stress-free  $a_0$  and  $c_0$  lattice parameters as well as for the unit cell volume,  $V_0$ . Validated  $a_0(x)$  and  $c_0(x)$  dependencies can further be applied for evaluation of  $x$  in  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  films with unknown composition.

Notably, positive bowing in  $V_0(x)$  correlates with positive enthalpy of mixing in  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  alloys. Possible origin of deviation from Vegard's law and its relation to thermodynamic properties in Al-Ga-N system will be discussed.