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Towards Molecular Dynamics Simulations of InGaN Nanostructures

X. W. Zhou, and R. E. Jones
Sandia National Laboratories, Livermore, CA 94550, USA

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Introduction

Molecular-dynamics (MD) simulations helps improve $In_xGa_{1-x}N$/GaN nanostructures that underpin solid-state-lighting applications. To enable such simulations, we have developed an InGaN Stillinger-Weber (SW) potential. We demonstrate that our potential not only captures well the experimental lattice constants, cohesive energies, and elastic constants of wurtzite GaN and InN, but also enables direct MD simulations of crystalline growth of InGaN structures.

Stillinger-Weber Potential

SW potential can be expressed as

$$E = \frac{1}{2}\sum_i \sum_{j\neq i}\left[V_{IJ}^R(r_{ij}) - V_{IJ}^A(r_{ij}) + u_{IJ}(r_{ij}) \sum_{k\neq i,j} u_{IK}(r_{ik}) \left(\cos\theta_{jik} + \frac{1}{3}\right)^2 \right]$$

$$V_{IJ}^R(r) = A_{IJ}\cdot\varepsilon_{IJ}\cdot B_{IJ}\left(\frac{\sigma_{IJ}}{r}\right)^4 \cdot \exp\left(\frac{\sigma_{IJ}}{r - a_{IJ}\cdot\sigma_{IJ}}\right)$$

$$V_{IJ}^A(r) = A_{IJ}\cdot\varepsilon_{IJ}\cdot \exp\left(\frac{\sigma_{IJ}}{r - a_{IJ}\cdot\sigma_{IJ}}\right)$$

$$u_{IJ}(r) = \sqrt{\lambda_{IJ}\cdot\varepsilon_{IJ}}\cdot \exp\left(\frac{\gamma_{IJ}\cdot\sigma_{IJ}}{r - a_{IJ}\cdot\sigma_{IJ}}\right)$$

Where ε_{IJ}, σ_{IJ}, a_{IJ}, A_{IJ}, B_{IJ}, λ_{IJ}, and γ_{IJ} are parameters.

InGaN SW Potential Parameters

Table I. SW potential parameters for In-Ga-N (energy in unit eV and length in unit Å).

pair ij	ε	σ	a	A	B	λ	γ
InIn	2.449833	1.938334	1.622254	7.9170	0.970030	32.5	1.2
GaGa	2.926384	1.759683	1.607120	7.9170	0.995618	32.5	1.2
NN	4.420186	1.726983	1.630012	7.0496	0.969832	32.5	1.2
InN	2.202060	1.852758	1.799906	7.0496	0.761521	32.5	1.2
GaN	2.289660	1.715927	1.799677	7.0496	0.641026	32.5	1.2
InGa	1.984319	1.769153	1.710916	7.0496	0.865982	32.5	1.2

InGaN SW Potential Characteristics

Table II. Relaxed energies (eV/atom) of selected structures: face-centered cubic (fcc); hexagonal-closely-packed (hcp); body-centered-cubic (bcc); simple-cubic (sc); diamond-cubic (dc); zinc-blende (zb); wurtzite (wz); NaCl (B1); and CsCl (B2). Note that numbers in bold highlight the lowest energies.

element	fcc, hcp (target)	bcc	sc	dc
In	**-2.4894**	-2.3823	-2.1875	-2.0974
Ga	**-2.7930**	-2.6426	-2.4023	-2.2398
N	**-3.8382**	-3.7026	-3.4863	-3.4572
alloy	wz, zb (target)	B1	B2	
InGa	**-2.3771**	-2.1595	-2.1930	
compound	wz, zb (target)	B1	B2	
InN	**-3.7702**	-3.0619	-2.8583	
GaN	**-4.4012**	-3.4481	-3.1706	

Table III. Predicted and experimental cohesive energies (eV/atom) of lowest energy phases of elements and compounds.

	In	Ga	N	InN	GaN
prediction	-2.4894	-2.7930	-3.8382	-3.7702	-4.4012
experiment	-2.4894	-2.7930	-3.8382*	-3.7702	-4.4012

experiment: I. Barin, Thermochemical Data of Pure Substances (VCH, Weinheim, 1993)

*: from our density function theory calculations

Table IV. Predicted and experimental (in parenthesis) lattice constants a and c (Å^3), bulk modulus B (eV/Å^3), and elastic constants C_{11}, C_{12}, C_{13}, C_{44} (eV/ Å^3) for wz and zb structures of InN and GaN.

phase	a	c	B	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}
InN-wz	3.517 (3.533[a])	5.743 (5.692[a])	0.897 (0.897[b])	1.566 (1.373[b])	0.598 (0.749[b])	0.526 (0.568[b])	1.637 (1.554[b])	0.441 (0.225[b])
InN-zb	4.974	-----	0.897	1.408	0.641	0.641	1.408	0.555
GaN-wz	3.175 (3.180[a])	5.184 (5.166[a])	1.206 (1.206[c])	2.274 (2.353[c])	0.717 (0.999[c])	0.626 (0.712[c])	2.365 (1.305[c])	0.716 (0.508[c])
GaN-zb	4.489	-----	1.206	2.059	0.780	0.780	2.059	0.869

a: J. D. H. Donnay, and H. M. Ondik, Crystal Data, Determinative Tables, 3rd ed., Vol. 2, Inorganic Compounds (U.S. Department of Commerce, National Bureau of Standards, and Joint Committee on Power Diffraction Standards, U.S.A., 1973).

b, c: B. Derby, Phys. Rev. B, 76, 054126 (2007).

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Growth Simulations

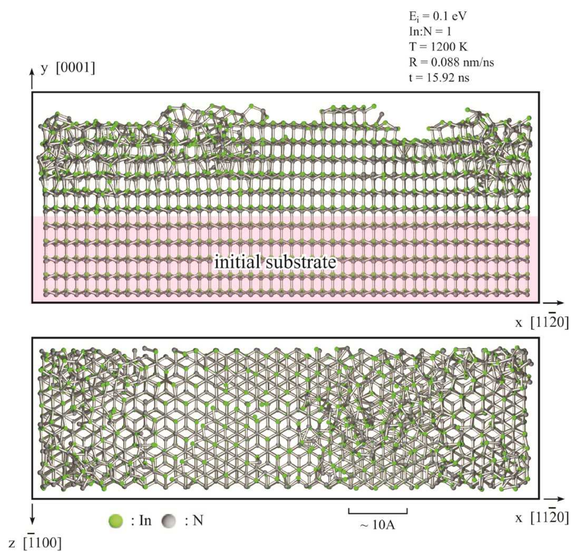

Fig. 1. Crystalline growth of InN.

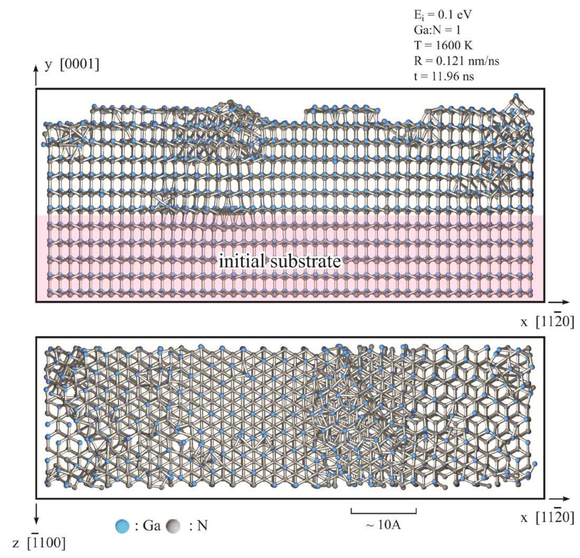

Fig. 2. Crystalline growth of GaN..

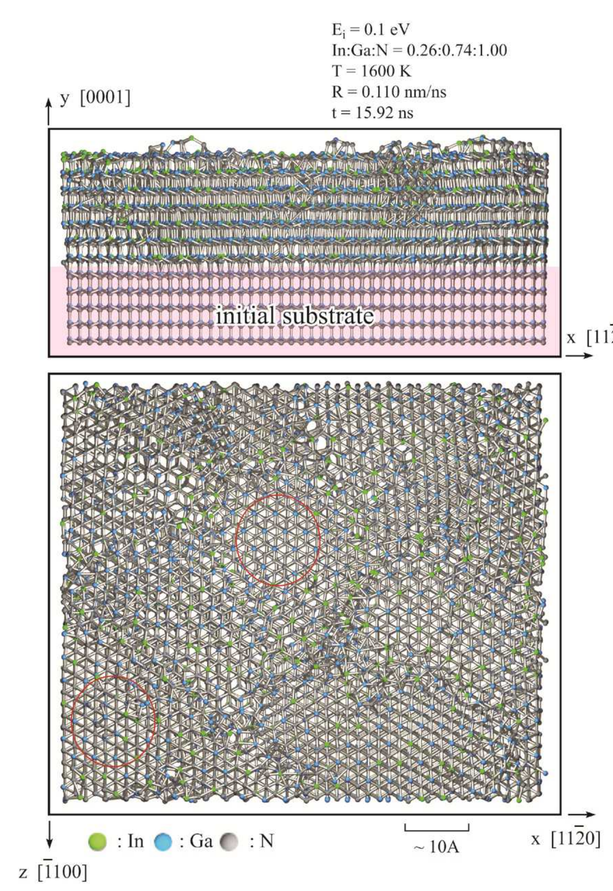

Fig. 3. Crystalline growth of $In_{0.26}Ga_{0.74}N$ on GaN.

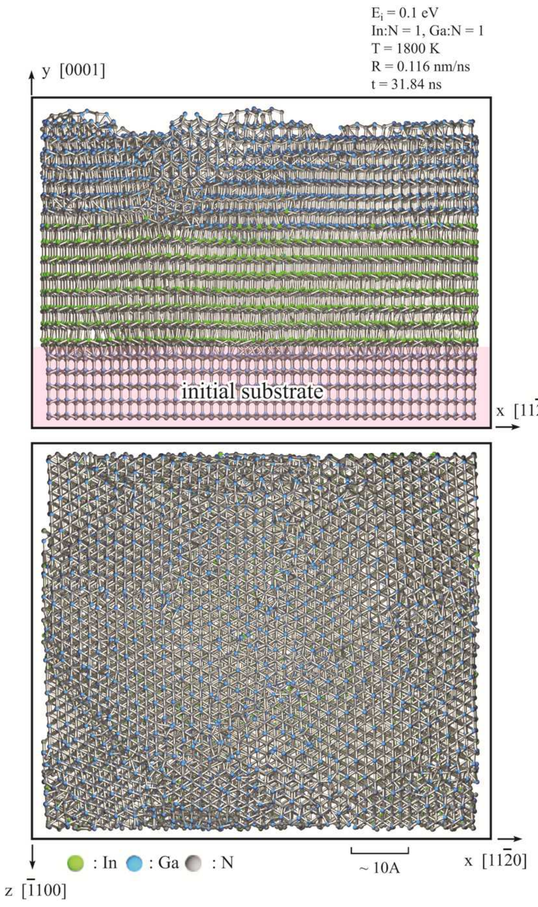

Fig. 4. Crystalline growth of GaN/InN bilayer on GaN.

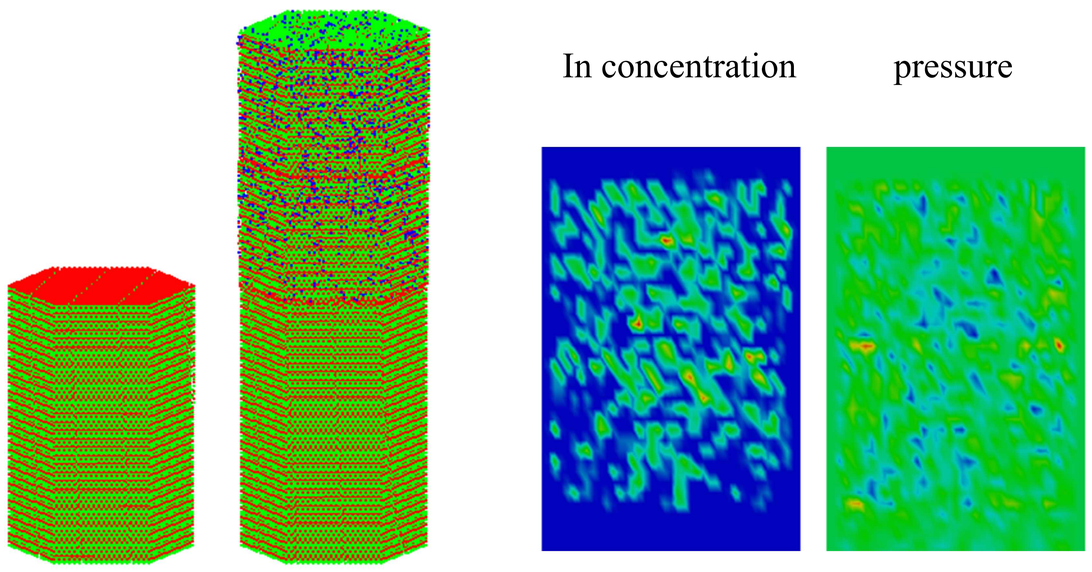

Fig. 5. Growth of a 10% In-GaN pillar on a pure GaN stock. In concentration and pressure distribution in the deposited region allow analysis of the structure.

Conclusions

New molecular dynamics models have been developed for In-Ga-N systems. These new methods are beginning to enable predictive simulations of InGaN growth, and theoretical exploration of nanostructures for defect reduction.