Strain effects on the electronic properties of 2-dimensional nitrides

Abdelhakim Meziani[a,b] , Nada Belmokhi[a] ,Hilmi Unlu,[c]
[a]Physics Department Frères Mentouri University Constantine, 25000 Algeria.
[b]Laboratory of Microelectronics and instrumentation,Electronics department, Frères Mentouri University Constantine, 25000 Algeria.
[c] Faculty of Science and Letters, Department of Physics Engineering, İstanbul Technical University, Istanbul, Turkey

2D nitrides

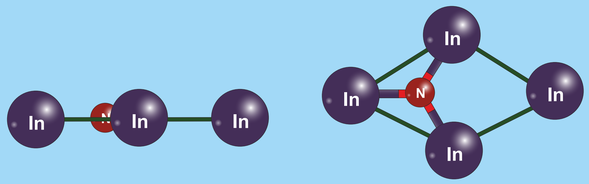
The Nobel Prize awarded to Nakamura acknowledged that bulk group-III nitrides like GaN, AlN and InN are important materials. They are used for a very wide range of applications such as solid-state lighting, LED, laser and photovoltaics [1].

Two-dimensional materials such as III-Nitrides (III-N) have been making a fuss in the material sciencefield lately because of their unique physico-chemical properties and rare physical phenomena, that might allow electronics to be smaller.

Experimentally, scientists successfully were able to grow AlN and GaN sheets by epitaxy growth techniques on transferred graphene Si substrates [2], but for 2D InN, its realization hasn't seen light yet.

Physical Properties of 2D Nitrides

Monolayered AlN, InN and GaN nano sheets have flat honeycomb structure of 2D nitrides is similar to that of graphene, but with polar bonds owing to the distinct electronegativity of the lattice atoms .



Unit cell atomic structure of 2D InN in different views

		AlN (Å)	GaN (Å)	InN (Å)
Lattice parameter 2D nitrides	Our work	3.129	3.212	3.570
	Others	3.123	3.25	3.616
Band gap 2D ntrides	Our work (HSE)	3.991	3.446	1.592
	Others	4.06 [i]	3.23 [i]	1.721
Experimental of bulk wurtzite nitrides	Lattice parameter	3.113	3.19	3.53
	Band Gap	6.2	3.4	0.6
	Experimental	3.113	3.19	3.53

Lattice parameter and band gap energy of 2D and bulk AlN, GaN and InN

Computational methods

Our first-principles calculations are based on DFT using the Quantum Espresso package and the pseudo-potential method and ultra-soft pseudopotentials.

The exchange-correlation potential is approximated the Perdew–Burke-Ernzerhof approximation (PBE) and the Heyd-Scuseria-Ernzerhof hybrid (HSE06) for the electronic structure calculation.

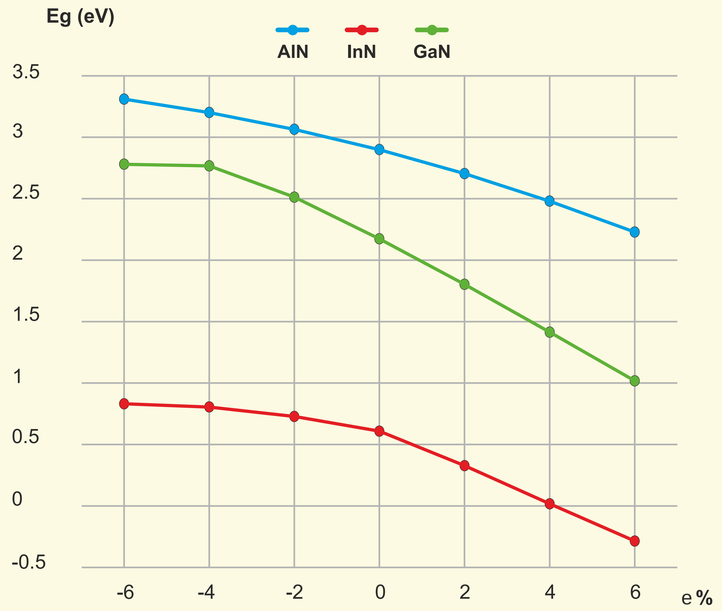
The plane wave basis set was defined by energy cut-off at 40 Ry and a 12x12x1 k-point grid in the first-Brillouin zone for all the previous 2D materials To exclude interactions between neighbor slabs, we used a 15 A° vacuum space in the z direction perpendicular to the monolayer surface

Effect of strain on the electronic structure

Among many techniques such as doping, chemical functionalization, biaxial strain also can be effective to tailor the electronic properties and energy band structure of a 2D semiconductor.

The strain results in a displacement of both the conduction and valence bands, leading to the variation of the primary band gap which is the main interest to fabricate under-strain operation devices.

A biaxial compressive and tensile strain from -6% to 6% was applied on our structures affecting their energy band structures, band gaps, effective masses.



2D AlN, InN and GaN's band gap energy in function of strain percentage

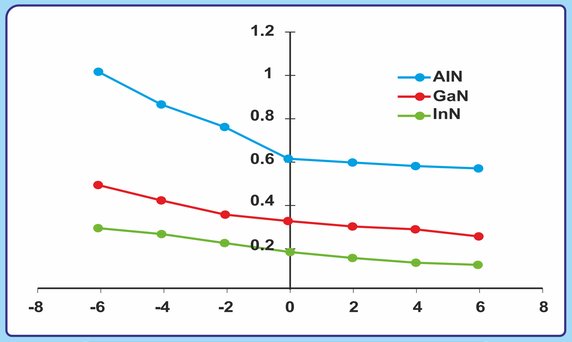
For 2D ALN InN and GaN, Gap energy increases whenapplied strain is compressive strain applied, and decreases when strain applied is tensile. With AlN gap remains indirect and shifts from direct to indirect at 2% of strain for InN and shift from indirect to direct at -4% of strain for GaN.

Variation of the electron effective mass with applied stress

The effective mass and of AlN, InN and GaN can be tuned effectively by different strain %

When the structures are under a compressive strain, we notice the increase of the effective mass of electron and the decrease of the effective mass of hole for all the compounds.

When the structures are under a tensile strain, we notice the decrease of the effective mass of electron and the increase of for all the compounds



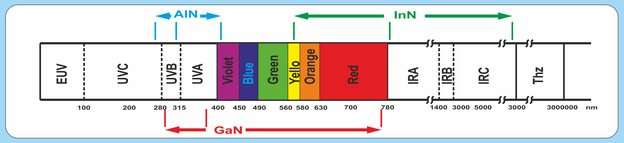
Calculated electron effective mass in function of strain percentages, for 2D AlN, GaN and InN

Change in emission spectra

The effective mass and of AlN, InN and GaN can be tuned effectively by different strain %

When the structures are under a compressive strain, we notice the increase of the effective mass of electron and the decrease of the effective mass of hole for all the compounds.

When the structures are under a tensile strain, we notice the decrease of the effective mass of electron and the increase of for all the compounds



References

[1] Nakamura, Shuji.. Reviews of Modern Physics 87, no 4 (2015): 1139 51
[2] Al Balushi et al. Nature Materials 15, no 11 (2016): 1166 71.
[3] Paolo Giannozzi; Stefano Baroni Journal of Physics: Condensed Matter. 21 (39)
[4] John P. Perdew, Kieron Burke, and Matthias Ernzerhof, Physical Review Letter, 77, 3865. (1996).
¡5] J. Heyd, G. E. Scuseria, and M. Ernzerhof, The Journal of Chemical Physics 118, 8207 (2003).