



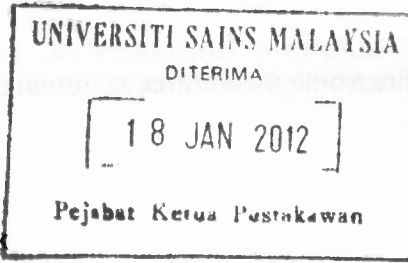
USM

**UNIVERSITI
SAINS
MALAYSIA**

Pejabat Pengurusan Dan Kreativiti Penyelidikan
Research Creativity and Management Office

No. Fail : F0358
Tarikh : 2nd Disember 2011

Dr. Yoon Tiem Leong
Pusat Pengajian Sains Fizik
Universiti Sains Malaysia



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Tuan,

LAPORAN AKHIR SKIM GERAN PENYELIDIKAN FUNDAMENTAL (FRGS)

Tajuk Projek : Ab Initio Study of Electronic Structures of Advanced Solid Materials
No. Akaun : 203/PFIZIK/671169

Dengan hormatnya perkara di atas dirujuk.

2. Terlebih dahulu saya ucapkan ribuan terima kasih di atas satu salinan laporan akhir untuk projek penyelidikan seperti tajuk di atas.
3. Adalah dimaklumkan walaupun projek ini telah selesai, kerjasama Jabatan Bendahari dipohon untuk menguruskan penutupan akaun projek pada selewat-lewatnya **31 Disember 2011**. Tempoh ini bertujuan untuk menyelesaikan semua urusan tuntutan dan bayaran yang telah dibelanjakan di dalam tempoh projek. Walau bagaimanapun, tuan dinasihatkan supaya tidak mengeluarkan borang-borang pesanan baru di dalam tempoh ini.
4. Selanjutnya sila ambil perhatian terhadap perkara-perkara berikut sekiranya berkaitan:
 - (i) Semua penerbitan harus merakamkan penghargaan kepada **Skim Geran Penyelidikan Fundamental (FRGS)** dan tuan dipohon mengemukakan satu salinan ke Pejabat ini.
 - (ii) Bahagian Penyelidikan & Inovasi boleh/akan mengagihkan semula peralatan yang telah dibeli menggunakan peruntukan geran ini seandainya terdapat penyelidik lain yang memerlukan peralatan tersebut.
5. Akhir sekali, tahniah di atas usaha dan kejayaan pihak tuan dapat menyelesaikan projek ini dengan jayanya.

Sekian, terima kasih.

“BERKHIDMAT UNTUK NEGARA”
‘Memastikan Kelestarian Hari Esok’

Yang menjalankan tugas,


(AMRA OTHMAN)
Penolong Pendaftar
Unit Pengurusan Geran & Kontrak

HAN, HAR. SM

LAPORAN AKHIR SKIM GERAN PENYELIDIKAN FUNDAMENTAL (FRGS)


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s.k. Dekan Penyelidikan
Pelantar Sains Fundamental
Pejabat Pelantar Penyelidikan
Universiti Sains Malaysia

Dekan
Pusat Pengajian Sains Fizik
Universiti Sains Malaysia

Timbalan Dekan
(Pengajian Siswazah & Penyelidikan)
Pusat Pengajian Sains Fizik
Universiti Sains Malaysia

 Ketua Pustakawan
Perpustakaan Hamzah Sendut
Universiti Sains Malaysia

Penolong Bendahari Kanan
Unit Kumpulan Wang Penyelidikan
Jabatan Bendahari
Universiti Sains Malaysia

Pegawai Sains
Pelantar Sains Fundamental
Pejabat Pelantar Penyelidikan
Universiti Sains Malaysia

} Disampaikan satu salinan laporan akhir projek untuk simpanan Perpustakaan

} Mohon kerjasama pihak puan untuk menguruskan penutupan akaun projek selewat-lewatnya pada **31 Disember 2011** dan mohon kemukakan satu salinan penyata kewangan terakhir ke Pejabat ini untuk tujuan rekod



FINAL REPORT FUNDAMENTAL RESEARCH GRANT SCHEME (FRGS)

Laporan Akhir Skim Geran Penyelidikan Asas (FRGS) IPT

Pindaan 1/2010

A RESEARCH TITLE : Ab initio study of electronic structures of advanced solid materials
Tajuk Penyelidikan

PROJECT LEADER : Dr. Yoon Tiem Leong
Ketua Projek

PROJECT MEMBERS : 1. Dr. AHMAD PUAAD HI. OTHMAN (SCHOOL OF APPLIED PHYSICS FACULTY OF SCIENCE (including GRA) AND TECHNOLOGY, Universiti Kebangsaan Malaysia)
Ahli Projek

PROJECT ACHIEVEMENT (*Prestasi Projek*)

ACHIEVEMENT PERCENTAGE					
Project progress according to milestones achieved up to this period	0 - 50%	51 - 75%	76 - 100%		
Percentage		√			
RESEARCH OUTPUT					
Number of articles/ manuscripts/ books <i>(Please attach the First Page of Publication)</i>	Indexed Journal		Non-Indexed Journal		
	Surface and interface phonon polaritons of wurtzite GaN thin film grown on 6H-SiC substrate, S. S. Nga, T. L. Yoon, Z. Hassan, and H. Abu Hassan, Applied Physics Letters, 94, 241912 (2009).		NIL		
Conference Proceeding <i>(Please attach the First Page of Publication)</i>	International		National		
	NIL		NIL		
Intellectual Property <i>(Please specify)</i>	NIL				
HUMAN CAPITAL DEVELOPMENT					
Human Capital	Number				Others <i>(please specify)</i>
	On-going		Graduated		
Citizen	Malaysian	Non Malaysian	Malaysian	Non Malaysian	
PhD Student	NIL	NIL	NIL	NIL	
Master Student	NIL	NIL	NIL	NIL	
Undergraduate Student	NIL	NIL	4	NIL	

Total

4

PROBLEMS / CONSTRAINTS IF ANY (*Masalah/ Kekangan sekiranya ada*)

E Despite earnest, I failed to find interest postgraduate candidates to take up the challenge to perform the ab initio calculation. The lack of research experience in such kind of first-principles calculations also leads to some technical difficulties to produce more concrete results.

RECOMMENDATION (*Cadangan Penambahbaikan*)

F Concerted collaboration between experimentalists with theoreticians should be the way how good physics research conducted. This ab-initio calculations research project has laid a good start for such kind of collaboration model. It is recommended to continue the existing research effort so that more quality research results could be produced as a result of such a collaborative research model.

EXPENDITURE (Perbelanjaan)

C Budget Approved (Peruntukan diluluskan) : RM 25200
 Amount Spent (Jumlah Perbelanjaan) : RM 19551.16
 Balance (Baki) : RM 5648.84

(Peratusan Belanja)

ADDITIONAL RESEARCH ACTIVITIES THAT CONTRIBUTE TOWARDS DEVELOPING SOFT AND HARD SKILLS
 (Aktiviti Penyelidikan Sampingan yang menyumbang kepada pembangunan kemahiran insaniah)

D

International		
Activity	Date (Month, Year)	Organizer
(e.g : Course/ Seminar/ Symposium/ Conference/ Workshop/ Site Visit)	14th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, January 2009.	ICTP, Italy
	Research visit for a two weeks research visit. 26 Nov 2007-14 Dec 2007.	Computational condensed matter physics group, National University of Singapore (Prof. Feng Yan Ping's group)
	14th WIEN2k – WORKSHOP, 6-9 July 2007.	Institute of High Performance Computing, Singapore
	Sabbatical leave for 7 Months, Jun 2009 – Dec 2010.	Delft University of Technology, the Netherlands.
MSSC 2009 ab initio Modelling in Solid State Chemistry (Workshop), 14 – 18 Sept 2009.	Imperial College, London.	
National		
Activity	Date (Month, Year)	Organizer
(e.g : Course/ Seminar/ Symposium/ Conference/ Workshop/ Site Visit)	KURSUS LATIHAN MATLAB, 26 Feb 2008	Solutions 4U Sdn. Bhd

G The physical properties of crystalline solid materials are determined by the electronic structure at the atomic scale. This is a many-body, complex quantum system governed by the Schroedinger equation. DFT is a Nobel-prize winning, well-established first-principles approach to calculate electronic and other physical properties of crystalline solids. DFT has made it a practical feasibility to carry out numerical computation to obtain realistic properties of solid state systems. On the other hand, many works have been done by USM school of Physics solid state experimentalists in Gallium-based materials (e.g. AlGa_N, GaN). We propose to make use of the current DFT software packages to simulate and compute the electronic, optical, magnetic and other physical properties of those solid state samples from first principles. This project proposes to check, reproduce, refine, and improve on the DFT results against the Gallium-based materials fabricated and characterized by our local experimental groups. The long term aim is to build up our local expertise in DFT research (not limited to only simulating Gallium-based materials) so that we could perform our own DFT calculations to complement local solid state experimental efforts in the research for other novel materials in the future. (193 words)

Date : 9 March 2011
Tarikh

Project Leader's Signature: Yoon Tiem Leong
Tandatangan Ketua Projek

Name:

Nama:

Date:

Tarikh:

Signature:

Tandatangan:

Surface and interface phonon polaritons of wurtzite GaN thin film grown on 6H-SiC substrate

S. S. Ng,^a T. L. Yoon, Z. Hassan, and H. Abu Hassan

School of Physics, Universiti Sains Malaysia, 11800 Minden, Pulau Pinang, Malaysia

(Received 13 April 2009; accepted 22 May 2009; published online 19 June 2009)

Surface and interface phonon polaritons of wurtzite GaN thin film grown on 6H-SiC substrate are investigated experimentally and theoretically. Two strong absorption peaks that correspond to the surface and interface phonon polaritons are clearly observed at 710 and 916 cm^{-1} , respectively. This observation is in good agreement with the results simulated using an anisotropy model. Finally, the obtained surface phonon polariton (SPP) mode is compared with the reported result. It is revealed that the SPP mode in the wurtzite GaN thin film is shifted toward higher frequency as compared to that in the wurtzite bulk GaN. © 2009 American Institute of Physics.

[DOI: 10.1063/1.3157130]

Gallium nitride (GaN) is a wide band gap III-V semiconductor. It is an important material for optoelectronic applications operating in the blue and near ultraviolet wavelength region.¹⁻³ For this reason, research activity in this material as well as its related alloys has experienced explosive growth in the past few decades.

To date, much of the research devoted to GaN has been directed toward the understanding of its Brillouin zone center optical phonon properties. In contrast, the study of surface phonon polariton (SPP) properties is rarely reported and has not received sufficient attention. In 1997, Davydov *et al.*⁴ studied the surface and interface phonon polariton (IPP) of cubic GaN epitaxial layers grown on (001) GaAs substrates by using Raman scattering. In 2000, Torii *et al.*⁵ carried out investigations on wurtzite bulk GaN by means of attenuated total reflection (ATR) method. Recently, we reported the SPP properties of wurtzite AlN, GaN, and Al_{1-x}Ga_xN (0 ≤ x ≤ 1) thin films grown on sapphire substrates using the ATR method.⁶⁻⁸ Due to both the superimposed of these films reststrahlen bands with that of the sapphire substrate and the complexity of the optical phonon modes of the sapphire substrate, we were unable to detect any IPP mode from these measurements. For GaN thin film, the obtained SPP is still a bulk-like mode due to the penetration depth of the evanescent waves (EWs) being comparable to the thickness of the GaN epilayer. Very recently, Zhang⁹ deduced the dispersion relations of the SPP modes in the wurtzite thin film. However, it was only based on vacuum-film-vacuum structure. Besides that, the effects of the substrate on the SPP mode are not taken into consideration. As a consequence, the fundamental properties of SPP and IPP of wurtzite GaN thin film grown on wurtzite substrate still remain unclear.

In this work, we report on the SPP and IPP of wurtzite GaN thin film grown on wurtzite 6H-SiC substrate. In order to investigate the SPP and IPP, a relatively thin wurtzite GaN thin film grown on 6H-SiC substrate is used. The other reasons for using this structure are that the GaN and 6H-SiC have single optical phonon mode and their reststrahlen regions are well separated. Thus, the SPP and IPP from this structure can be figured out more clearly.

Hydride vapor phase epitaxial growth GaN wafer from Technologies and Devices International, Inc., USA, was used in this study. The GaN epilayer was grown on 6H-SiC substrate using a relatively thin AlGaN buffer layer. The wurtzite structure GaN epilayer was unintentionally doped n-type with carrier concentration of about $3 \times 10^{17} \text{ cm}^{-3}$, and its thickness was about 0.34 μm . The full width at half maximum (FWHM) of (0002) diffraction plane of the GaN thin film is about 259 arcsec, as measured by x-ray diffraction rocking curves at omega scan mode. The cross sectional structure of this sample was scanned with field emission scanning electron microscope (SEM, Leo Supra 50 VP) at an accelerating potential of 10 kV.

Room temperature p-polarized IR ATR measurements were carried out using a Fourier transform IR spectrometer (Spectrum GX FTIR, Perkin-Elmer) and an optional ATR with germanium (Ge) single reflection plate (MIRacle, PIKE Technologies). The polarized spectra were recorded at a spectral resolution of 2 cm^{-1} , and the number of scans was 128. Detailed description of the experimental setup is given elsewhere.⁷

Figure 1 shows the cross sectional SEM image of the GaN thin film grown on 6H-SiC substrate at magnification of 50 000 \times . It is clearly seen that there is only one single layer (GaN epilayer) above the 6H-SiC substrate; whereas the

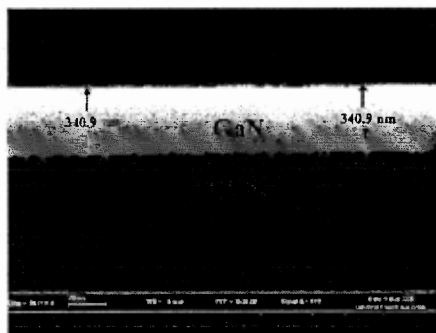


FIG. 1. SEM cross sectional image of GaN thin film grown on 6H-SiC substrate measured at magnification of 50 000 \times .

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