Effect of thermal stresses on electronic properties of GaN/AlN nanowire superlattices

Patil, S. and Melnik, R.V.N.

Proceedings of the 8th International Congress on Thermal Stresses, June 1-4, 2009, University of Illinois, Urbana-Champaign, Ostoja-Starzewski, M., Marzocca, P. (Eds), Vol. II, pp. 579-582, 2009.

ISBN 10: 0615282334 || ISBN 13: 978-0-615-28233-6

Proceedings of
The Eighth International Congress on Thermal Stresses
1–4 June 2009
University of Illinois at Urbana-Champaign, Illinois, USA

Thermal Stresses 2009

Co-Editors
Martin Ostoja-Starzewski
University of Illinois at Urbana-Champaign

Pier Marzocca
Clarkson University

VOLUME II

International Congresses on Thermal Stresses are affiliated with IUTAM

ISBN 10: 0615282334

ISBN 13: 978-0-615-28233-6

Preface

The *Eighth International Congress on Thermal Stresses*, *TS 2009*, was held from May 31 to June 4, 2009, at the University of Illinois at Urbana-Champaign. The Organizing Committee received nearly 150 contributions from a number of countries. Following a review process, 137 papers were accepted for final presentation at the congress and publication in these proceedings. Nearly half of all the papers were submitted directly to special symposia, and these, with their respective organizers, are

- Professor Liviu Librescu Memorial Symposium organized by *Pier Marzocca*
- Fracture and Deformations in Functional Materials and Structures organized by *Sei Ueda, Nao-Aki Noda, Cun-Fa Gao, and Zheng Zhong*
- Second Sound and Thermal Shock Phenomena organized by *Pedro Jordan*

At the congress we were also privileged to have outstanding keynote lectures by

- Louis M. Brock, University of Kentucky, USA
- David G. Cahill, University of Illinois at Urbana-Champaign, USA
- Ching-Kong Chao, National Taiwan University of Science and Technology, Taiwan
- Artur Ganczarski and Jacek Skrzypek, Cracow University of Technology, Poland
- Paul M. Goldbart, University of Illinois at Urbana-Champaign, USA
- Gerard A. Maugin, Université Pierre et Marie Curie, France
- Walter Noll, Carnegie Mellon University, USA
- Yoshihiro Ootao, Osaka Prefecture University, Japan

The Congress gratefully acknowledges the valuable efforts of the special symposia organizers and all the reviewers. As Congress Chair, I am greatly indebted to the Congress Co-Chairs, Professors Richard B. Hetnarski and Pier Marzocca, for their guidance in planning the congress. Special thanks go to Ms. Michelle Chappell with the Conferences & Institutes division of the Office of Continuing Education at the University of Illinois for continuing assistance, efficient planning, and patient management of a multitude of tasks associated with the organization of the congress. Last, but not least, the Congress gratefully acknowledges the support by the University of Illinois (and especially the Department of Mechanical Science & Engineering), Clarkson University, The Air Force Office of Scientific Research, and the National Science Foundation.

MartinO stoja-Starzewski
Congress Chair

Proceedings of the 8th International Congress on Thermal Stresses, TS2009
1–4 June, University of Illinois at Urbana-Champaign

Effect of thermal stresses on electronic properties of GaN/AlN nanowire superlattices

Sunil R. Patil and Roderick V. N. Melnik

M^2NeT Lab, Wilfrid Laurier University,

75 University Ave W., Waterloo, ON, N2L 3C5, Canada

Abstract

We report the effects of thermal stresses on electromechanical and electronic properties of GaN/AlN cylindrical nanowire supperlattices (NWSLs). In order to study thermal stress effects on electromechanical properties we develop a fully coupled generalized 3D model. We consider the nanowire supperlattices having alternate layers of GaN and AlN in an AlN matrix. The resulting thermoelectromechanical properties are then incorporated in the 8-band $k \cdot p$ Hamiltonian to calculate the bandstructure of GaN/AlN NWSLs. Next, we analyze the effect of various thermal loadings up to 1000 K on electromechanical properties and subsequently on electron localization. It is observed that the thermal loading results in strain in addition to the lattice mismatch induced strain. Since GaN/AlN are piezoelectric and pyroelectric in nature, thermal stresses also have a significant effect on the internal electric field. The thermoelectromechanical properties are observed to modify significantly the bandstructure properties of the GaN/AlN NWSLs.

Keywords: *Thermal stress, electronic properties, coupled effects, nitride semiconductors, nanowire superlattice*

1 Introduction

Studies on low-dimensional systems, such as nanowires and superlattices, have attracted considerable attention in pursuit to develop smaller and faster electronic devices and to exploit their unusual properties for improved performance in various applications, such as thermoelectrics [1]. Today's technology allows finite-length modulated quantum-wire heterostructures to be grown in what is known as nanowire superlattice (NWSL) structures. NWSLs are nanoscale building blocks that could, through bottom-up assembly, enable diverse applications [2]. One can expect a straightforward analogy to the planar electronic/optoelectronic industry to extrapolate that complex compositionally modulated superlattice structures could greatly increase the versatility and power of these building blocks in nanoscale applications.

The NWSLs are often strained as they consist of alternate layers of different materials and also they are normally embedded in a host material with different structural properties [3]. The lattice mismatched strain in addition to thermal stresses can induce electric field in piezoelectric materials such as GaN/AlN. Further, the strain can exhibit strong couplings with thermal field in thermoelastic materials and with electric field in thermoelectric materials [4]. The role of the lattice mismatched strain on optoelectronic properties of nanostructures is now better understood, however, very little is known about the effects of thermal stresses. These effects can become more important at the nanoscale. Recently, it has been reported that GaN/AlN quantum dots exhibit a significant modification in electromechanical properties and the bandstructure. Considered here GaN/AlN semiconductors are wurtzite crystals and are also known as potentially important thermoelectric materials [5]. Thermoelectromechanical properties can also have a prominent effect on the bandstructure properties of the corresponding NWSLs. In addition there exist additional effects such as barrier localization due to the presence of multi-layers [6]. Understanding thermally dependant electronic localization is of vital importance from both technological and fundamental points of views.

In this paper, we develop a fully coupled generalized 3D model to study thermal stress effects on electromechanical properties of GaN/AlN cylindrical NWSLs. In our study we take a sufficiently wide range of thermal loadings of our structures, up to 1000 K, keeping in mind their potential applications as thermoelectrics and their operations in various temperature regimes. It is for this entire range of thermal loadings, electromechanical fields and electronic properties are studied. The resulting thermoelectromechanical properties are then incorporated in the 8-band $k \cdot p$ Hamiltonian to determine electronic properties. Finally, we analyze the effect of thermal stresses on electromechanical properties and subsequently on electron localization in GaN/AlN NWSLs.

2 Theory

A mathematical model is formulated in order to study thermal stress effects in GaN/AlN cylindrical NWSLs. The 3D linear fundamental equations for the thermoelectromechanical body occupying volume $\boldsymbol{\Omega}$, under steady state conditions can be summarized as follows [5]:
mechanical equilibrium equation

$$\nabla \bullet \boldsymbol{\sigma} + f = 0\,, \tag{1}$$

the equation of electrostatics

$$\nabla \bullet D - q = 0\,, \tag{2}$$

the thermal energy balance equation

$$\nabla \bullet h - k = -\Theta_0 \dot{S}\,. \tag{3}$$

Here $\boldsymbol{\sigma}$ is the stress tensor, D is the vector of electric displacement, h is the vector of heat flux, f, q and k are body mechanical forces, electric charges and heat sources in $\boldsymbol{\Omega}$, respectively. $\dot{S}$ and Θ_0 represent the change in entropy and the reference temperature, which is taken as 300K in the present study. Coupling of equations (1)-(3) is implemented through constitutive equations for the special case of wurtzite symmetry,

$$\begin{aligned}
&\boldsymbol{\sigma}_{xx} = c_{11}\boldsymbol{\varepsilon}_{xx} + c_{12}\boldsymbol{\varepsilon}_{yy} + c_{13}\boldsymbol{\varepsilon}_{zz} - e_{31}E_z - \boldsymbol{\beta}_{11}\boldsymbol{\Theta}\\
&\boldsymbol{\sigma}_{yy} = c_{12}\boldsymbol{\varepsilon}_{xx} + c_{11}\boldsymbol{\varepsilon}_{yy} + c_{13}\boldsymbol{\varepsilon}_{zz} - e_{33}E_z - \boldsymbol{\beta}_{22}\boldsymbol{\Theta}\\
&\boldsymbol{\sigma}_{zz} = c_{13}\boldsymbol{\varepsilon}_{xx} + c_{13}\boldsymbol{\varepsilon}_{yy} + c_{33}\boldsymbol{\varepsilon}_{zz} - e_{33}E_z - \boldsymbol{\beta}_{33}\boldsymbol{\Theta}\\
&\boldsymbol{\sigma}_{xy} = (c_{11} - c_{12})/2\ \boldsymbol{\varepsilon}_{xy},\ \boldsymbol{\sigma}_{yz} = c_{44}\boldsymbol{\varepsilon}_{yz} - e_{15}E_x\\
&\boldsymbol{\sigma}_{zx} = c_{44}\boldsymbol{\varepsilon}_{zx} - e_{15}E_y\,,\\
&D_x = e_{15}\boldsymbol{\varepsilon}_{yz} + \in_{11} E_x,\quad D_y = e_{14}\boldsymbol{\varepsilon}_{zx} + \in_{22} E_y\,,\\
&D_z = e_{31}(\boldsymbol{\varepsilon}_{xx} + \boldsymbol{\varepsilon}_{yy}) + e_{33}\boldsymbol{\varepsilon}_{zz} + \in_{33} E_z + p_3\boldsymbol{\Theta} + P_z^{sp},\\
&S = \boldsymbol{\beta}_{11}\boldsymbol{\varepsilon}_{xx} + \boldsymbol{\beta}_{22}\boldsymbol{\varepsilon}_{yy} + \boldsymbol{\beta}_{33}\boldsymbol{\varepsilon}_{zz} + p_3E_z + a_T\boldsymbol{\Theta}.
\end{aligned} \tag{4}$$

Here c_{ij}, e_{ij} and χ_{ij} are elastic moduli, piezoelectric constants and dielectric constants respectively. P_i^{sp} is the spontaneous polarization; p_i and $\boldsymbol{\beta}_{ij}$ are thermo-electric and thermo-mechanical coupling constants, respectively, and ε, E and Θ are strain tensor, electric field and temperature, respectively. This model can also be used for zinc blend materials with appropriate constitutive relations [7].

The resulting thermoelectromechanical properties are then incorporated in the 8-band $k \cdot p$ Hamiltonian for band structure calculations. We consider two conduction bands coupled with six valance bands including heavy-hole, light-hole and spin-orbit bands. The crystal-field splitting is also accounted for. Electron-hole states are the eigenstates of the 8-band envelope function equation:

$$H\boldsymbol{\Psi} = E\boldsymbol{\Psi}\,, \tag{5}$$

where H is the 8 x 8 matrix of the Hamiltonian, $\boldsymbol{\Psi}$ is the envelope wave function and E is the energy. The unstrained valance band edge of AlN at 300K is taken as a reference. The strain dependent electron-hole part of the Hamiltonian, piezoelectric potential and energy band edges are temperature dependent. Detailed expressions for elements of the Hamiltonian, computational procedures to solve Eqns. (1)-(3) and (5) and physical parameters used in this paper are given in [5, 8].

3 Results and discussion

First, we obtain electromechanical fields for cylindrical GaN/AlN NWSLs without accounting for thermal stress effects. Next, we account for thermal stress effects and analyze the influence of these effects on electromechanical properties of the NWSL. Further, we also account for external thermal loadings and analyze their effect. We assume that the NWSL consists of alternate layers of AlN/GaN and is embedded in an AlN matrix. The dimensions and geometrical details of the NWSL are given in Fig. 1.

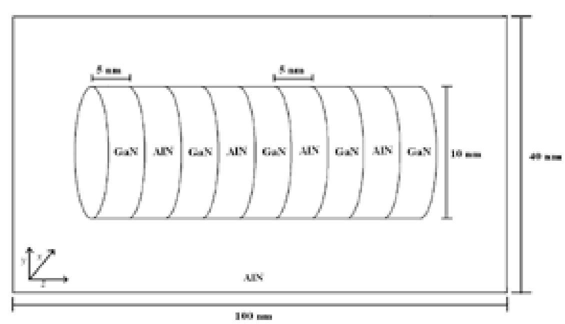

Figure 1: Geometry of the NWSLs

The values of lattice mismatch for GaN/AlN systems are -2.41 % and -4.07% along a and c directions of the WZ crystal unit cell, respectively. As the AlN matrix is relatively large compared to NWSL, we follow common practice to neglect lattice mismatch inside the matrix. However, we account for mismatch along the z-direction (c-direction of the unit cell) in inner AlN layers.

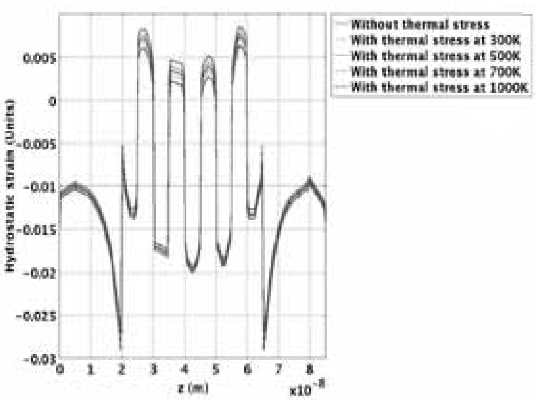

Figure 2: Hydrostatic strain as a function of thermal loadings

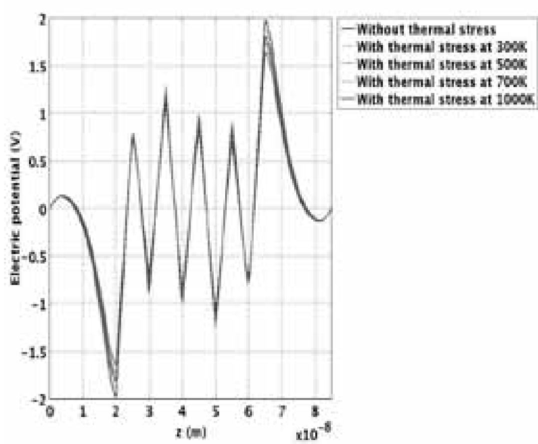

Figure 3: Piezoelectric potential as a function of thermal loadings

In Fig. 2 we present the hydrostatic strain component along the central line of NWSL and its variation when thermal stresses are accounted for. The magnitude of the hydrostatic strain increases with increase in thermal loadings. Without accounting for thermal stresses the magnitude of hydrostatic strain at the center of the NWSL is 0.0190. However, when thermal stresses are accounted for, without external loadings, it increases to 0.0195 and increases even further on external loadings, 0.0205 at 1000K. Since it is known that hydrostatic strain leads to a rigid shift in the band edges, even small changes caused by thermal stresses become important [5, 7].

In Fig. 3 we present the piezoelectric potential for different cases of thermal stresses. The electric potential decreases when thermal stresses are accounted for. In the case when thermal stresses are neglected, the electric potential is the highest at 3.9 V and further decreases to 3.3 V at 1000K, with accounting for thermal stresses. The potential difference creates a deeper potential well, for holes at the negative side and at the positive side for electrons. Thus, the decrease in potential difference with temperature leads to a shallower potential well, which will result in relatively less confinement [5]. In the present case we observe the highest value of electric potential in the second layer of GaN (from left to right in Fig.1). Also we note that the variation of potential in the NWSL may lead to band splitting. In order to analyze this issue further, electronic localizations for the ground state of the GaN/AlN NWSLs under different thermoelectro-mechanical loadings are determined using 8-band $k \cdot p$ model.

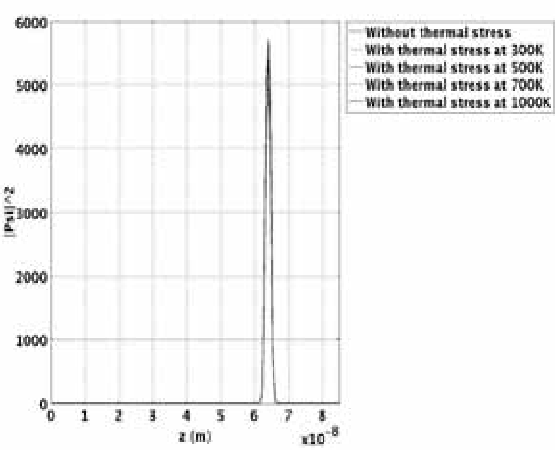

Figure 4: Electronic ground state as a function of thermal loadings

In Fig. 4, we show the probability density of the ground state variation with various cases of thermal loadings. In the absence of any kind of loadings we observe the localization in the central well of the NWSLs with the ground state energy, E_1, at about 4.3116 eV. However, the electrons are localized in the lower second layer (from the left) of GaN when electromechanical effects are taken into account. This is due to the higher value of the electric potential in that layer. The localization probability decreases with increase in thermal loading. However, the ground state energies, presented in Table 1, decrease when the influence of piezoelectric effects on band structure is taken into account. Furthermore, a significant reduction in energies of the electronic states highlights the importance of taking into account operating temperature contributions in the analysis of the NWSLs. The qualitative behavior of electron localizations is dominated by the piezoelectric potentials even at higher temperatures. The lowest state energies have been significantly reduced as compared to the case without accounting for thermal effects. This is due to the fact that the energy band gap decreases as temperature increases.

Sr. No.	Conditions	Ground state energy (eV)
1	Without any loading	4.3116
2	With electromechanical loading induced by lattice mismatch	3.2329
3	With thermoelectromechanical loading induced by lattice mismatch	3.3129
4	With thermoelectromechanical loading induced by lattice mismatch and external thermal loading of 500K	3.3328
5	With thermoelectromechanical loading induced by lattice mismatch and external thermal loading of 700K	3.3035
6	With thermoelectromechanical loading induced by lattice mismatch and external thermal loading of 1000K	3.2026

Table 1: The ground state energies of the electrons in various cases.

In Table 1, we summarize the ground state energies of the electrons for various situations. In the first case (without any loading) the electrons take the highest energy which is further reduced by electromechanical effects (case 2). A slight increase in energy is observed when thermal stresses are accounted for, shown by case 3. On applying external thermal loadings the energy decreases with increase in external temperature. At higher temperatures the energies are substantially reduced as the temperature effect on band gap dominates [5, 7].

4 Conclusions

In this study, based on a fully coupled multi-physics model, combined contributions of thermo-electromechanical effects in GaN/AlN NWSLs have been analyzed for the first time. It has been found that accounting for thermal loadings can significantly modify electromechanical and electronic properties of GaN/AlN NWSLs. Thermal loadings can lead to the increase in magnitude of hydrostatics strain and piezoelectric potential. Significant reductions and shifts in localizations in electronic state energies due to thermal loadings are observed. Thus, in addition to electromechanical tuning, operating temperature can also provide an additional tuning parameter in band gap engineering of NWSLs. The observed phenomena emphasize the importance of the fully coupled thermopiezoelectric models in studying the properties of NWSLs.

Acknowledgment

This work, conducted in the M²NeT Laboratory (http://www.m2netlab.wlu.ca), was made possible by the facilities of the SHARCNET. R.M. acknowledges the support from the NSERC and CRC programs.

References

(1) Lin Y. M. and Dresselhaus M. S., Phys. Rev. B, Vol. 68 (7), 075304, 2003.

(2) Lieber C. M., Nano Lett., Vol. 2 (10), 1137–1141, 2002.

(3) Niquet Y. M., Phys. Rev. B, Vol. 74 (15), 155304, 2006.

(4) Snyder G. J. and Toberer E. S. Nature Mater., Vol. 7, 105-114, 2008.

(5) Patil S. R. and Melnik R. V. N. Nanotechnology Vol. 20 (12), 125402, 2009.

(6) Voon L. C. L. Y., Lassen B., Melnik R., and Willatzen M., J. Appl. Phys. 96 (8), 4660-4662, 2004

(7) Patil S. R. and Melnik R. V. N. physica status solidi (a), in press, 2009.

(8) Fonoberov V. A. and Balandin A. A., J. Appl. Phys., Vol. 94 (11), 7178-7186, 2003.

THERMOMECHANICS & NANOEFFECTS 573

WAVE PROPAGATION 595

AUTHOR INDEX FOR VOLUMES I AND II 613