Strain dependence of Internal Displacement and Effective Charge in Wurtzite III-N semiconductors

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Abstract. The elastic and dielectric properties of binary III-N wurtzite semiconductors have been investigated as a function of strain. Using an ab initio density functional theory (DFT), we concentrate on the internal displacement (u) and Born effective charge (Z*) and show that our model provides a unique non linear dependence of the III-N material properties as a function of strain.

1. Introduction

Group III-V semiconductors are gaining popularity by virtue of the wide range of prospective applications as optoelectronic devices such as lasers and LEDs along with electronic devices1 such as HEMTs, HBTs, Gunn diodes, transducers and micropositioners. III-Nitrides can be employed in high frequency and high power devices for radar and avionics exploiting material properties such as their wide bandgap and high electron mobility.2 Strain induced electrical and optical along with electromechanical properties of the III-N materials are well known to strongly affect device behaviour.3,4,5 Substantial nonlinear effects in the strain to second order have been reported already in wurtzite III-N6,7,8,9,10,11 following previous analogous reports for zincblende InGaAs12,13

2. The Physical Model And DFT Calculations

Our previous work6 has already reported the methodology for computing the piezoelectric coefficients (PZCs). Such methodology is based on a semi empirical formalism within Density Functional Theory (DFT), Local Density Approximation (LDA) and plane wave pseudopotentials. The same approach has been exploited previously to obtain predictions for InGaAs which seem to provide excellent agreement with experimental data.12,14 The piezoelectric polarization is calculated as the sum of a direct dipole contribution and a bond contribution, a semi empirical approach, originally proposed by Harrison15.
In Eq.1, \( \hat{x}_i \) is the direction of the Cartesian axes, \( \delta r \) is the displacement vector of cations in respect of anions from the initial position (i.e. the condition when all the bonds in the tetrahedron are equal in nature), \( r_q \) and \( \delta R_q \) are the distance and displacement (deviation from the initial position) vectors of the nearest neighbour \( q \) from the atom at the centre of the tetrahedron, respectively, \( \alpha_p \) is the bond polarity and \( \Omega \) is the atomic volume, \( Z_{H^*} \) is the atomic charge, not to be confused with the transverse effective charge or Born charge (\( Z^* \)), calculated with DFPT. Our previous work on wurtzite III-N\(^6\) and zincblende GaAs and InAs\(^12,14\) has already reported that the value of the atomic charge \( Z_{H^*} \) needs to be 25\% of the value for the dynamic Born effective charge (\( Z^* \)) to attain precise estimates of piezoelectric polarization compared to the experimental values. However \( Z^* \) is linked to the bond polarity \( \alpha_p \) so it is still an important quantity.

In this work, we report the non linear behaviors of two quantities, the deformation or internal displacement parameter \( u \) and \( Z^* \), which are fundamental for calculating Eq.1. These have been calculated for both bulk and strained cases using pseudopotentials derived with the Troullier–Martin scheme (for \( u \)),\(^16\) along with the Hamann scheme (for \( Z^* \)),\(^17\) in the CASTEP\(^18\) code.

Both Density functional theory in the local density approximation (DFT-LDA)\(^19\) and density functional perturbation theory (DFPT) have been used in the calculations. Single-particle orbitals expressed in a plane-wave basis set with kinetic energy of up to 1keV and Brillouin zone summations of up to 10x10x6 Monkhorst-Pack k-point grids\(^20\) were sufficient to make the simulations converge below a remaining error of about 1\%. \( Z^* \) was computed using the Berry phase approach\(^21\) with application of periodic boundary conditions and finite electric field perturbation.

3. Results

Our previous works reported the DFT calculated equilibrium values for the lattice parameters, internal displacement parameter \( u \), \( Z^* \) and the resulting bond polarity \( \alpha_p \) (obtained from \( Z^* \)) for all three III-N semiconductors and in Table I we showed these to be in good agreement with the existing values in the literature.\(^22,23,24,25\)
Table I: Comparison of the physical parameters of Group-III Nitrides (GaN, AlN and InN) used in this work\textsuperscript{6} with other calculated values in brackets.

| Parameters | GaN     | AlN     | InN     |
|------------|---------|---------|---------|
| a (Å)      | 3.155   | 3.063   | 3.523   |
|            | (3.196)\textsuperscript{22} | (3.076)\textsuperscript{22} | (3.524)\textsuperscript{22} |
|            | (3.131)\textsuperscript{23} | (3.069)\textsuperscript{23} | (3.509)\textsuperscript{23} |
| c (Å)      | 5.149   | 4.906   | 5.725   |
|            | (5.220)\textsuperscript{22} | (4.980)\textsuperscript{22} | (5.773)\textsuperscript{22} |
|            | (5.104)\textsuperscript{23} | (4.910)\textsuperscript{23} | (5.656)\textsuperscript{23} |
| u (Å)      | 0.376   | 0.382   | 0.377   |
|            | (0.376)\textsuperscript{22,23} | (0.380)\textsuperscript{22} | (0.377)\textsuperscript{22,24} |
|            | (0.377)\textsuperscript{24} | (0.382)\textsuperscript{23,24} | (0.379)\textsuperscript{23} |
| Z*         | 2.583   | 2.553   | 2.850   |
|            | (2.510)\textsuperscript{23} | (2.652)\textsuperscript{23} | (3.045)\textsuperscript{23} |
| \(\alpha_p\) | 0.517   | 0.511   | 0.578   |
|            | (0.511)\textsuperscript{25} | (0.508)\textsuperscript{25} | (0.542)\textsuperscript{25} |

In Fig. 1 we show the distribution of the dimensionless internal displacement parameter (u) with parallel and perpendicular strain (varying from -10% to 10%).

The results show a wide variation of the u-parameter. Different combinations of strain applied to the system leads to different values for AlN, GaN and InN, but essentially the same behaviour.

The range of the internal displacement parameter with applied strain differs with different materials. While for both GaN and InN, the u-parameter dips to 0.34 for 10% strain along c-axis and to 0.35 for AlN. Application of strain parallel to growth direction reveals different trends altogether, where the u-parameter for AlN and InN grows to 0.44 and for GaN to 0.43 for 10% strain.
Fig. 1: Strain dependence of internal displacement parameter $(u)$ as a function of in-plane and perpendicular strain (from -0.1 to 0.1 in steps of 0.02) for a) GaN, b) AlN and c) InN respectively.

The $u$-parameter is dimensionless.
We also investigated the strain dependence of $Z^*$ for all III-N materials for various arrangements of strain along in-plane and perpendicular to the growth plane directions. The outcomes of the $Z^*$ calculations reflect an unusual trend of non-linearity on strain which again is common to GaN, AlN and InN.

In Fig.2, the strain effects on $Z^*$ for strain along perpendicular as well as in-plane strain varying ±10% with steps of 2% are shown. While GaN and AlN show almost identical behaviour, InN shows a less pronounced non-linear dependence on perpendicular strain. But $Z^*$ for all the three different III-Nitride materials, namely GaN, AlN and InN, increases with more tensile strain in the plane of the direction of growth.

We have not explored the non-linear dependence of $u$ and $Z^*$ on shear strain in the growth direction or growth plane. It could have a significant influence on nanostructures such as quantum dots, but not on the bulk semiconductors or 2-dimensional thin films, which has been the primary aim of this work.

4. Conclusions

Our semi empirical formalism has been employed to investigate the effect on fundamental and critical elements of III-N materials. We have already illustrated non-linear effects on piezoelectric coefficients in our previous work$^6$ leading towards new and improved sets of parameters for III-N binary and ternary materials. In this work, we have shown that a strong strain effect of second-order is prevalent on material properties such as internal displacement ($u$) and born effective charge ($Z^*$). As this data was obtained in the framework of DFT-LDA, it can be useful in fitting other semiempirical model such as force fields for Molecular Dynamics simulations.

References

1. S. Nakamura, G. Fasol, The Blue Laser Diode: GaN Based Light Emitters and Lasers (Springer-Verlag, Berlin, 1997)
2. W. D. Hu, X. S. Chen, F. Yin, J. B. Zhang, and W. Lu, J. Appl. Phys., 105, 084502 (2009).
3. A. D. Andreev and E. P. O’Reilly, Phys Rev B 62, 15851 (2000)
4 S. Tomic and N. Vukmirovic, Phys. Rev. B 79, 245330 (2009)
5 L. C. Lew Yan Voon and M. Willatzen, J. Appl. Phys. 109, 031101 (2011)
6 J. Pal, G. Tse, V. Haxha, M. A. Migliorato, S. Tomic, Phys. Rev. B 84, 085211 (2011)
7 G. Vaschenko, C. S. Menoni, D. Patel, C. N. Tomic, B. Clausen, N. F. Gardner, J. Sun, W. Goetz, H. M. Ng and A. Y. Cho, Phys. Stat. Sol. B 235, 238 (2003)
8 D. Cai and G-Y. Guo, J. Phys. D: Appl. Phys. 42, 185107 (2009)
9 K. Shimada, T. Sota, K. Suzuki and H. Okumura, Jpn. J. Appl. Phys. 37, Pt.2, 12A (1998)
10 G. Vaschenko, D. Patel, C. S. Menoni, N. F. Gardner, J. Sun, W. Go’tz, C. N. Tomé and B. Clausen, Phys. Rev. B 64, 241308 (2001)
11 O. Ambacher, J. Majewski, C. Miskys, A. Link, M. Hermann, M. Eickhoff, M. Stutzmann, F. Bernardini, V. Fiorentini, V. Tilak, B Schaff and L F Eastman, J. Phys.: Condens. Matter 14, 3399 (2002)
12 M. A. Migliorato, D. Powell, A. G. Cullis, T. Hammerschmidt and G. P. Srivastava, Phys. Rev. B 74, 245332 (2006)
13 G. Bester, X. Wu, D. Vanderbilt, and A. Zunger, Phys. Rev. Lett. 96, 187602 (2006)
14 R. Garg, A. Hue, V. Haxha, M. A. Migliorato, T. Hammerschmidt and G. P. Srivastava, Appl. Phys. Lett. 95, 041912 (2009)
15 W. A. Harrison, Electronic Structure and Properties of Solids, Dover Publications Inc., New York, (1989).
16 N. Troullier and J. L. Martins, Phys. Rev. B 43, 1993 (1991).
17 D. R. Hamann, Phys. Rev. B 40, 2980 (1989)
18 S. J. Clark, M. D. Segall, C. J. Pickard, P. J. Hasnip, M. J. Probert, K. Refson, M. C. Payne, Zeitschrift für Kristallographie 220(5-6) pp.567-570 (2005)
19 J. P. Perdew and A. Zunger, Phys. Rev. B 23, 5048 (1981).
20 H. J. Monkhorst and J. D. Pack, Phys. Rev. B 13, 5189 (1976)
21 M.V. Barry, Proc. R. Soc. Lond. A 392, 45 (1984)
22 F. Bernardini, V. Fiorentini, D. Vanderbilt, Phys. Rev. B 56, R10024 (1997)
23 A. Zoroddu, F. Bernardini, P. Ruggerone and V. Fiorentini, Phys. Rev. B 64, 045208 (2001)
24 S. Y. Karpov, Phys. Status Solidi C 7, 1841 (2010)
25 S. Q. Wang, H. Q. Ye, J. Phys. Condens. Matter, 17, 4475 (2005)