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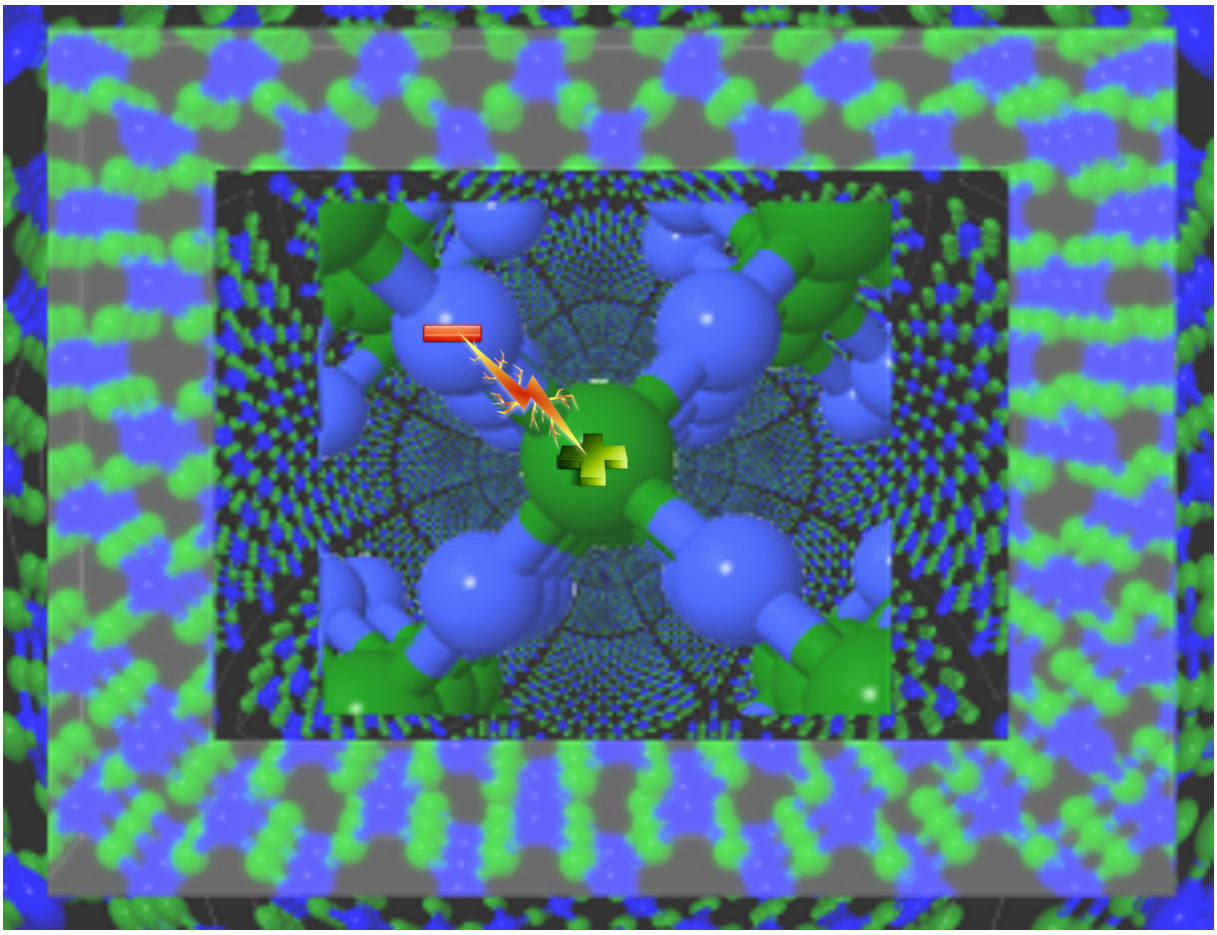
Newsletter



Piezoelectricity: An atomic phenomena of generating electricity when atomic bonds are put under any kind of strain; above a tetrahedral III-V atomic model.
(image courtesy of Dr Joydeep Pal)

Newsletter Contents

This Newsletter...

Dear Readers,

The feature article for this bumper edition of the newsletter is an invited contribution by Joydeep Pal from the University of Manchester, our winner of the 2013 IoP Computational Physics Group PhD Prize, on *'Exploiting Non Linear Piezoelectricity in novel semiconductor based electronic devices'*.
Joydeep also kindly provided the cover image for this edition.

In addition, we have a comprehensive report from the CompMat 2014 Symposium.

Most URLs in the newsletter have web hyperlinks and clicking on them should take you to the corresponding page. The current edition of the newsletter can be found online at:

`www.iop.org/activity/groups/subject/comp/news/page_40572.html`

with previous editions at:

`www.iop.org/activity/groups/subject/comp/news/archive/page_53142.html`
`www.soton.ac.uk/~fangohr/iop_cpg.html`

As always, we value your feedback and suggestions. Enjoy this edition!

Marco Pinna, Newsletter Editor ✉ mpinna@lincoln.ac.uk)

(on behalf of the The Computational Physics Group Committee).

Exploiting Non Linear Piezoelectricity in Novel Semiconductor based Electronic Devices

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Introduction

The field of Piezotronics began in 2006 when Regent Professor Zhong Lin Wang at Georgia Institute of Technology (USA) coined a new term to describe the exploitation of strain induced piezoelectricity in nanostructured semiconductors to develop electronic devices with new functionalities.[1] A piezoelectric potential (PZP) can be created in any bulk or nanostructured semiconductor crystal having non central symmetry, such as the Group III-V and II-VI materials, due to polarization of ions under applied stress and strain. Because of the presence of both piezoelectric (PZ) response and semiconductor behaviour, the piezoelectric polarization (PZP) in the crystal affects significantly the carrier transport at the interface/junction and their optical properties.[2, 3, 4, 5, 6] Unique applications have been proposed in areas such as sensing and actuating in nanorobotics, human-computer interfacing, nanorobotics, smart MEMS/NEMS, smart and personalized electronic signatures and energy harvesting.[7, 8] In recent years a new theoretical understanding, obtained through sophisticated computer simulations, of the nature of the PZ polarization and resulting electric fields in semiconductor crystals has emerged[9, 10] which advocated the necessity to include non-linear piezoelectric coefficients (PZCs) even in the limit of vanishing strain in order to correctly estimate the effect of the presence of strain induced electric fields on the electro-optical properties of polar semiconductor nanostructures.[11, 12, 13] Such studies have demonstrated that the assumption that the PZ effect is a linear effect in the strain is incorrect and that the magnitude of the second order PZCs is of the same order of magnitude as the first order, even in the range of $[-0.1 \div 0.1]$ of strains, which is typical for nanostructures.[14] Furthermore non-linear effects, because of their ability to switch the sign of the PZP from negative to positive depending on the applied strain,[14] have been shown to provide an additional and unexpected degree of freedom in the design of optoelectronic components. Although non-linearities have been experimentally observed in III-Nitrides (III-Ns), second order PZCs had not yet been reported, making it difficult to assess the influence of second-order piezoelectricity in nanostructures. While we report the strong non-linear strain induced piezoelectric behaviour with second order coefficients, all spontaneous polarization terms are substantially smaller than the previously proposed values. We show that, unlike existing models, our calculated piezoelectric coefficients and nonlinear model provide a close match to the internal piezoelectric fields of quantum well and superlattice structures. Also, pressure dependence of the piezoelectric field in InGaN based LEDs predicts a significant improvement of the spontaneous emission rate can be achieved as a result of a reduction of the internal field. The LED devices using the proposed structures including a metamorphic layer under the active region of the device are expected to increase their light output power by up to 10%. We also explored the impact of the non-linear piezo effect in nanowires and present a further theoretical computational study of single photon sources optimization in InGaN based wurtzite single quantum dots. We observed the light emission can be made by those single photon sources covering the entire visible spectrum through suitable change in the alloy composition.

Physical Model and Results

To resolve the issue of calculating the spontaneous and strain-induced PZ effect beyond the linear model, we present a semiempirical method that produced accurate predictions for InGaAs.[9, 14] The physical model, as originally proposed by Harrison,[15] is used to represent the influence of atomic displacement

Coefficient	GaN	AlN	InN
P_{sp}(C/m^2)	-0.007	-0.051	-0.012
e_{31}(C/m^2)	-0.55	-0.60	0.55
e_{33}(C/m^2)	1.05	1.47	1.07
e_{15}(C/m^2)	-0.57	-0.60	-0.65
e_{311}(C/m^2)	6.185	5.850	5.151
e_{333}(C/m^2)	-8.090	-10.75	-6.685
e_{133}(C/m^2)	1.543	4.533	1.280

Table 1: Linear and non-linear piezoelectric coefficients for III-N semiconductors. (Values taken from Ref [22]).

and atomic charge on the creation of an electrical dipole in a WZ crystal, while the variations of these quantities as a function of strain are calculated in the framework of ab initio density functional theory (DFT) in supercomputing clusters.
The total polarization resulting from both spontaneous and strain induced polarization is given by the sum of a direct dipole contribution and a bond contribution:[15]

$$P_{\hat{x}_i} = \frac{Z_H^* \delta r + 2\alpha_p \left(1 - \alpha_p^2\right) \cdot \sum_{q=1}^{4} \left(\vec{r}_q \cdot \hat{x}_i\right) \delta R_q}{2\Omega} \tag{1}$$

where x_i is the Cartesian direction, δr is the displacement vector of cations in respect of anions from the ideal position (i.e. the situation where all bonds in the tetrahedron are equal to each other), r_q and δR_q are the distance and displacement (deviation from the ideal position) vectors of the nearest neighbour q from the atom at the centre of the tetrahedron, respectively, α_p is the bond polarity and Ω is the atomic volume. Borrowing from the language of tight binding, Z_H^* is the atomic charge, generally different from the transverse effective charge, which instead has its direct equivalent in the dynamic effective charge, or Born charge (Z^*), calculated with density functional perturbation theory (DFPT). The elastic deformation and Z^*, for both the bulk and strained cases, were evaluated by using planewave pseudopotential, with pseudopotentials derived with the Troullier Martin scheme,[16] density functional theory in the local density approximation (DFT-LDA)[17] and density functional perturbation theory (DFPT), with pseudopotentials derived with the Hamann scheme,[18] within the CASTEP[19] code. Single-particle orbitals expressed in a plane-wave basis set with kinetic energy of up to 10^3 eV, and Brillouin zone summations of up to $10 \times 10 \times 6$ Monkhorst-Pack k point grids[20] were sufficient to converge the simulations below a remaining error of about 1% for multiple combinations of k-point grids and kinetic energy. The dynamic effective charge was computed from the Born charge matrix, studied via the Berry phase approach[21] by applying a finite electric field perturbation in periodic boundary conditions. The matrix was then diagonalized and an average of the eigenvalues was taken as the effective charge. Both its bulk and strain dependence were determined in the same way. The wurtzite structure, with its 3 independent PZCs e_{13}, e_{33} and e_{15} and the presence of spontaneous polarization (P_{sp}), i.e. polarization present even in the absence of any external or in built pressure, provides a much more stringent test for Harrison's model (HM). Pal $et\ al$[22] first reported the non-linear PZCs for all III-N semiconductors (TABLE 1), with the limitation of isotropic strain in the growth plane (c-plane). The non linear PZCs fit the following equation:

$$P_{Tot} = P_{sp} + e_{33}\epsilon_{\perp} + 2e_{31}\epsilon_{\parallel} + e_{311}\epsilon_{\parallel}^2 + e_{333}\epsilon_{\perp}^2 + e_{133}\epsilon_{\parallel}\epsilon_{\perp} \tag{2}$$

The most notable prediction of HM is the fact that P_{sp}, for which no direct experimental values can be obtained, must be substantially lower than those reported in the past from theoretical calculations.[23]

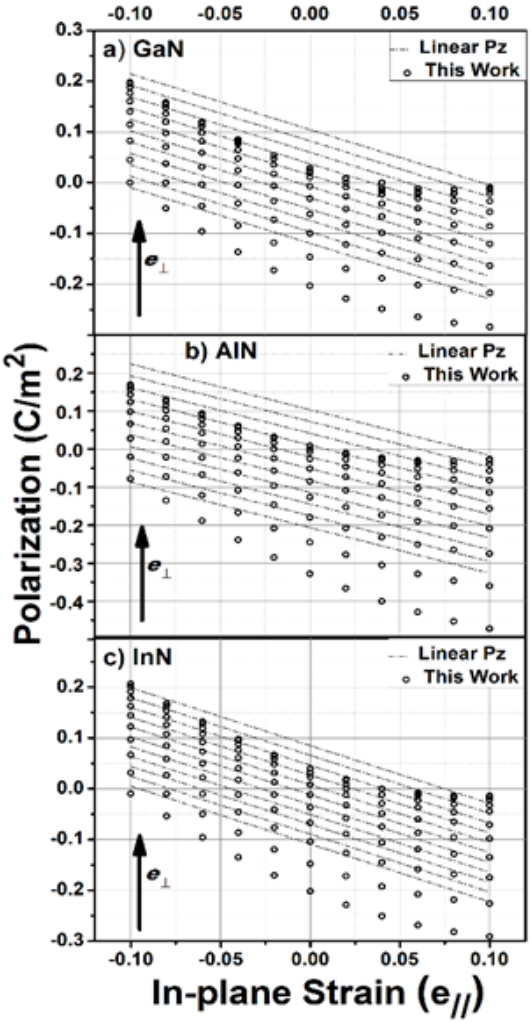

Figure 1: Reproduced with permission from Ref [22]. Dependence of the total polarization of III-N semiconductors upon combinations of strain in both the c-plane and c-axis. Comparison between the linear and non linear (this work) is given.

This discrepancy was attributed to an incorrect interpretation in the earlier theoretical work[23] of the role of Z^* vs Z^*_H within the direct dipole contribution to the total polarization. Further work from Pedesseau $et\ al$[24] using the Linear Response (LR) method reported non-linear piezoelectric coefficients, albeit similar issues as discussed in the context of InAs and GaAs remain, together with the expected discrepancy in the values of P_{sp}. The total non-linear polarization compared with the classic linear model (LM) with the parameters of Bernardini $et\ al$[23] is given in Figure 1. The difference is substantial and in particular much larger PZP can be expected compared to the LM in the same range of strain, which could be potentially exploited in the field of piezotronics to synthesize combination of materials with increased PZ response. The PZCs given by Pal $et\ al$[22] were tested by Suski $et\ al$[25] alongside the LM and other suggested parameters in the literature.[23, 26] Authors acknowledged that the non-linear PZCs of Pal $et\ al$[22] lead to correct predictions of the experimentally observed trends in electro-optical measurements of InGaN quantum wells, but also pointed out that for quantitative agreement there is the need to also take non-linear elasticity (NLE)[27] into account.

Comparison with experimental results on binary materials

To test the validity of our method and the PZCs obtained (listed in Table 1) we compared with the experimental values for AlN/GaN superlattices.[28, 29, 30, 31] For this comparison we have evaluated the field in the AlN and GaN regions (conventionally referred to as the barrier (b) and well region (w) respectively) using the well-known superlattice equations.[31]

$$F_z^w = \frac{P_{SP}^b + P_{PZ}^b - P_{SP}^w - P_{PZ}^w}{\epsilon^w + \epsilon^b(L_w/L_b)} \tag{3}$$

$$F_z^b = \frac{-L_w}{L_b} F_z^w \tag{4}$$

In the Figure 2, we show the comparison of the fields in the well region between our calculated fields (cross) with the experimental fields (squares) along with the linear model[23] (triangles) with different estimates of the ratio of the lengths of the well and the barrier used in the superlattice equations.[32]

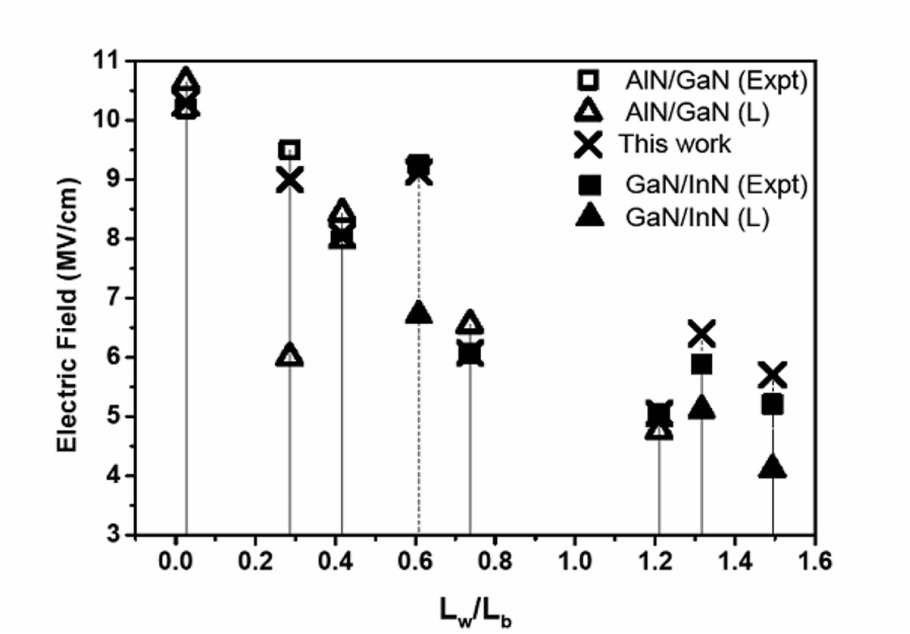

Figure 2: Comparison of the fields in the well region between our calculated fields (cross) with the experimental fields (squares) along with the linear model (triangles) with different estimates of the ratio of the lengths of the well and the barrier used in the superlattice equations.[32] The linear model parameters are taken from Ref.[23]. We compared the field in GaN/AlN (hollow symbols) and InN/GaN (solid symbols) QWs. Reproduced from this work of Ref[33].

The substantial agreement confirms the correctness of our PZCs for GaN and AlN. In particular it validates the proposed lower values of the P_{sp} term, which is probably the most interesting outcome of our model. While, in case of nanostructures with InN/GaN layers, the field predictions have been matched with the theoretical calculations from Ref [34]and again, the linear model[23] provide substantial differences with the values of the field from our calculations.

III-N Light Emitting Diodes

One of the major factors limiting the light output power of InGaN-based emitters is the presence of in built polarization fields that originate from the wurtzite crystal structure of III-N semiconductors.[35, 36, 37, 38]

Coulomb repulsion of localized carriers creates energy barriers that hinder carrier transportation. The need to manage piezoelectric polarization in InGaN/GaN superlattices[34] has led to attempting to synthesize devices on substrates with non-polar and semi-polar crystal orientations.[39, 40, 41, 42] However, the output powers at high injection current of these devices currently do not outperform the best devices grown on (0001) planes (c−planes).[14, 43, 44]

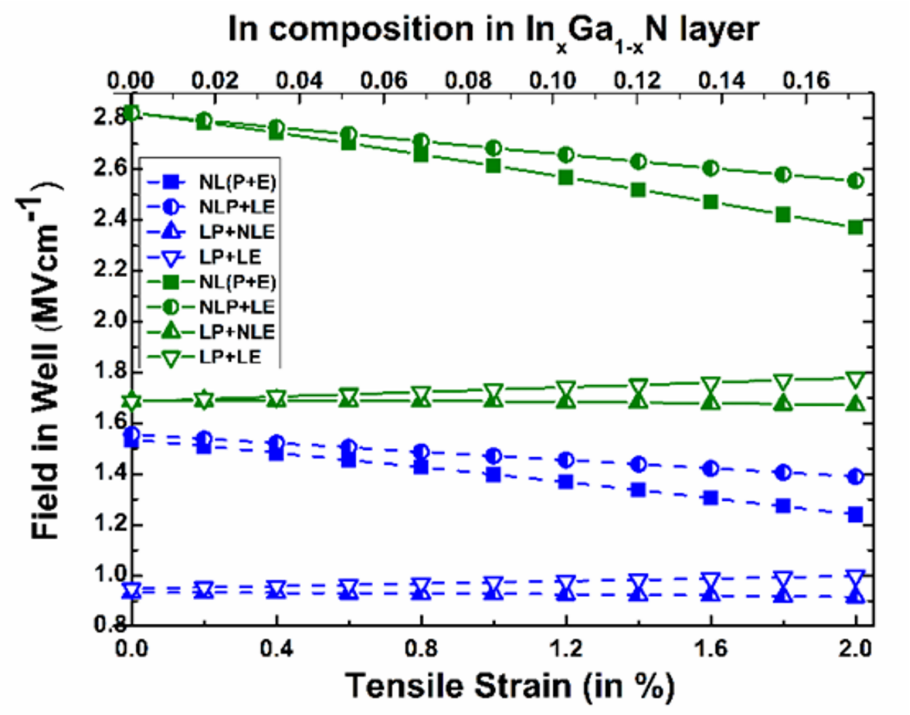

Figure 3: Reproduced with permission from Ref [45]. Dependence of the piezoelectric field in the well region as a function of tensile strain in the c plane, for both the blue and the green LED structures. Comparison of the calculations using the both linear and non linear piezoelectric and elasticity models.

Crutchley $et\ al$[46] showed experimentally that there appears to be a linear correlation between the change in internal field and the reduction of the optical efficiency in c−plane GaN based LED devices. This was concluded after observing optical efficiency as a function of applied hydrostatic pressure. Applying pressure (hydrostatic compressive strain) from 0 to 1GPa led to a reduction in wells with metamorphic layer vs the conventional quantum well structure of 4% in the light output power for both green and blue LEDs at an operating current of 260mA. In the same range of pressures, HM in the non-linear regime predicts an equivalent 4% increase of the PZ field in the quantum well regions, which would explain the efficiency drop. LM instead predicts a reduction of 2%, which should lead to higher optical efficiency. The calculations of the PZ field in the quantum well region of a blue and a green LED structures (Figure 3) as a function of external strain confirm the expected reduction of the field.[45] Based on this data Pal $et\ al$[22] made the suggestion that if hydrostatic pressure reduces efficiency then tensile pressure might instead increase it. On the top axis of Figure 3 the strain is equated to the composition of a metamorphic InGaN layer (Figure 4) that if inserted below the active region would generate the same tensile strain of the bottom axis.

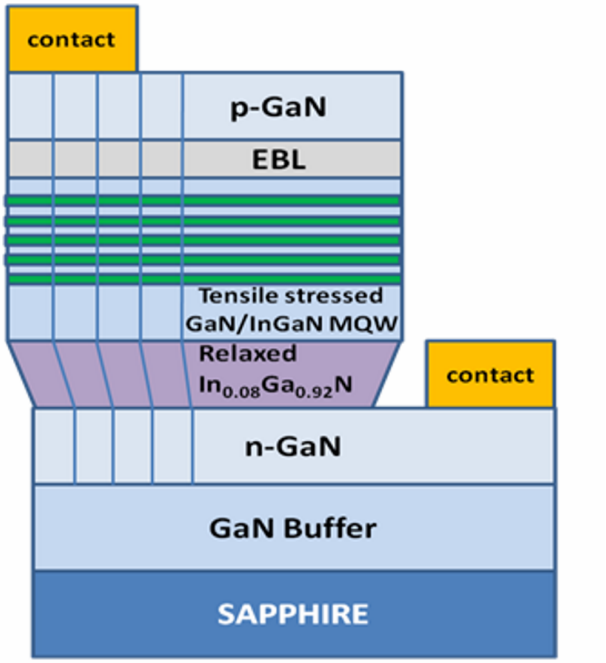

Figure 4: Reproduced with permission from Ref [45]. Proposed c-plane InGaN LED device structure using a metamorphic layer before the MQW region which is grown on the top of n−type GaN layer. The InGaN quantum well has either 14% or 26% for the blue or green emission respectively models.

Further analysis of the radiative emission rate utilizing a self consistent Poisson and 6 X 6 $k \cdot p$ Schrödinger solver[47] also confirmed the expectations of higher efficiency for tensile strained devices.

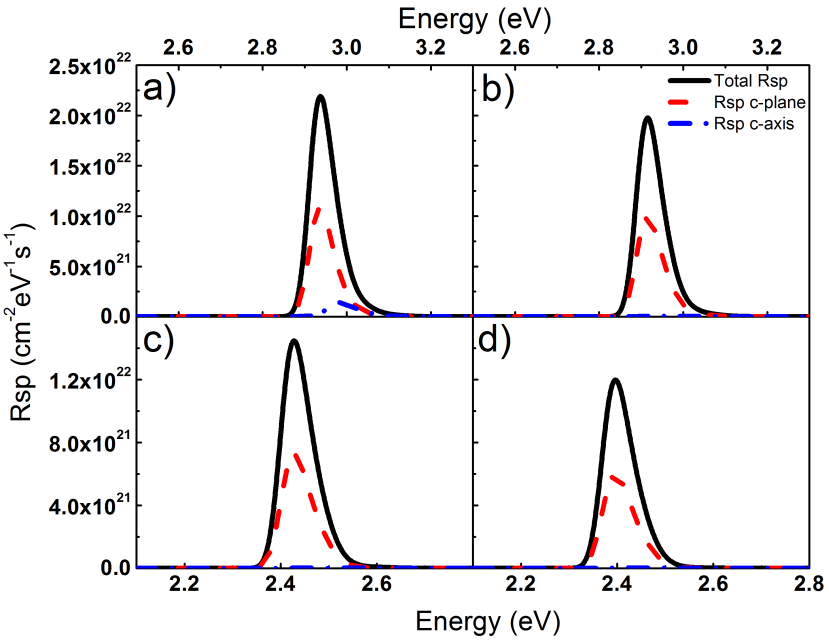

Figure 5: Spontaneous emission spectra at injection carrier density equal to $2.5 \times 10^{12}\ cm^{-2}$ for both the blue (x=14%) and green (x=26%) LED structures having $In_xGa_{1-x}N$/GaN quantum wells with metamorphic layer (a and c) and the conventional quantum well structure (b and d).

In Figure 5 we show the difference in emission strength, by comparison of the spontaneous emission

Led Structure	Overlap $\lvert\langle\psi_e\lvert\psi_h\rangle\rvert$	Emission Energy eV	Peak Spontaneous Emission rate R_{sp}(max) 10^{22}(cm^{-2} eV^{-1}s^{-1})	Integral of Spontaneous Emission Rate (R_{sp}) 10^{21}(cm^{-2} s^{-1})
Blue with ML	**0.5070**	**2.94**	**2.190**	**1.801**
Blue without ML	**0.4525**	**2.92**	**1.975**	**1.619**
Green with ML	**0.3652**	**2.42**	**1.447**	**1.214**
Green without ML	**0.3329**	**2.40**	**1.197**	**1.003**

Table 2: Wavefunction overlap, peak emission energy, peak spontaneous emission rate and integrated spontaneous emission for both the blue (x=14%) and green (x=26%) LED structures having InxGa1-xN/GaN quantum wells with and without metamorphic layer.

spectra for both the blue (x=14%) and green (x=26%) LED structures having $In_xGa_{1-x}N$/GaN quantum wells with metamorphic layer (Figures 5a and 5c) and the conventional quantum well (Figures 5b and 5d).

At injection carrier density equal to $2.5 \times 10^{12}\ cm^{-3}$, the conventional LED structures light emissions is significantly lower than the proposed ones with the metamorphic layer. The results are summarized in Table 2. The results clearly indicate that the addition of tensile strain to the active region is beneficial to the efficiency of LED devices. This was also experimentally observed by Zhang and Tansu,[48] further confirming that the non linear model of piezoelectricity appears to be not just qualitatively but also quantitatively correct. In conclusion, we have analyzed the strain dependence of the piezoelectric field in the active region of two pseudomorphically strained $In_xGa_{1-x}N$ MQWs with different In content and designed for blue (x=0.14) and green (x=0.26) light emission. A significant reduction of the total internal piezoelectric field as a function of tensile strain is found in both cases, when both non-linear piezoelectricity and non-linear elasticity models are taken into account in the calculations. Since tensile strain could be generated by growing the QW region on a semiconductor layer with a lattice parameter larger than that of GaN, a proposal to use a relaxed InGaN metamorphic layer has been presented. We have evaluated the optical matrix elements and the resulting spontaneous emission rate for the proposed structures and confirmed that, consistent with experimental data in the literature, an increase of the optical emission can be predicted. Since we have previously experimentally showed that the change in value of the internal piezoelectric fields is proportional to the change in optical efficiency, LED devices made using the proposed structures are expected to increase their light output power by up to 10%.

Nanowires

To compare the LM and NLM in deformed NWs, we calculated the polarization in a ZnO and GaN nanowires[49, 50] subjected to a bending force deforming the cylindrical shape into an arch. For simplicity the assumption was used that such deformation would result in a polarization that is isotropic for each circular cross section of the nanowire. The resulting perpendicular strain was taken as antisymmetric along the section of the bent cylinder. Since in most materials compressibility is always lower than the ability to withstand tensile deformation, this is a correct assumption only for small strains. The perpendicular strain was related to the parallel strain $\epsilon_{\|}$ through Poissons ratio and the elastic constants of the material. The combination of parallel and perpendicular strain was then used in Eq. 3 to evaluate the polarization. In Figures 6 and 7 we show the variation of the polarization for the case where the perpendicular (parallel) strain varies from -2.8% (+2.8%) to +2.8% (2.8%) for ZnO and -4% (+4%) to +4% (-4%) for GaN. There are marked differences between the predictions of the LM and NLM.

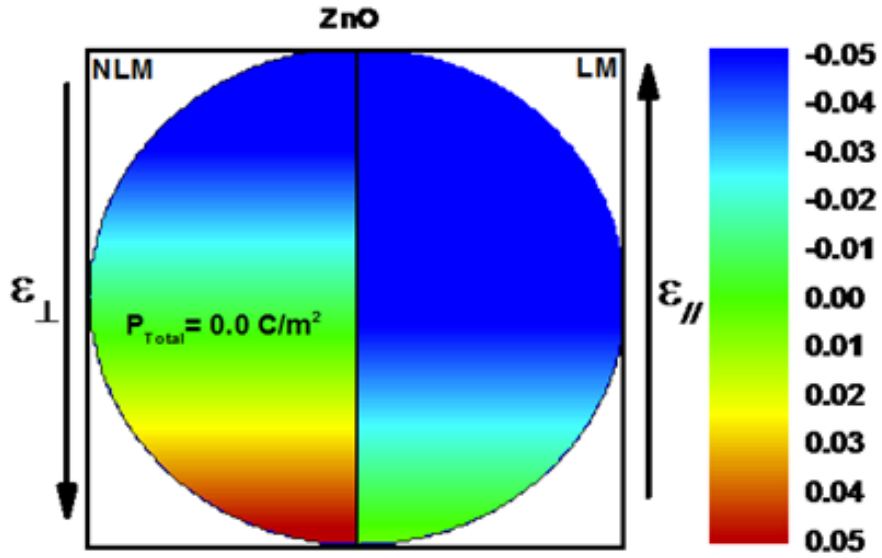

Figure 6: Reproduced with permission from Ref [49]. Variation of the polarization (C/m^2) in a cross section of a ZnO nanowire. The perpendicular (parallel) strain varies from -2.8% (+2.8%) to +2.8% (-2.8%). The calculated polarization of the non-linear (quadratic) model (NLM) is on the left half and the classic linear model (LM) on the right.

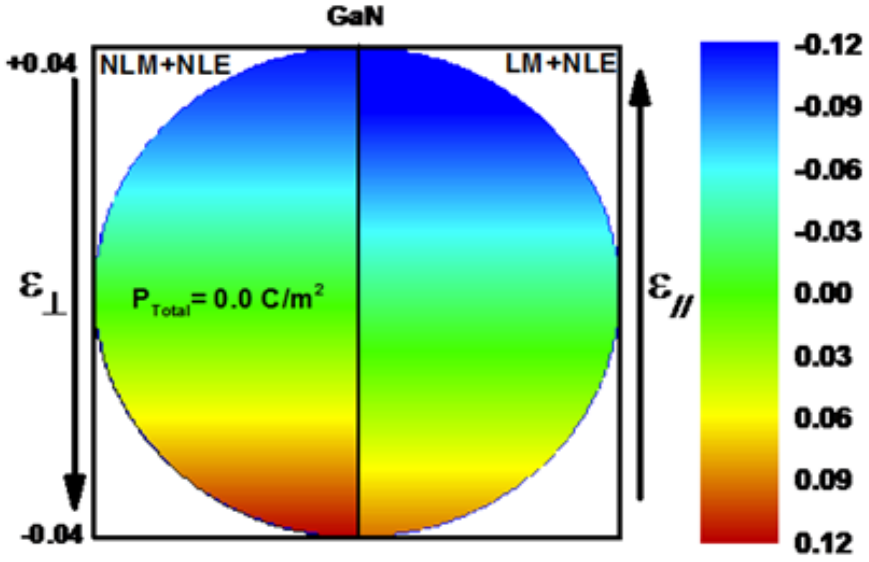

Figure 7: Reproduced with permission from Ref [51]. Variation of the polarization (C/m^2) in a cross section of a GaN nanowire. The perpendicular (parallel) strain varies from -4% (+4%) to +4% (-4%). The calculated polarization using NLE parameters of the non linear (quadratic) model (NLM) is on the left half and the classic linear model (LM) on the right.

In particular, For ZnO, the NLM and LM (in brackets) predict a gradient of the polarization ranging from 0.08 C/m^2 (0.12 C/m^2) at the compressed end of the section, to +0.06 C/m^2 (0.0 C/m^2) at the tensile end. While, for GaN, the NLM and LM (in brackets) predict a gradient of the polarization ranging from -0.12 C/m^2 (-0.15 C/m^2) at the compressed end of the section, to +0.12 C/m^2 (+0.09 C/m^2) at the tensile

Alloy content ($\%$)	Excitonic energy (eV)
20	**3.251**
30	**3.043**
40	**2.832**
50	**2.610**
60	**2.394**
70	**2.219**

Table 3: Alloy composition dependence of the excitonic energy levels in InGaN/GaN quantum dots for bound biexcitons (having a negative biexcitonic shift B_{XX}<0). The calculations are done over different aspect ratios (D/h) of 4, 5, 6 and 7.

end. The conclusion was that LM and NLM can at times produce opposite predictions of the distribution of the total polarization in bent NWs in ZnO and marked differences are observed in GaN, between the predictions of the LM and NLM using the NLE parameters. Nevertheless there are sufficient grounds to assume that non-linear PZ must be considered as one of the possible reasons behind reports of giant PZ coefficients in III-N NWs and pronounced dependence on NW diameter. [51]

III-N Quantum Dots

Here, we analysed the impact of our non linear piezoelectricity model on the Quantum Dots (QDs) formed by $In_xGa_{1-x}N$. We performed modelling of wurtzite $In_xGa_{1-x}N$/GaN QD single particle electron and hole states using an 8-band k.p Hamiltonian [52] including second order piezoelectricity (with our parameters) and P_{sp}, strain, spin-orbit interaction and crystal-field interaction. We obtained the biexciton states using configuration interaction (CI)[53] and finally computed the biexcitonic shift, namely the difference between the energy of the exciton transition line and the energy of the transition line from the biexciton to exciton state. The biexcitonic shift is given by $B_{XX} = (E_{XX} - E_X) - E_X$ and in order to obtain bound biexcitons, B_{XX} needs to be negative. We found that using the parameters from our model, bound biexcitons are achievable over a wide range of structures having an alloy composition varying from 20$\%$ to 70$\%$. All calculations for the exciton and biexciton have been performed for a series of InGaN QDs with aspect ratios (D/h) of 4, 5, 6 and 7 and the outcomes suggest the presence of bound biexcitons across different sizes of the QDs under consideration. In Table 3, we show the variation of the excitonic emission energy with the In alloy composition in InGaN/GaN QDs. Thus, similar to QW nanostructures, the effect of strain induced PZ polarization with second order coefficients and P_{sp} has a large influence over the excitonic properties of QDs. This also forms the basis for highly tunable devices emitting over a wide range of the visible spectra (from 2.2 -3.25 eV).[33] Thus, similar to QW nanostructures, the effect of strain induced PZ polarization with second order coefficients and Psp has a large influence over the excitonic properties of QDs.

Conclusions and Future Scope

This work explores the origin of non-linear piezoelectricity and its influence on the polar III-V, III-N and II-VI semiconductors. The field of piezotronics is emerging and its research impacts a wide range of applications in self-powered circuits for wireless sensors, nanorobotics, interfacing between human and computer, medical science, tactile sensors imitating human skin, nanogenerators for portable devices, solar cells, LEDs and other optoelectronic devices.

The existence of non linear piezoelectric effects in nanostructured polar semiconductors is well established primarily because of my own work. Previous works on the topic has been performed in zincblende III-V semiconductors, but this work reported the strain dependent non linear piezoelectric coefficients for III-N in wurtzite for the very first time. Wurtzite crystals semiconductors such as III-N, by virtue of the existence of four piezoelectric coefficients, i.e. spontaneous polarization, e_{13}, e_{33} and e_{15}, provide sufficiently stringent tests compared to the zincblende semiconductors.
Non linearities in III-N quantum well structures used for light emitting diodes have been shown to provide an important pathway to designing devices with increased optical efficiency. In ZnO and III-N nanowires, non linearities can be exploited in designing composite heterostructured combinations capable of increased piezoelectric response, thus having the potential for becoming the engine in future piezotronic devices such as pressure sensors and nanogenerators. The tunability of the emission spectra of the excitons and biexcitons in different InGaN QDs will be of great interest for development of futuristic optoelectronic devices such as multi exciton generation solar cells and applications based on photon entanglement.
In summary, we developed a computational model on non linearities in piezoelectricity, validated it on real devices and experimental data, also confirmed by others, and exploited the non linear effect to make unexpected predictions of electro optical behaviour in a variety of nanostructures. This research is now an integral part of the global piezotronics effort and will play a pivotal role in computational modelling and design of devices for the better future, providing better fundamental understanding of the underlying physics.

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Computational Physics Group News

• The Computational Physics Annual PhD Thesis Prize

Each year, the IoP Computational Physics Group awards a Thesis Prize to the author of the PhD thesis that, in the opinion of the Committee, contributes most strongly to the advancement of computational physics.

The winner of the 2014 Thesis Prize is is Be$\tilde{n}$at Gurrutxaga-Lerma for his thesis entitled *A Dynamic Discrete Dislocation Plasticity Model for the Study of Plastic Relaxation under Shock Loading*, which was undertaken at Imperial College London.

Runner-up prizes are awarded to Tom Goffrey, for his thesis entitled *A Cylindrical Magnetohydrodynamic (MHD) Arbitrary Lagrangian Eulerian (ALE) Code*, carried out at the University of Warwick, and Bartomeu Monserrat, for his thesis entitled *On the vibrational properties of solids*, carried out at the University of Cambridge.

Thanks to the generosity of the Smith Institute (`www.smithinst.co.uk`) and AWE (`www.awe.co.uk`) Be$\tilde{n}$at receives £450 and Tom and Bartomeu receive £150 each for their achievements.

Summaries of their PhD research will appear in forthcoming issues of this newsletter.

For this year's prize applications are encouraged across the entire spectrum of computational physics. Entry is open to all students from an institution in the UK or Ireland, whose PhD examination has taken place since 1st January 2015 and up to the submission deadline.

Prize winners will be invited to write a feature article in the Computational Physics Group newsletter.

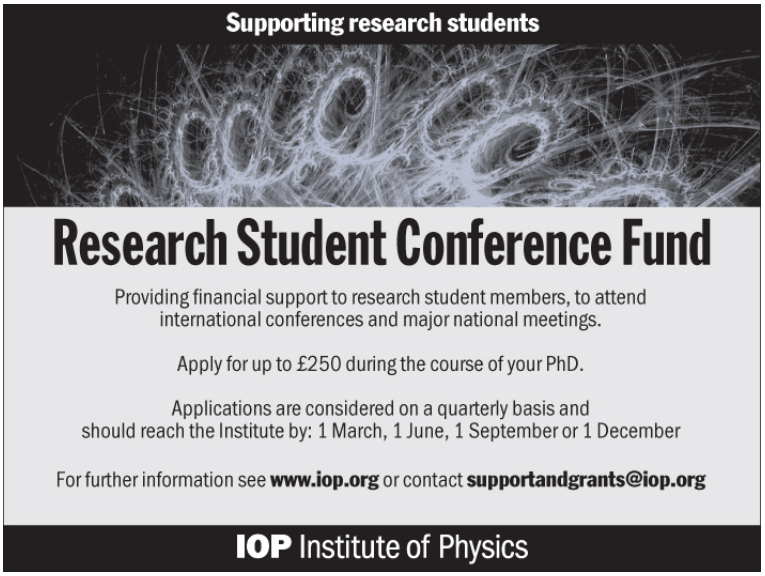
The submission deadline is **30 April 2016**.

The submission format is as follows:

- A four page (A4) abstract describing the background and main achievements of the work
- A one page (A4) citation from the PhD supervisor
- A one page (A4) confidential report from the external thesis examiner

Entries (PDF documents preferred) should be submitted by email, with "IOP CPG Thesis Prize" as the subject header, to Dr Arash Mostofi (a.mostofi@imperial.ac.uk). Any queries should also be directed to Dr Arash Mostofi.

- **IoP Computational Physics Group - Research Student Conference Fund**



The Institute of Physics Computational Physics Group is pleased to invite requests for partial financial support towards the cost of attending scientific meetings relevant to the Group's scope of activity. The aim of the scheme is to help stimulate the career development of young scientists working in computational physics to become future leaders in the field.

Further details on this award can be found at:

`www.iop.org/about/grants/research student/page_38808.html`

Conference and Workshop reports

- **Computational Condensed Matter: advances and challenges (CompMat 2014)**

8-9 September 2014: Whitehavean, The Lake District, UK.
Website: `https://compmat2014.wordpress.com/`

On 7-9 September 2014 the Computational Physics Group based in the University of Lincoln organized an International Symposium and PhD students Workshop **Computational condensed matter: advances and challenges**(`https://compmat2014.wordpress.com/`). The event took place in the seacoast town of Whitehaven in western part of the Lake District National Park in Cumbria (UK), the most westerly and most tranquil of the lakes. The venue was UCLan (University of Central Lancashire) Westlakes campus, which was provided for free and allowed to minimize the costs for the participants. The event marked 10 years of our group. Coincidentally, it was the first scientific event organized by newly founded Lincoln School of Mathematics and Physics at the University of Lincoln, where our group relocated from UCLan on 1st September 2014. The event attracted 37 participants (one of 38 registered participants got not well before the event and could not come) from 10 countries: Spain, Norway, France, Italy, Germany, UK, Japan, Canada, USA and the Netherlands. The small number of the participants allowed for an intensive networking (see Figure 8).

Figure 8: Group Photo on the 9th of November before Symposium dinner at Moresby Hall.

On Sunday 7th of September there was a Pre-symposium workshop delivered by 6 international lecturers. The workshop was oriented on PhD students and postdocs, but was also well attended by many other participants (see Figure 9). The lectures were delivered by Prof. Lev Kantorovich, Prof. Toshihiro Kawakatsu, Dr Lianheng Tong, Dr Attilio Vargiu, Prof. Ignacio Pagonabarraga and Prof. David Q. Wang.

Figure 9: Symposium reception on 7th of September.

The material taught in the symposium covered codes in ab initio materials simulations, hybrid fields, mesoscopic computational approaches, introduction to Monte Carlo simulation and force-field based

molecular simulations. The main program was held on 8 and 9 September, consisting of 15 invited talks, 6 short oral presentations of 20 minutes, 2 poster sessions and substantial discussion time. Pre-dinner key-note lecture was delivered by Professor Daan Frenkel, University of Cambridge (see Figure 10). Daan was talking on the role of entropy and cooperativity in complex self-assembly and his talk was captivating as always providing an unrivalled mixture of depths and entertainment. Two poster sessions combined with the afternoon tea provided plenty of opportunity for discussion. Several scientific publishers offered 7 generous poster prizes in the form of books and journal subscriptions which included poster prizes from Elsevier, Springer, Wiley (Macromolecular Journals), Royal Society of Chemistry and Soft Matter. Special Feature of this computational symposium was the Guest Experimentalist lecture by Philip Moriarty from the University of Nottingham who delivered a fascinating talk on application dynamics of force microscopy in materials science and its connection to the Pauli principle which underpins the ability to achieve submolecular resolution.

Figure 10: Keynote “pre-dinner” lecture by Daan Frenkel, closing 1st day scientific program.

The symposium program was accompanied by the symposium dinners, where discussions continued. The symposium was finished by the symposium dinner at Moresby Hall with a lively string quartet performance by Elysia String Quartet from the South Lakes. The event was financially supported by IOP Computational Physics Group, RSC Materials Chemistry Division, J-OCTA of JSOL Corporation and Polymers (MDPI). Thanks to this and other support, we kept the fee low, in particular for PhD students, and in some cases we waived participation fee for some PhD students. As a result of the symposium new collaboration emerged and old collaborations were refreshed.

Report kindly provided by Marco Pinna, School Mathematics and Physics, Lincoln, CompMat2014 committee

Upcoming Events of Interest

Upcoming events of interest to our readers can now be found via the following web links.

- IOP's index page for scientific meetings, including conferences, group events and international workshops:

  `www.iop.org/events/scientific/index.html`

- IOP Conferences page for conference information, calendar and noticeboard:

  `www.iop.org/events/scientific/conferences/index.html`

- All events being run or supported by IOP Groups including calendar and links to event web pages:

  `www.iop.org/events/scientific/group/index.html`

- Thomas Young Centre: The London Centre for Theory and Simulation of Materials organises many different kinds of scientific events on the theory and simulation of materials, including Highlight Seminars, Soirees and Workshops. For further details of upcoming events please visit:

  `www.thomasyoungcentre.org/events/`

- CECAM is a European organization devoted to the promotion of fundamental research on advanced computational methods for atomistic and molecular simulation and their application to important problems in science and technology. CECAM organises a series of scientific workshops, tutorials and meetings. For further details please visit:

  `www.cecam.org`

Computational Physics Group Committee

The current members of the IoP Computational Physics Group committee with their contact details are as follows:

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Some useful web links related to the Computational Physics Group are:

- CPG webpages
  comp.iop.org
- CPG Newsletters
  Current issue:
  www.iop.org/activity/groups/subject/comp/news/page_40572.html
  Previous issues:
  www.iop.org/activity/groups/subject/comp/news/archive/page_53142.html
  www.soton.ac.uk/∼fangohr/iop_cpg.html

Related Newsletters and Useful Websites

The Computational Physics Group works together with other UK and overseas computational physics groups. We list their newsletter locations and other useful websites here:

- Newsletter of the Computational Physics Division of the American Physical Society:
  www.aps.org/units/dcomp/newsletters/index.cfm
- Europhysicsnews newsletter of the European Physical Society (EPS):
  www.europhysicsnews.org/
- Newsletter of the Psi-k (Ψ_k) network:
  www.psi-k.org/newsletters.shtml