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Microelectronics and Nanostructures (M&N)

Microelectronics and Nanostructures group

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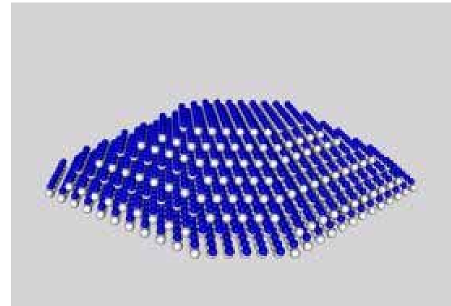
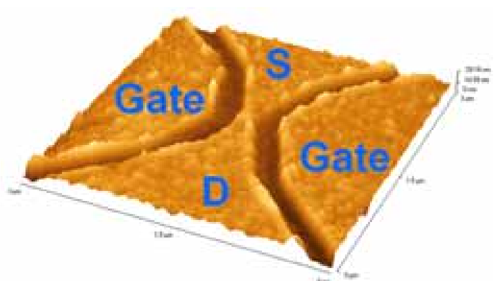
- 3 MBE reactors: 1 V100+, 2 V90
- clean-rooms (class 100 & 1000): IC, III-V, Si, polymer
- e-Beam & AFM nano fabrication facilities
- Optical spectroscopy: including μ-Raman
- Electrical measurements: Laplace DLTS
- AFM / STM / EFM: cryogenic UHV state of art



Quantum Dots



plastic nano-transistor

- Imaging and spectroscopy of Nanomaterials and Devices
- THz Photonics & Terahertz Technologies.
- Nanostructured Semiconductors based Devices
- VLSI Design for IP architecture
- Polymer based Electronics
- Modelling of Semiconductor Materials & Nanostructures

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Piezoelectric coefficients of strained InAs and GaAs

Dr Max Migliorato

RAENG-EPSRC and RCUK Research Fellow
Microelectronics and Nanostructures Group

School of Electrical and Electronic Engineering

The Royal Academy of Engineering

EPSRC
Engineering and Physical Sciences Research Council

NUSOD-Nottingham, September 2008

Outline

- **Introduction:**
  - **Classic theory of Piezoelectricity**
  - **Piezoelectric Quantum Wells**
- **II order piezoelectric effects in (111) growth**
  - **The effect of strain**
  - **Harrison's model**
  - **DFT-LDA calculations**
- **II order piezoelectricity in (001) growth**
  - **I order Piezoelectric effect in Quantum Dots**
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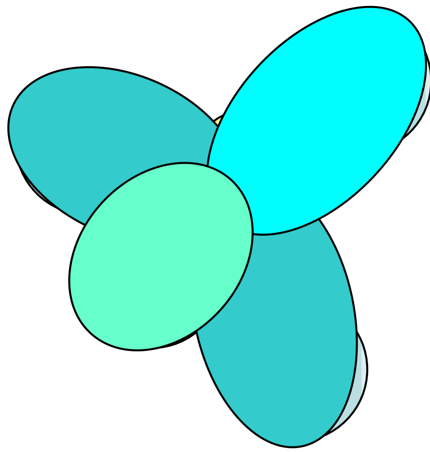
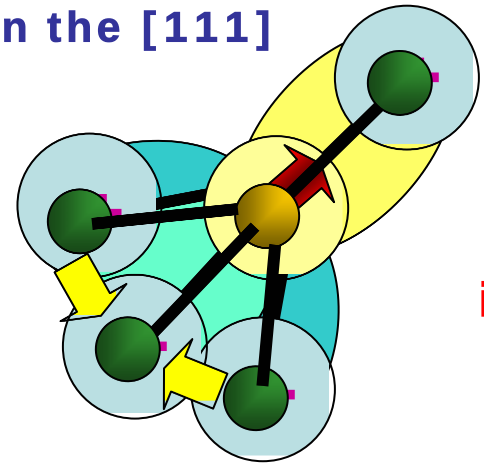
- **Conclusions & Acknowledgements**

Piezoelectricity in III-V Semiconductors

Strain in the [111]

4 identical sp^3 orbitals



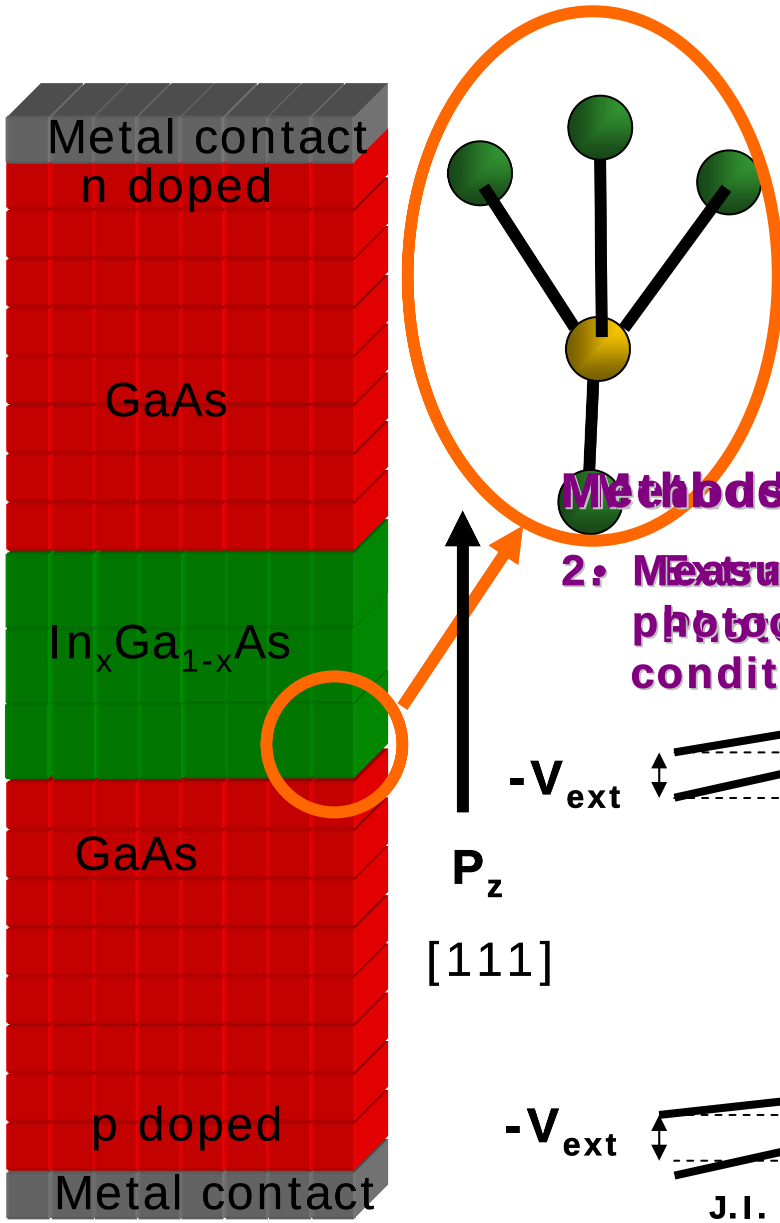


Only 3 identical sp^3 orbitals

Polarisation $$P_i = \sum_{k,l} \tilde{e}_{ikl} e_{kl}$$

Charges $$\rho(\mathbf{r}) = -\nabla \cdot \left(2e_{14}(\mathbf{r})[e_{yz}(\mathbf{r})\mathbf{i} + e_{xz}(\mathbf{r})\mathbf{j} + e_{xy}(\mathbf{r})\mathbf{k}]\right)$$

Piezoelectricity in [111] QWs

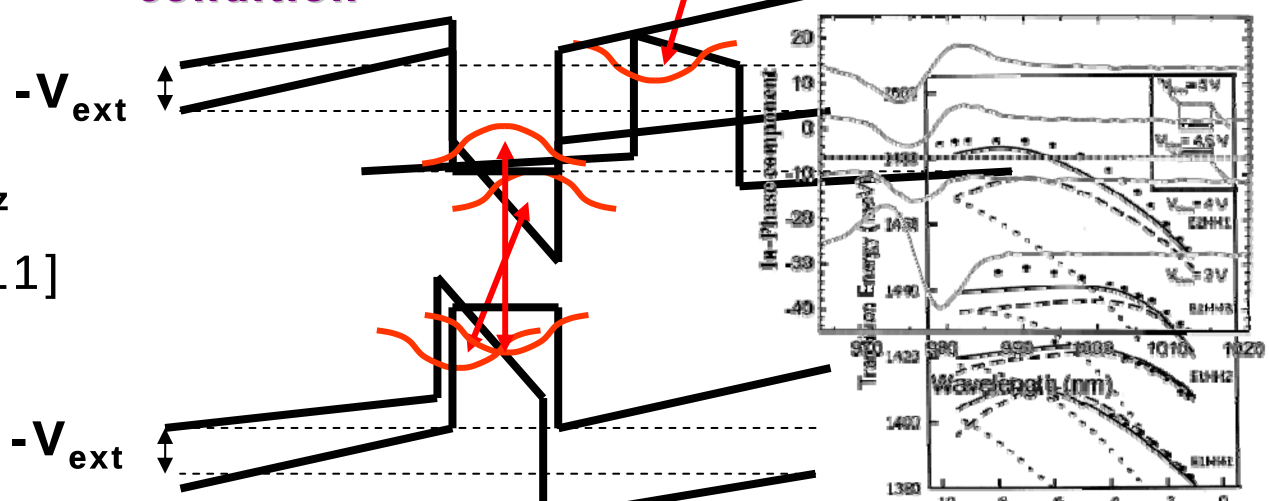


Methods to obtain P_z

Methods to obtain P_z

2. Measure directly through Differential photocurrent looking at the flat band condition

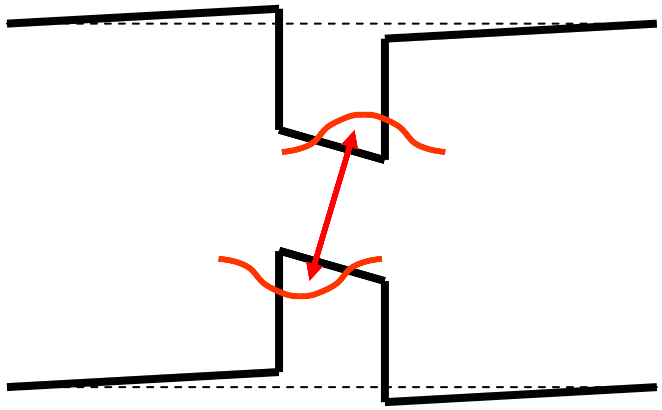
Extrapolate from Model Photocurrent vs External bias

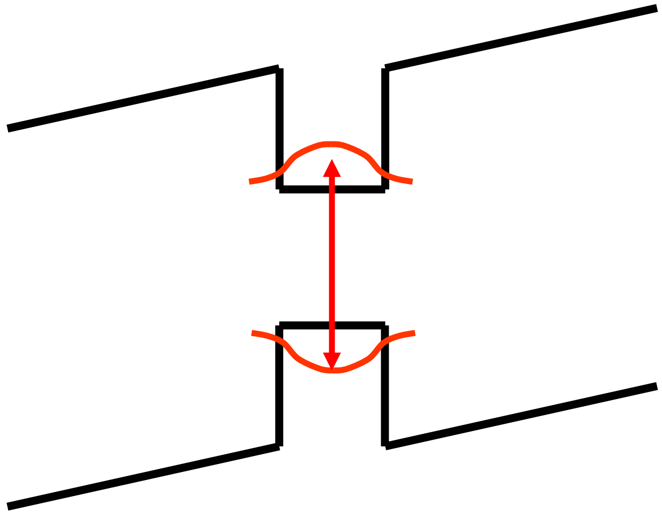


J.I. Izpura *et al*, Microelectronics Journal 30, 439 (1999)

Hogg *et al,* Phys Rev B 48, 8491 (1993)

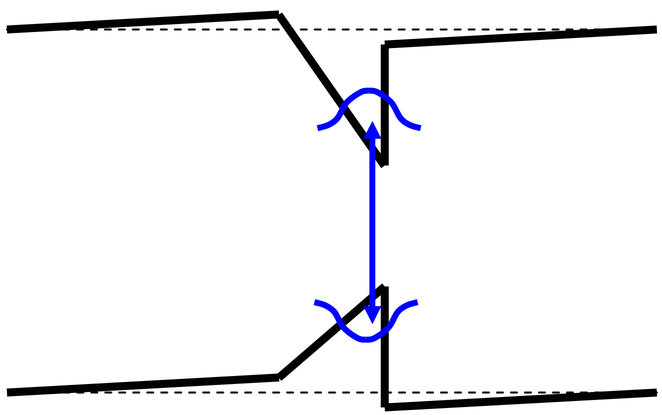
Piezoelectricity in [111] QWs

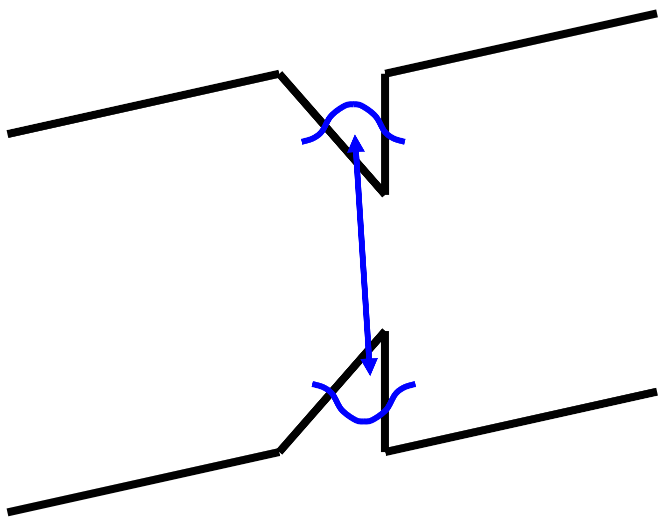




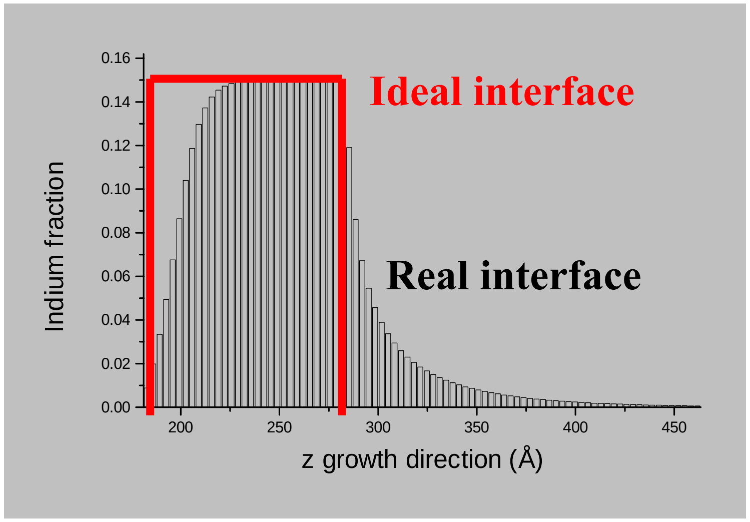
Photocurrent vs External bias

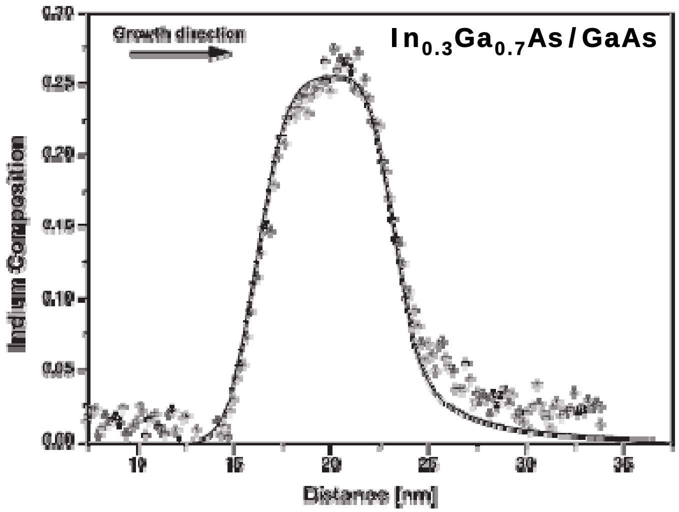
Differential Photocurrent

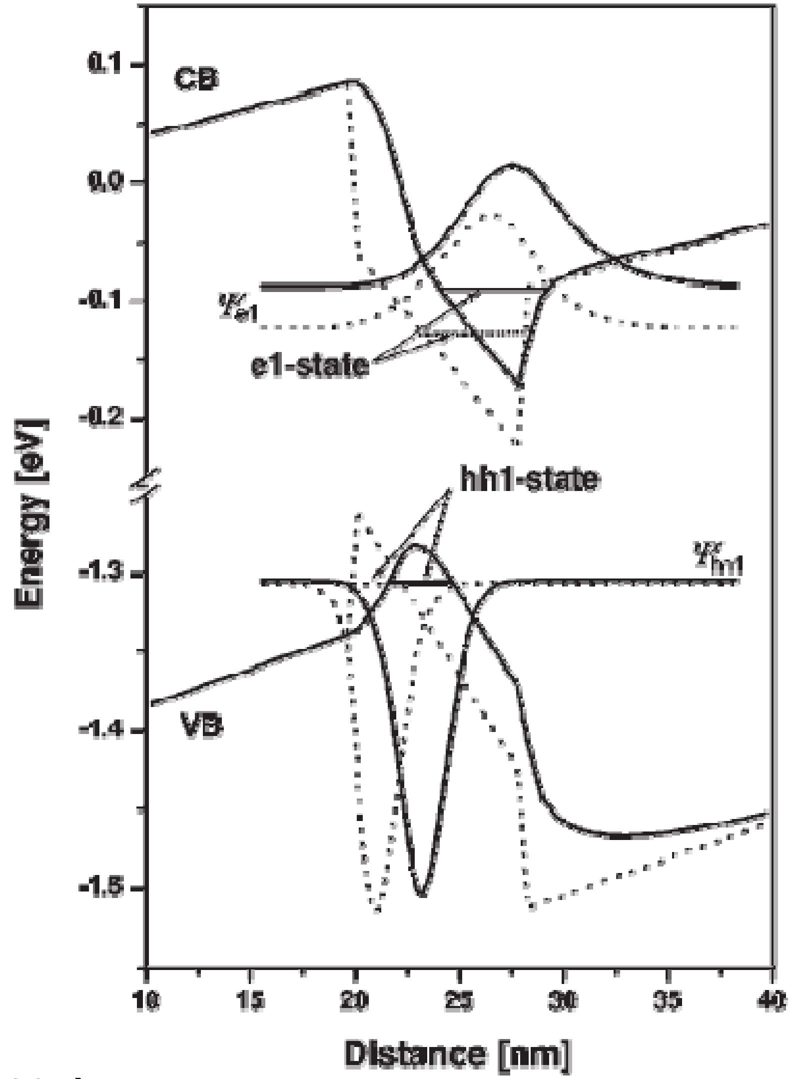




Piezoelectricity in real [111] QWs







Moran *et al*, J. Phys. D: Appl. Phys. 34, 1943 (2001)

Piezoelectricity in real [111] QWs

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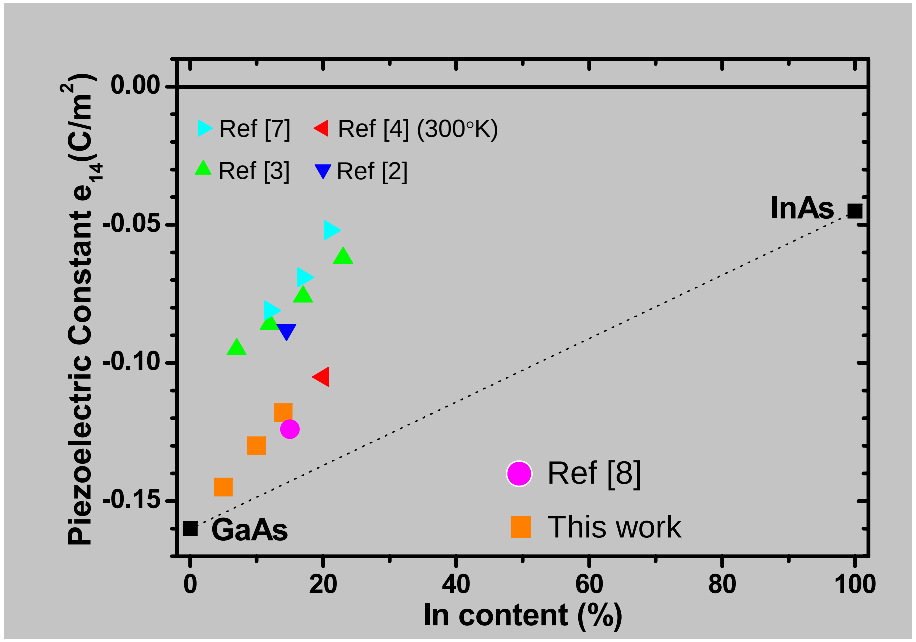
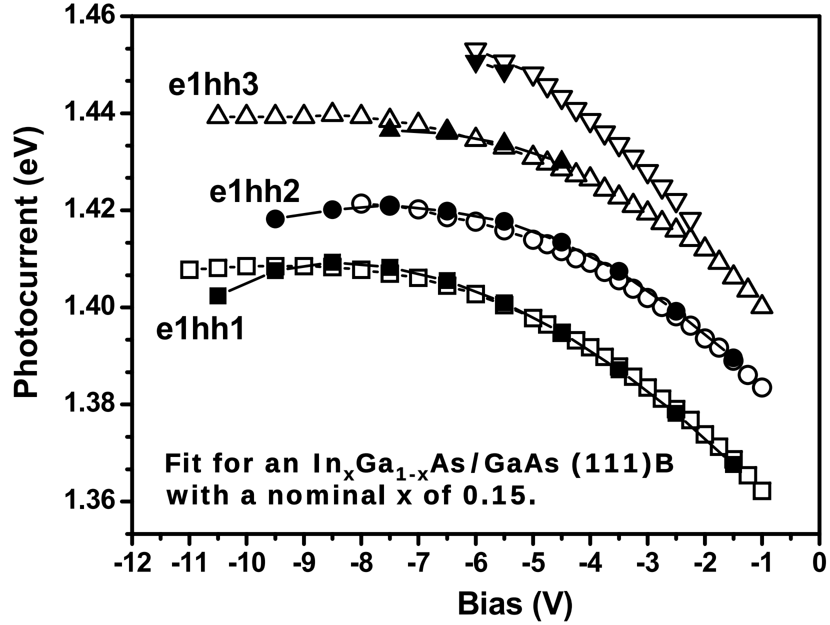


[2] R.A. Hogg et al 48, 8491 (1993)
[3] J.L. Sanchez-Rojas et al Appl. Phys. Lett. 65, 2042 (1994)
[4] C.H. Chan et al, Appl. Phys. Lett. 72, 1208 (1998)
[7] S. Cho et al, phys. stat. sol. (a) 195, 260 (2003);
J. Appl. Phys 90, 915 (2001); J. Appl. Phys 96, 1909 (2004)
[8] P. Ballet, Phys. Rev. B 59, R5208 (1999) (with Segregation)

The best fit is obtained including segregation and with e_{14} 83 % of the linearly interpolated value. Linear regression to the GaAs bulk value was also used.



M.A. Migliorato *et al*, Phys. Rev. B 74, 245332 (2006)

Outline

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Piezoelectricity and Strain

The problem is that bulk and strained layers have different piezoelectric properties!!!! (G Bester, X Wu, D Vanderbilt and A Zunger, Phys Rev Lett 96, 187602 (2006))

$$\hat{x}' = (1+\varepsilon)\hat{x} + \frac{\gamma}{2}\hat{y} + \frac{\gamma}{2}\hat{z}$$

$$\hat{y}' = \frac{\gamma}{2}\hat{x} + (1+\varepsilon)\hat{y} + \frac{\gamma}{2}\hat{z}$$

$$\hat{z}' = \frac{\gamma}{2}\hat{x} + \frac{\gamma}{2}\hat{y} + (1+\varepsilon)\hat{z}$$

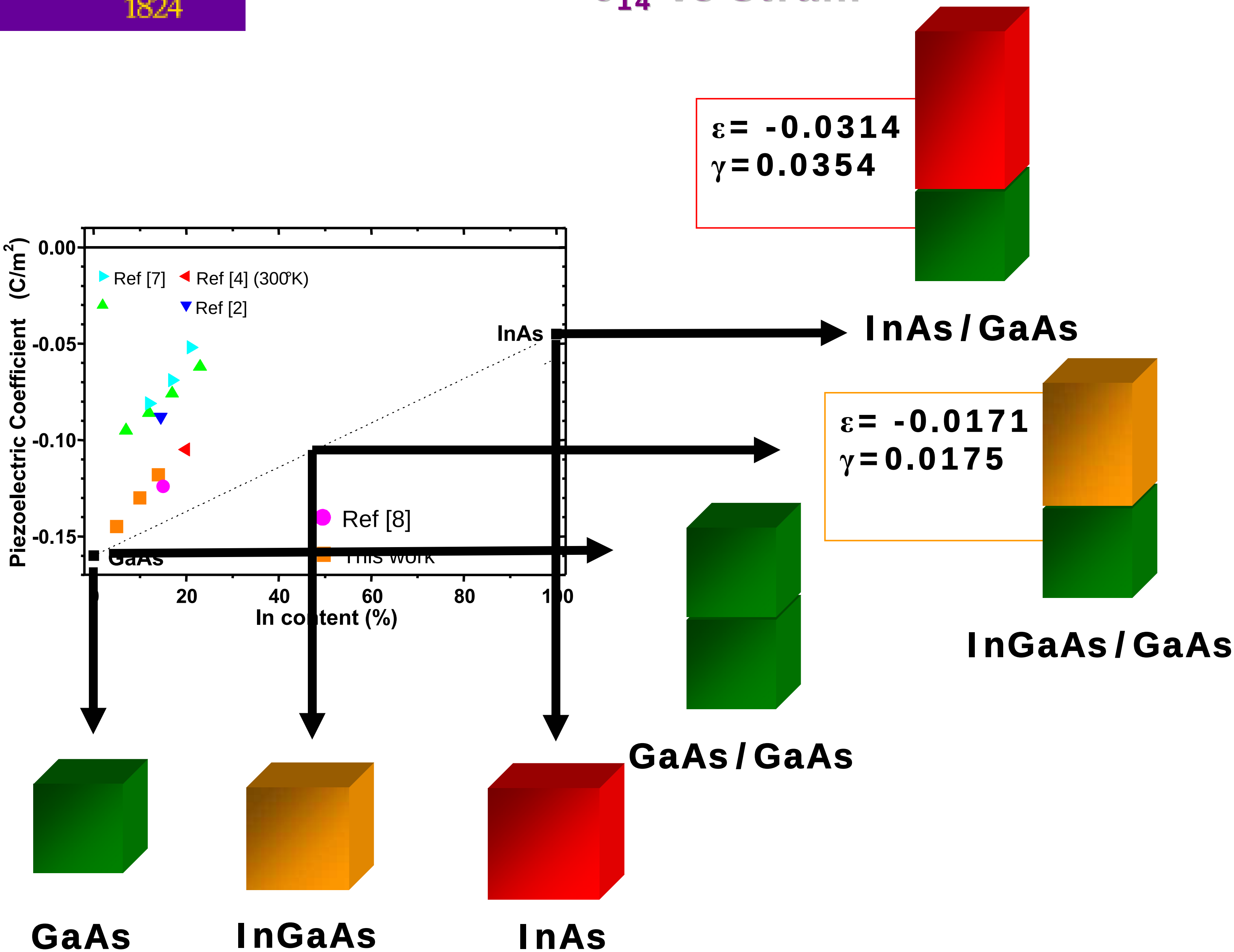
Strain Tensor in (111) growth: Only two strains!!

Polarisation $$P_i = \sum_{k,l} \tilde{e}_{ikl} e_{kl}$$

Charges $$\rho(\mathbf{r}) = -\nabla \cdot \left(2e_{14}(\mathbf{r})[e_{yz}(\mathbf{r})\mathbf{i} + e_{xz}(\mathbf{r})\mathbf{j} + e_{xy}(\mathbf{r})\mathbf{k}]\right)$$

$$\mathbf{P} = \mathbf{e}_{14} * \gamma$$

e_{14} vs Strain



Harrison’s model

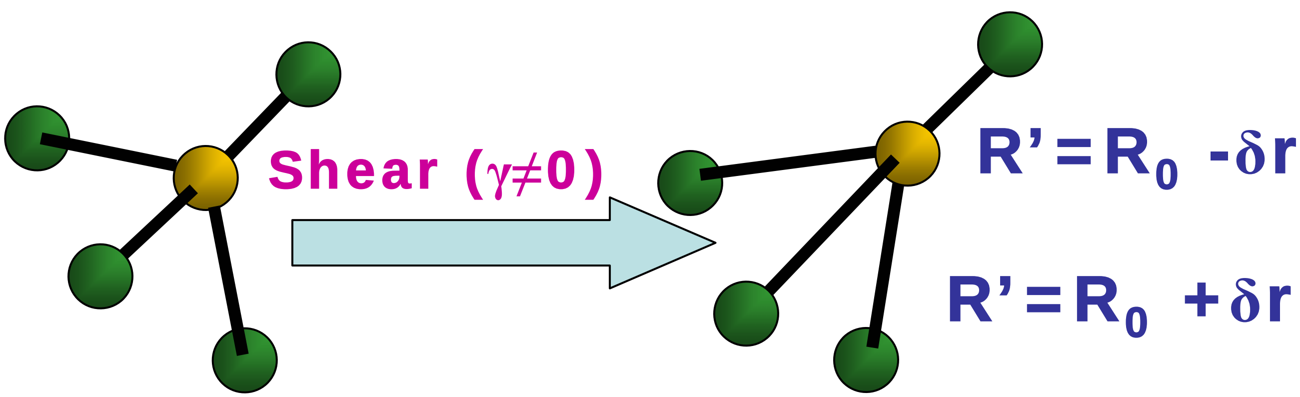
PHYSICAL REVIEW B VOLUME 10, NUMBER 2 15 JULY 1974

Effective charges and piezoelectricity*

Walter A. Harrison
Applied Physics Department, Stanford University, Stanford, California 94305

(Received 26 December 1973)

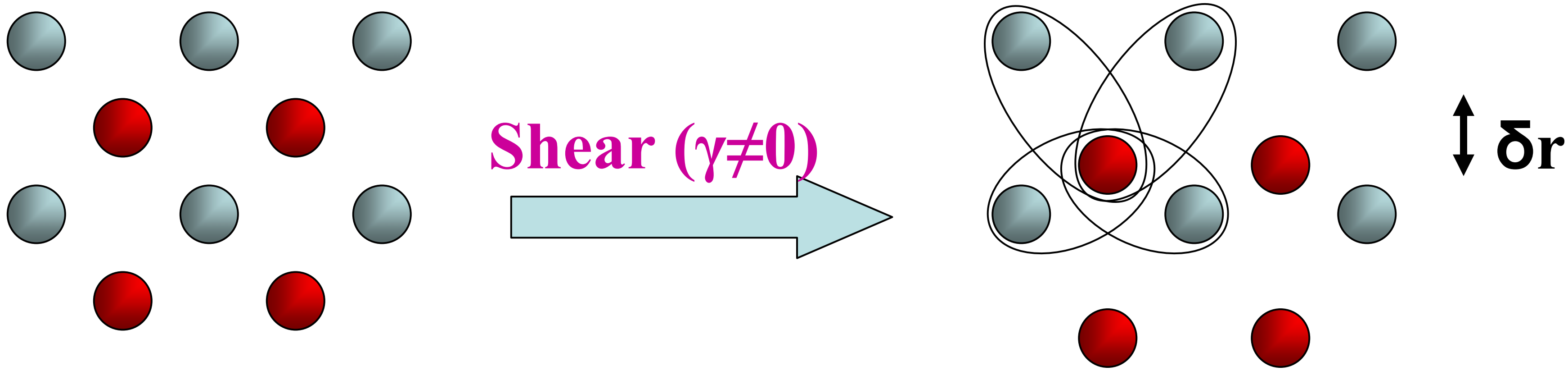
The effective charge for piezoelectricity is calculated using the bond-orbital model and Martin's internal-displacement parameters. Direct and simple calculations made with no additional parameters lead to a semiquantitative description of this effect. The qualitatively different trend with polarity shown by this charge and by the macroscopic transverse effective charge is elucidated. It is noted that this approach is essentially equivalent to the approach used by Lannoo and Decarpigny in studying the transverse effective charge, but is very different from the approaches used in other current studies of effective charges.



$$\delta r = \frac{\sqrt{3}}{4} a \gamma \zeta$$

Kleinman Parameter

Harrison's model



$$P^{\mathrm{direct}} = \mathrm{e}Z_{\mathrm{H}}{}^{*} \cdot \delta \mathrm{r}$$

$$P_k^{dipoles} = 2\alpha_p\left(1-\alpha_p{}^2\right)\sum_{i=1}^{4}\left(\vec{r}_q \cdot \vec{k}\right)\delta R_q$$

Material parameters in the Tight Binding expressions:

α_p: bond polarity

Z_H*: effective ionic charge (depends on α_p)

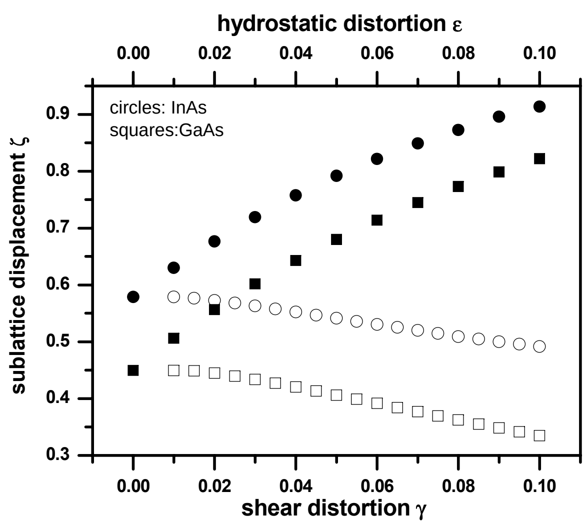
ζ: Kleinman parameter

Problem: No reliable values for Z_H*, α_p, ζ so only semi-quantitative

DFT and Harrison's model

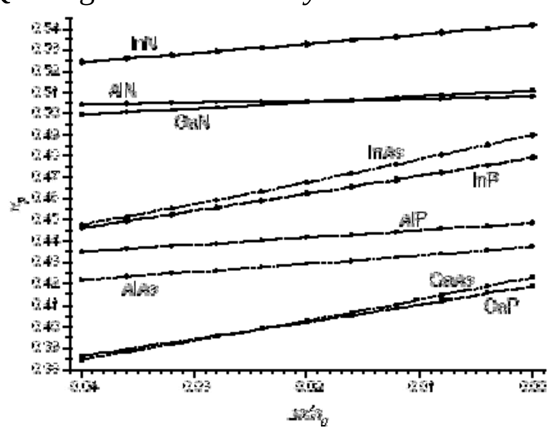
- Harrison's model is based on Tight Binding (BOM)
- ab initio for the 3 Tight Binding quantities
- include strain effects in the DFT calculations
- DFT-LDA, 1000eV, MP-K grid 8x8x8
- DFPT, Born Charges, CASTEP

$$Z^*_{DFT} = \Delta Z + 4\alpha_p + 4\alpha_p(1-\alpha_p^2)$$



Kleinman parameter ζ

S Q Wang *et al* 2005 *J. Phys.: Condens. Matter* **17 4475**



Bond Polarity α_p

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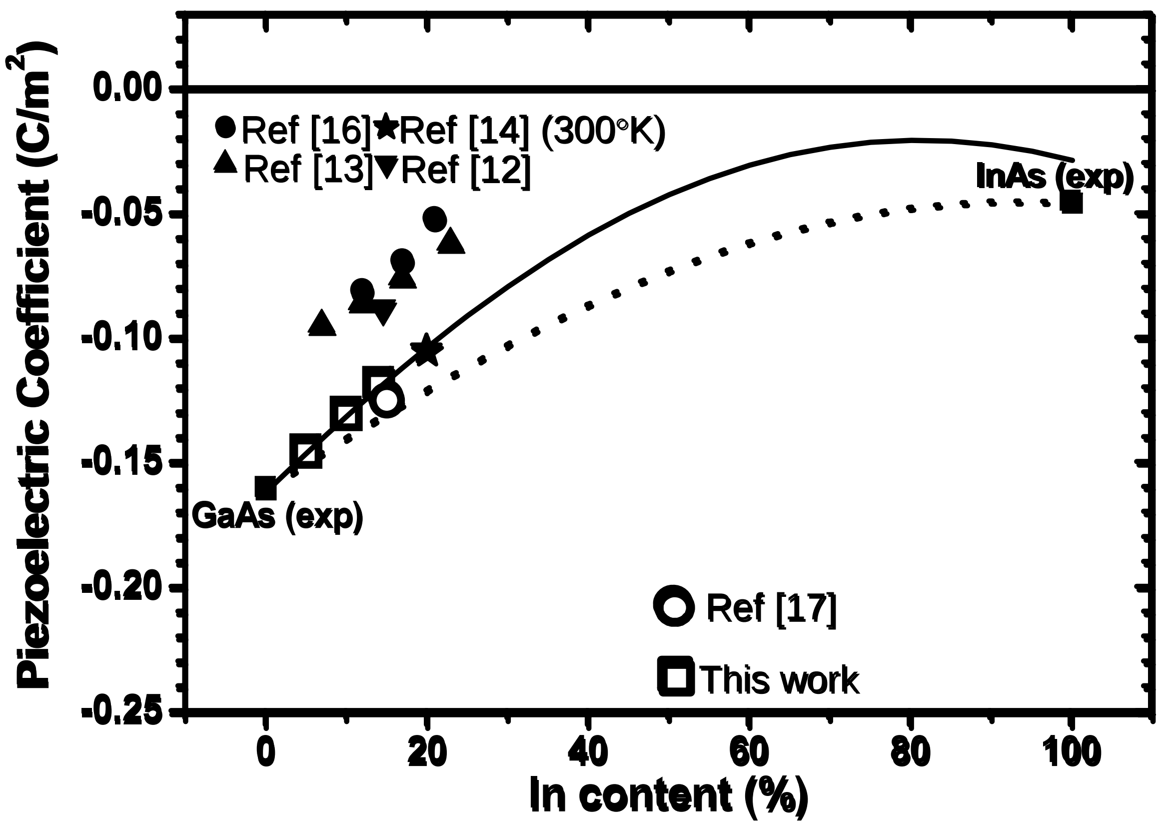
Piezo-coefficient for (111) Growth

M.A. Migliorato *et al*, Phys. Rev. B 74, 245332 (2006)



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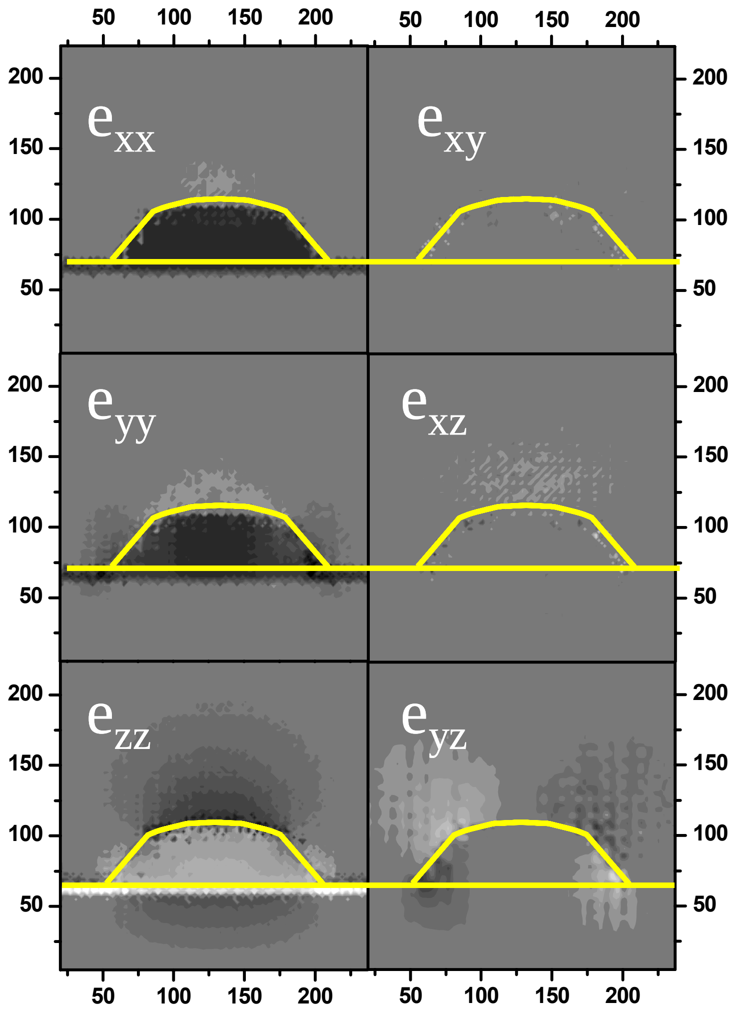
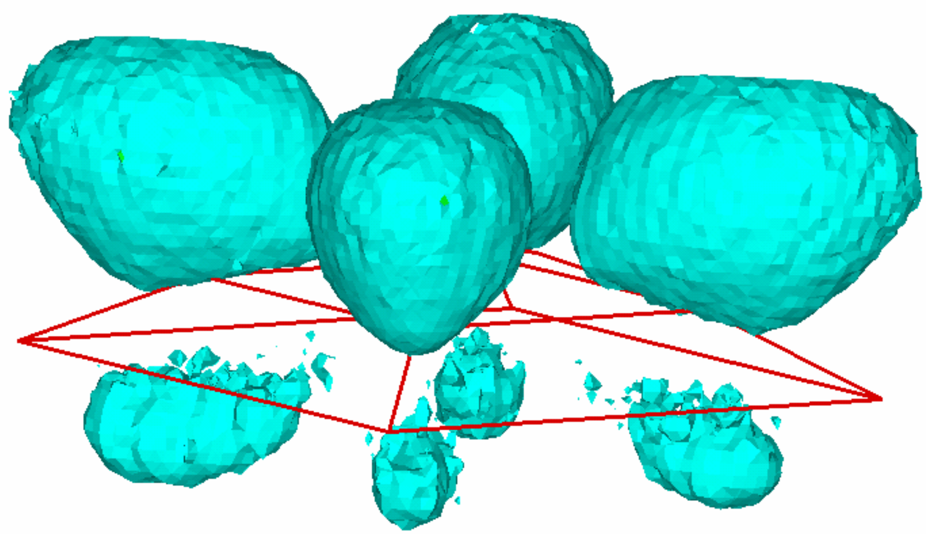
Piezo-effect in QDs for (001) Growth

6 components of the strain tensor



potential



e_{14} vs Pseudomorphic Strain.

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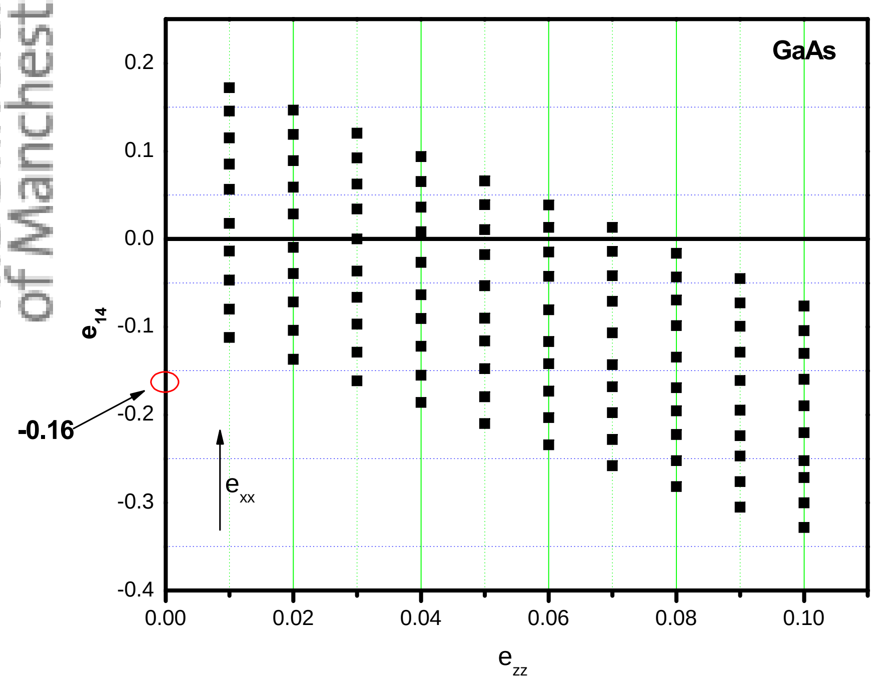

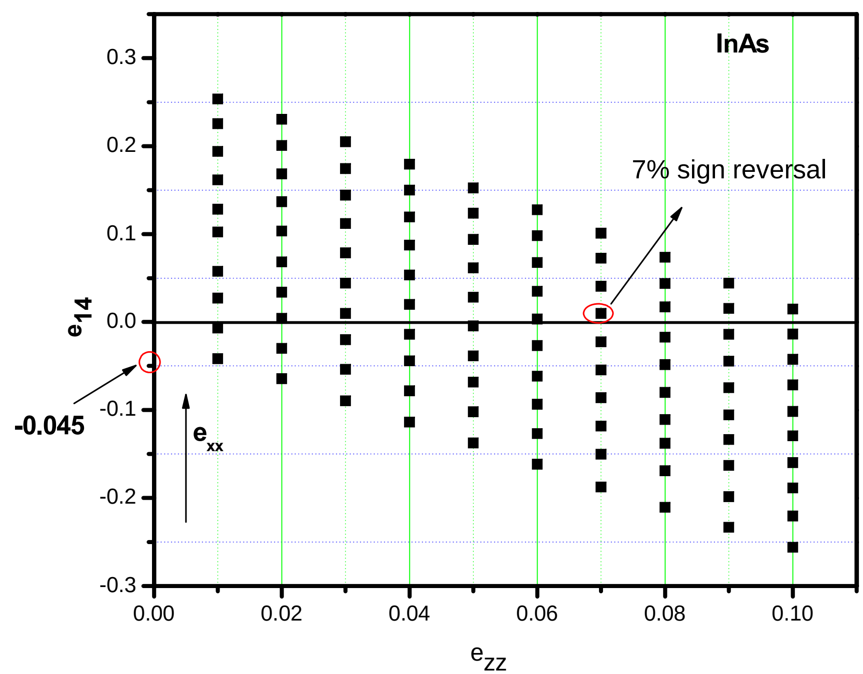

$$\vec{P} = 2[e_{14}(\mathbf{r})\varepsilon_{yz}(\mathbf{r})\mathbf{i} + e_{25}(\mathbf{r})\varepsilon_{xz}(\mathbf{r})\mathbf{j} + e_{36}(\mathbf{r})\varepsilon_{xy}(\mathbf{r})\mathbf{k}]$$

We are now dealing with a general form of the expression for P

As a result of strain the 3 piezo coefficients are not generally identical

For [001]: identical behaviour for e_{25} , similar for e_{36}

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Conclusions

- First order piezoelectricity is only valid for material that is strained by very small non diagonal strains.
- II order piezoelectric effects in the strain can be efficiently calculated in the framework of Harrison's model and DFT-LDA calculations
- In (111) growth this model shows excellent agreement with experimental data and the predicted values of e_{14} are always in the range 0-25% lower than the linearly interpolated values.
- In (001) growth the framework can result in inversion of the piezoelectric coefficients compared to bulk.

Acknowledgements

Many thanks and gratitude go to:

- EPSRC grant EP/C534352/1
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- G.P Srivastava (Exeter)
- Thomas Hammerschmidt (Oxford)
- CDG: CASTEP Development Group, Dr Matt Probert & Dr Phil Hasnip (York)
- Tony Cullis, Dave Powell (formerly), Luke Wilson, Evgeny Zibik (Sheffield)
- Andrei Schliwa (Berlin)
- (the late) HPC Team in Manchester

DFT and Harrison's model

- **Interpolation scheme for Alloys:**

GaAs Z_H^*, α_p, ζ →	**$In_xGa_{1-x}As$** $Z_H^*(x), \alpha_p(x), \zeta(x)$	← **InAs** Z_H^*, α_p, ζ

↓

Include Strain dependence

↓

$$P_k = Z_H^* * \delta r + 2\alpha_p\left(1-\alpha_p{}^2\right)\sum_{i=1}^{4}\left(\vec{r}_q \cdot \vec{k}\right)\delta R_q$$

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ζ & α_p vs Pseudomorphic Strain