Microelectronics and Nanostructures (M&N)

- 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

V100+
E-Beam/SEM
DLTS
LT STM

- 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

Quantum Dots

plastic nano-transistor
NUSOD-Nottingham, September 2008
Piezoelectric coefficients of strained InAs and GaAs

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Microelectronics and Nanostructures Group

School of Electrical and Electronic Engineering
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
  • DFT-LDA calculations

• Conclusions & Acknowledgements
Piezoelectricity in III-V Semiconductors

4 identical sp$^3$ orbitals

Only 3 identical sp$^3$ orbitals

Polarisation

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

Charges

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

NUSOD-Nottingham, September 2008
Piezoelectricity in [111] QWs

\[ \text{Methods to obtain } P_z \]

1. Extrapolate through modeling of photocurrent vs. external bias
2. Measure directly from differential photocurrent looking at the flat band condition


Piezoelectricity in [111] QWs

Photocurrent vs External bias

Differential Photocurrent
Piezoelectricity in real [111] QWs

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.


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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))

\[
\begin{align*}
\hat{x}' &= (1 + \varepsilon) \hat{x} + \frac{\gamma}{2} \hat{y} + \frac{\gamma}{2} \hat{z} \\
\hat{y}' &= \frac{\gamma}{2} \hat{x} + (1 + \varepsilon) \hat{y} + \frac{\gamma}{2} \hat{z} \\
\hat{z}' &= \frac{\gamma}{2} \hat{x} + \frac{\gamma}{2} \hat{y} + (1 + \varepsilon) \hat{z}
\end{align*}
\]

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

Polarisation

\[ P_i = \sum_{k,l} \tilde{e}_{ikl} e_{kl} \]

Charges

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

\[ P = e_{14} \gamma \]
Piezoelectric Coefficient (C/m$^2$)

- GaAs
- InGaAs
- InAs

Ref [8]
Ref [2]
Ref [4] (300°K)
Ref [7]

Piezoelectric Coefficient vs In content (%)

- $\varepsilon = -0.0314$
- $\gamma = 0.0354$

- $\varepsilon = -0.0171$
- $\gamma = 0.0175$

NUSOD-Nottingham, September 2008
Effective charges and piezoelectricity*

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(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.

\[ R' = R_0 - \delta r \]

\[ R' = R_0 + \delta r \]

\[ \delta r = \frac{\sqrt{3}}{4} a \gamma \xi \]

Kleinman Parameter
Harrison’s model

Shear ($\gamma \neq 0$)

\[ P_{\text{direct}} = eZ_H^* \cdot \delta r \]

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

Material parameters in the Tight Binding expressions:

- $\alpha_p$: bond polarity
- $Z_H^*$: effective ionic charge (depends on $\alpha_p$)
- $\zeta$: Kleinman parameter

Problem: No reliable values for $Z_H^*$, $\alpha_p$, $\zeta$ so only semi-quantitative
• 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

\[ Z_{DFT}^* = \Delta Z + 4\alpha_p + 4\alpha_p (1 - \alpha_p^2) \]

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Piezo-effect in QDs for (001) Growth

6 components of the strain tensor

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

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 \( e_{36} \).
Outline

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Conclusions

- First order piezoelectricity is only valid for material that is strained by very small non-diagonal strains.
- Second 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.
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- 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:

\[ P_k = Z_H^* \delta r + 2\alpha_p (1 - \alpha_p^2) \sum_{i=1}^{4} (\vec{r}_q \cdot \vec{k}) \delta R_q \]
$\zeta$ & $\alpha_p$ vs Pseudomorphic Strain