Non Linear Piezoelectricity in ZincBlende GaAs and InAs Semiconductors

G. Tse, J. Pal, R. Garg, V. Haxha and M.A. Migliorato
School of Electrical and Electronic Engineering, University of Manchester, United Kingdom
Joydeep.pal@postgrad.manchester.ac.uk

***Abstract*- We investigate the strain dependence of piezoelectric effect, both linear and non linear, in zincblende GaAs and InAs semiconductors. We expanded the polarization in terms of the ionic and dipole charges, internal displacement and the exploited the ab-initio Density Functional Theory (DFT) to evaluate the dependence of all quantities on the strain tensor. By this detailed study of the non linear piezoelectric effect, we report that even third order effects are significant.**

I. INTRODUCTION

It is well known that the piezoelectric effect in bulk III-V semiconductors arises from lack of inversion symmetry along particular crystallographic directions[1,2] and is found in devices as diverse as light-emitting diodes (LEDs), lasers, power electronics, transducers and micropositioners [3]. In III-V semiconductors and their nanostructures, strain with a component along the polar axis of the crystal leads to the generation of the electric dipoles. In epitaxially grown zincblende (ZB) materials such dipoles are linked to off-diagonal strain tensor components and manifest themselves as a piezoelectric field that exists in nanostructures grown on [111] oriented substrates. A similar effect is also noticeable in wurtzite (WZ) semiconductors along the polar axis of [0001] orientation and diagonal strain components are able to generate dipoles. Though non linear effect in the strain have long been recognized as important in the calculation of piezoelectric fields in ZB II-VI [4], ZB III-V [5,6,7] and WZ III-N [8] semiconductors, the two most widely used methods in the calculation of such non linearities, namely the linear response method [9] and Harrison's method[10], appear to produce different results. The predictions from those two methods have not been compared before mainly because the work using Harrison's method [5,6] has always been presented for subsets of the full strain tensor. In this work, we have tried to address this issue and report the dependence of the piezoelectric coefficients on a full set of diagonal components of the strain tensor.

II. NUMERICAL RESULTS AND DISCUSSION

In the framework of Harrison's theory and the scheme previously established by Migliorato et al [5] we use ab initio density functional theory in the local density approximation to extract the elastic and dielectric properties of single crystals under various degrees of pressure in the 3 main crystallographic directions. The results properly combined in a formulation that takes into account the dipole formation between cations and anions, together with the modification of the dipoles along all bonds in the tetrahedron of the zincblende structure, leads self consistently to the identification of strain induced polarization coefficients. As already noticed in our previous work [5,6], our data shows strong strain dependence and hence non linear piezoelectric effect, with a marked lack of inversion antisymmetry $\varepsilon_i \leftrightarrow -\varepsilon_i$ suggesting the existence of at least quadratic terms in the strain. To further prove this point we obtain the non linear piezoelectric coefficients by fitting a third order polynomial to the DFT calculated after we impose conditions on the coefficients based on the cubic symmetry of the crystal. The recent work by Beya-Wakata et al [9] presented a comprehensive study based on DFPT and linear response theory of non linear polarization in various III-V zincblende semiconductors. The method used differs from ours as it relies entirely on ab-initio calculation without any fitting parameters, which are instead used in our model (Z_H*). One of the major differences between the two models is that while the non linear response method introduces the small dependence on the quadratic shear strain, it neglects higher order contributions such as the quadratic and cubic terms in the diagonal strain components that our model instead obtains via a fitting procedure of the DFT data. The two models discussed in this paper obviously produce very different results. We pick two critical cases for comparison: InAs pseudomorphically strained on GaAs (001) ($\boldsymbol{\varepsilon}_1$= $\boldsymbol{\varepsilon}_2$= -0.7, $\boldsymbol{\varepsilon}_3$=+0.7, with a further shear given by $\boldsymbol{\gamma}$=0.02) or GaAs (111) ($\boldsymbol{\varepsilon}_1$= $\boldsymbol{\varepsilon}_2$= $\boldsymbol{\varepsilon}_3$= -0.223, $\boldsymbol{\gamma}$=0.268). The Beya-Wakata et al [9] model predict a polarization in the growth direction equal to +0.069 C/m2 for the (001) and +0.808 C/m2 for the (111) case. We note that the linear term alone would in both cases predict a negative polarization. Our model too predicts a positive sign of the polarization, but of a much smaller magnitude: +0.002 C/m2 for the (001) and +0.201 C/m2 for the (111) case. This is a crucial difference and should be observable in experiment. The present work showcases the importance of the non-linear terms, namely second and third order, for zincblende GaAs and InAs in calculating the piezoelectric field.

ACKNOWLEDGMENT

The authors thank Dave Powell for the parameterization routines used in the work.

REFERENCES

[1] R. M. Martin, Piezoelectricity, Phys. Rev. B **5**,1607(1972)
[2] W. G. Cady, Piezoelectricity (McGraw-Hill, New York, 1946)
[3] S. Nakamura, G. Fasol, The Blue Laser Diode: GaN Based Light Emitters and Lasers (Springer-Verlag, Berlin, 1997)
[4] L. C. Lew Yan Voon and M. Willatzen, Electromechanical phenomena in semiconductor nanostructures, Journal of Applied Physics **109**, 031101 (2011)
[5] M. A. Migliorato, D. Powell, A. G. Cullis, T. Hammerschmidt and G. P. Srivastava, Composition and strain dependence of the piezoelectric coefficients in $In_xGa_{1-x}As$ alloys, Phys. Rev. B **74**, 245332 (2006)
[6] R. Garg, A. Hüe, V. Haxha, M.A. Migliorato, T. Hammerschmidt, G. P. Srivastava: Tunability of the piezoelectric fields in strained III-V semiconductors, Appl. Phys. Lett. **95**, 041912-1–3 (2009)
[7] G. Bester, X. Wu, D. Vanderbilt, and A. Zunger, Importance of Second-Order Piezoelectric Effects in Zinc-Blende Semiconductors, Phys. Rev. Lett. **96**, 187602 (2006)
[8] J. Pal, G. Tse, V. Haxha, M. A. Migliorato and S. Tomic´, Second-order piezoelectricity in wurtzite III-N semiconductors, Physical Review B **84**, 085211 (2011).
[9] A. Beya-Wakata, P-Y Prodhomme and G. Bester, First- and second-order piezoelectricity in III-V semiconductors,Phys. Rev. B **84**, 195207 (2011)
[10] W. A. Harrison, Electronic Structure and Properties of Solids, Dover Publications Inc., New York, (1989).