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Volumetric piezoelectric effect and artificial pyroelectricity in GaAs

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Abstract

Multifunctional properties of semi-insulating GaAs type crystals could be essentially expanded under special boundary conditions. These crystals partial strain limitation makes possible to obtain electrical response on such external *scalar influence* as hydrodynamic pressure or temperature change. This gives rise to a new generation of microelectronic *one-crystal sensors* in which transducers, amplifiers and read-out electronics are various parts of the same crystal. In these devices, semi-insulating wafer itself is employed as matrix of sensor elements while amplifiers and other micro-electronics are no more than very thin semiconductor epitaxial layers.

Introduction

It is anticipated that future sensor devices will be manufactured by the use of microelectronics. By this is meant that sensor elements should be integrated with semiconductor chip to amplify and convert information. Integration of this sort occurs naturally for *semi-conductor* sensors but sometimes their possibilities and sensitivity are limited. In this connection, *dielectric* sensors might have generous advantages.

Unfortunately, based on dielectrics microelectronic sensors should be combined in various materials *hybrid* structure: "active" dielectric and semiconductor read-out chip. It is well known that constituent hybrid structures processing comes up against problems because their components have quite different chemical and physical properties.

It is significant that III-V crystals could be very close in their conductivity to dielectrics. Semi-insulating GaAs and moreover its solid solutions with AlP is considered as a dielectric other than semiconductor. Consequently, the only electrical polarization should be taken into account. In other words, *charge generation process* diminishes to nothing while *charge separation mechanisms* are the main features being considered.

Moreover, crystals of GaAs type have polar (piezo-electric) structure and are capable to convert external influences into electric signals, even if they are not pyroelectrics. So these crystals would be very promising as sensor materials if their polar potentialities would be unveiled. In such in event, the sensor and amplifying as well as read-out functions could be joined in a *one-crystal* device. That is why we have devoted our efforts to the conversion of piezoelectric type of response into a pyroelectric one. This idea was realized by the artificial controlling of crystal *boundary conditions*.

Response nature

Semiconductor microelectronic sensors of pressure (p) or temperature (T) are based on *electrical conductivity* (σ) *change*. For this object in view, scalar variables δp or δT are indicated through the effects of piezoresistivity $\sigma(\delta p)$ or far-infrared photoconductivity $\sigma(\delta T)$ [1].

In a similar manner, *dielectric* sensors for δp or δT evaluation use *spontaneous polarization* (P_s) *change*. The last provides so cold **volumetric piezoeffect** ($\delta P_i = e_i\ \delta p$) as well as **pyro-electric effect** ($\delta P_i = \gamma_i\ \delta T$). At this point, δP_i is the change of spontaneous polarization vector; thus volumetric piezoelectric coefficient ν_i as well as pyroelectric coefficient γ_i inherent to the polar dielectrics only.

By the symmetry, both of above mentioned effects are prohibited for free-stress III-V crystals (under conditions when crystals are free to expand). Of course, specials cuts of GaAs type crystals exhibit longitudinal and transverse piezoelectric effects as responses on *vectorial* or other *tensor type* external influences. However, free-stress III-V crystals are not capable to electrical response to any *scalar* influence like hydrodynamic pressure, uniform change of temperature etc.

It is significant that polar material characteristics e_i and γ_i are *vectorial* quantities. It was considered that lasts are possible only in the crystals which symmetry belongs to one of 10 *pyroelectric* classes that have "intrinsic vector" - spontaneous polarization P_s [2]. Nevertheless, this work is devoted to the possibility to obtain artificially vectorial γ_i or e_i responses in non-pyroelectric but piezoelectric crystals, among them in crystals of GaAs symmetry.

One of the mentioned artificial effects, namely, thermo-mechanically induced pyroelectricity is demonstrated on Fig.1 where "classical" pyroelectric response from pyroelectric (a) and ferroelectric (b) crystals are shown in comparison with two new types of responses (c,d). Following a common practice for pyroelectricity, the idea about temperature change of spontaneous polarization is applied. However, P_s decrease to zero could not be examined in "classical" pyroelectrics (Fig.1a) because of their melting at $T = T_m$. Nevertheless, decrease $P_s \to 0$ in ferroelectrics by the law $P_s \sim (\Theta\text{-}T)^{0.5}$ is shown on Fig.1b. The last is associated with long-range dipole interaction in one-dimensional (1D) ordered system. Correspondingly, their pyroelectric coefficient rises steeply near phase transition: $\gamma_i = dP_s/dT \sim (\Theta\text{-}T)^{-0.5}$. That is why γ_i in ferroelectrics could have very high magnitude.

Piezoelectrics are capable only to “artificial pyroeffect” possible in the conditions of partial clamping. Their intrinsic polar moments are second or third rank tensors, so vectorial component ΔP on Fig.1,c,d represents so cold “dipole projection” of spatially arranged complicated polarities. Because of this, artificial values ΔP and γ_i temperature changes are dissimilar from pyroelectric $P_s(T)$ and $\gamma_i(T)$ dependencies.

Theoretical background

Unit cell electric arrangement of any piezoelectric crystal may be described by various multipole (dipole/ quadrupole /octupole) electric moments that correlates with one/two/ three/-dimensional intrinsic polarity. Such *latent polar structure* is non-compensated in pyroelectrics that is represented for simplicity by 1D dipole cell, Fig.2,a. By virtue of the fact, dipole potential energy decreases with distance as $\sim r^{-2}$. These corresponds to $P_s \sim (\Theta-T)^{0.5}$ temperature dependence shown on Fig.1a.

However, polar structure is totally self-compensated in the free-stress piezoelectrics. Fig.2b shows 2D polar unit cell arrangement with three polar axes crossed at the angle 120^0 and characterized by energy decrease as $\sim r^{-3}$ (this model is close to quartz crystal). Crystals of GaAs type correspond to octupole 3D configuration with four polar axes crossed at $109{,}5^0$ angle and energy demagnification law of $\sim r^{-4}$.

Temperature change alters ionic and electronic forces in piezoelectric unit cells. Thermal disorganizing increases or decreases octupole or hexapole electric moment magnitudes. By way of illustration, octupole intrinsic polarity space distribution is represented on Fig.3a. Due to its high symmetry, *uniform* change of temperature or pressure could not separate electrical charges in piezoelectric crystal of GaAs type and no electrical response is excited.

It is the anisotropic limitation of thermal strains that makes possible artificial pyroelectricity and volumetric piezoeffect in such a crystals. Fig.3b demonstrates “octupole” moment distortion under the partial clamping: new spatial moment distribution shows dipole component appearance that is equivalent to P_s. In such a manner, uniform but anisotropic partial clamping destroys total self-compensation of non-central crystal 2D or 3D intrinsic polarity. This decompensation allows to observe polar responses which are "dipole projections" ΔP_i from broken by clamping spatial polar arrangement of piezoelectrics. The main ΔP_i temperature functions are shown on Fig.1: $\Delta P \sim (\Theta-T)$ if piezoelectric polar axes arrangement is planar (2D), but obeys to law $\Delta P \sim (\Theta-T)^2$ in the case of 3D (spatial) arrangement of these axes. These laws was established by the experimental study of artificial pyroelectric response in piezoelectric samples in the conditions of partial clamping, Fig.4. Dipole projection ΔP decreases with temperature in line with Fig.1c,d. From $\Delta P(T)$ temperature Θ = 843 K was obtained in quartz but in GaAs type crystals intrinsic polarity disappears only while melting (T_m) similarly to pyroelectrics, Fig.1a.

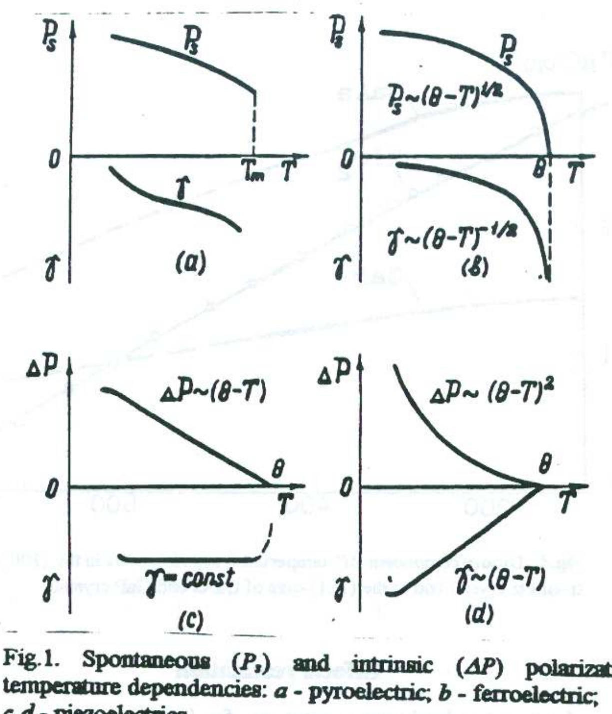

Fig.1. Spontaneous (P_s) and intrinsic (ΔP) polarization temperature dependencies: *a* - pyroelectric; *b* - ferroelectric; *c,d* - piezoelectrics.

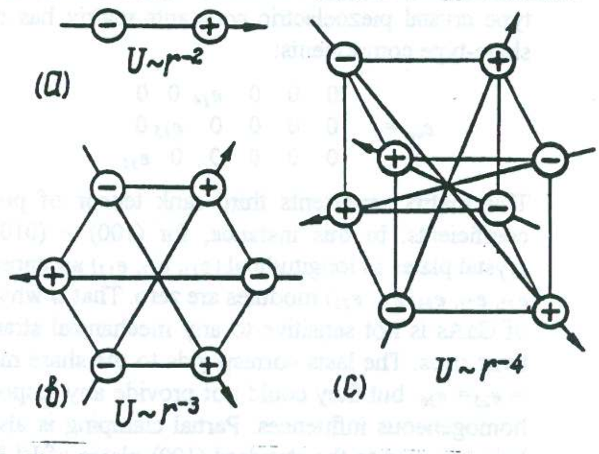

Fig.2. Simulation of non-central symmetric crystals unit cells electrical moments: *a* - dipole moment (1-st rank tensor); *b* - hexapole moment (2-nd rank tensor); *c* - octupole moment (3-rd rank tensor).

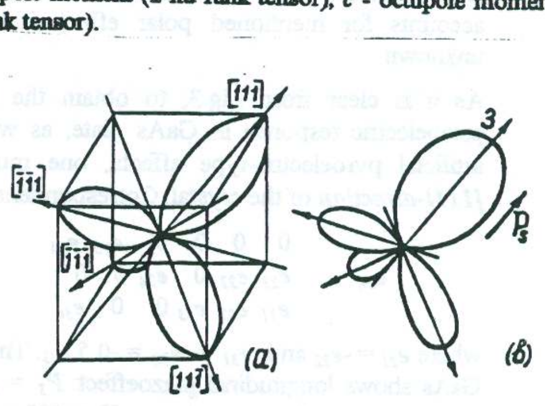

Fig.3. Spatial distribution of III-V crystals piezoelectric responsibility: *a* -free-stress crystal in which (111)-type axes are polar ones but totally compensated; *b* - partially clamped crystal with the artificially increased in [111] direction dipole-type responsibility.

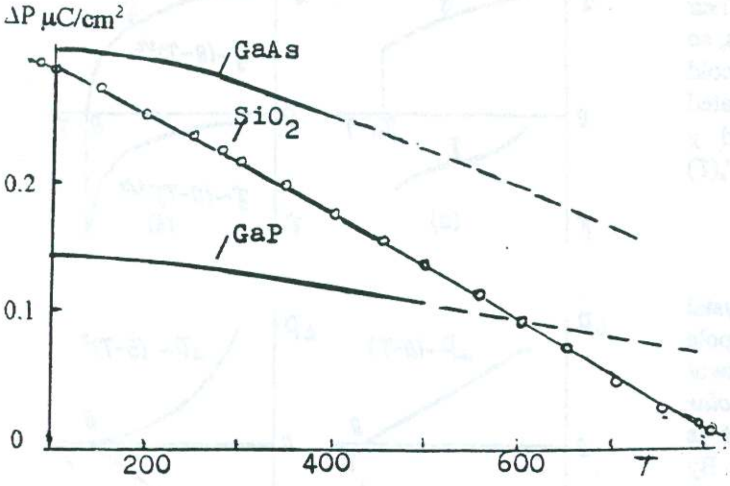

Fig.4. Dipole component ΔP temperature dependencies in the (100)-cut of α-quartz crystal and in the (111)-cuts of GaAs and GaP crystals.

Effects realization

In the standard representation, for [100] direction of GaAs type crystal piezoelectric constants matrix has only three share-type components:

$$e_{im} = \begin{matrix} 0 & 0 & 0 & e_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & e_{15} & 0 \\ 0 & 0 & 0 & 0 & 0 & e_{36} \end{matrix}$$

This matrix represents third rank tensor of piezoelectric coefficients. In this instance, for (100) = (010) = (001) crystal plates as longitudinal (e_{11}, e_{22}, e_{33}) so transverse (e_{12}, e_{13}, e_{21}, e_{23}, e_{31}, e_{23}) modules are zero. That is why (100)-cut of GaAs is not sensitive to any mechanical strains except twist ones. The lasts corresponds to the share modules $e_{14} = e_{25} = e_{36}$ but they could not provide any response under homogeneous influences. Partial clamping is also useless, being applied to the standard (100) plates of III-V crystals. However, the lasts are conceptually the sole material for GaAs devices. It is not improbable, that this is the main accounts for mentioned polar effects previously were unknown.

As it is clear from Fig.3, to obtain the maximum of piezoelectric response in GaAs plate, as well as wanted artificial pyroelectric-type effects, one must use ***polar [111]-direction*** of the crystal. Correspondent matrix is

$$e_{im} = \begin{matrix} 0 & 0 & 0 & 0 & e_{15} & e_{16} \\ e_{21} & e_{22} & 0 & e_{24} & 0 & 0 \\ e_{31} & e_{32} & e_{33} & 0 & 0 & e_{36} \end{matrix}$$

where $e_{21} = -e_{22}$ and $e_{31} = e_{32} = -0.5\ e_{33}$. Therefore, (111)-GaAs shows longitudinal piezoeffect: $P_3 = e_{33}\ x_3$ and the transverse one: $P_3 = e_{31}x_1 + e_{32}x_2$. Here "3" is the [111]-axis and all x_m are strains induced by external influence. The lasts are equivalent: $x_1 = x_2 = x_3$ if excitation is homogeneous and if studied plate is free to expand or contract. Because crystal is non-pyroelectric, sum of piezoelectric coefficients of transverse and longitudinal piezoelectric cofficints should be zero, e.g. $e_{31} + e_{32} + e_{33} = 0$ and no response is possible.

In just the same way, while thermal treatment, in the stress-free crystal longitudinal strain component $x_3 = \alpha dT$ in its piezoelectric transformation should be totally compensated by two transverse components: $x_1 = x_2 = \alpha dT$. Consequently, even the polar (111)-plate of GaAs type crystals could not be sensible to homogeneous excitations (if crystals are ***free-stress***).

The simplest experimental realization of partial strain limitation is demonstrated on Fig.5a: by this method, the first experimental data on artificial pyroelectricity in piezoelectrics have been obtained [3]. Planar strains in the semi-insulating (111)-cut crystal plate are banned by the "ideally hard" substrate. For volumetric piezoeffect, a hard steel substrate would be used. As a result, ***planar strains are limited by rigid substrate*** ($x_1 = x_2 = 0$) and the only response $P_3 = e_{33}x_3$ is non-compensated. So the possibility of volumetric piezoeffect is maid artificially, while e_{33} transfer to the first rank tensor - vector v_i.

In similar fashion crystal plate could be activated for pyroelectric response: if rigid substrate on Fig.5a has thermal expansion coefficient $\alpha \sim 0$ (in our experiments a fused silica was used). Under this conditions, planar thermal strain is forbidden and polarization $P_3 = e_{33}\alpha\delta T = \gamma_3\delta T$ imitates "pyroelectricity".

For GaAs (111) thin plate $\gamma_3 = 1.5\ \mu C/m^2K$ was obtained. Correspondent voltage sensitivity is $S_V = 0.02\ m^2C^{-1}$. It is worthy of notice that GaAs sensitivity is almost identical with S_V of commonly used PZT-type pyroelectric ceramics. Later investigations show that some of III-V (capable to form solid solution and epitaxial layer with GaAs) have γ and S_V parameters 10 times more [5]. Above all, they are much closer to dielectrics than semi-insulating GaAs.

Feasibility of GaAs-based sensor array

Other possibility of planar strain limitation is shown on Fig.5b: for device application, the decrease of response symmetry can be obtained in the immediate region of GaAs substrate by special etching to create cavities in basis plate. Such a finned design can be realized by micromachinery methods [5].

Thin and "soft" membranes separated by thick and "hard" edges of substrate provides a way for artificial volumetric effect as well for "pyroelectricity". Experiment shows that finned structure has a response 2-4 times more than simple element. This amplification is due to the membrane effect when e_{31} and e_{32} add to the e_{33}. Thin epitaxial GaAs FET amplifier is usually located on membrane that works as a piezo- or pyro-gate. For ***piezotransistor*** etched cavities should be closed while ***pyrotrasistor*** need the cavity covered by infrared absorbent layer.

The last one consists of MESFET with submicron channel that can be realized on thin epitaxial layer deposited onto (111)-cut wafer operating as the "pyrogate" [7]. Infrared radiation could be absorbed as by special IR-absorbent covering the back side of wafer so due to internal IR absorption of wafer. The last could be explained as by III-V crystal polar lattice peculiarities, so by its imperfections and doping.

The first method is usually used in pyroelectric detectors based on the ferroelectric materials with a very high IR reflection and large near-surface IR absorption. Unfortunately, slow thermal diffusion from IR-absorbent to pyroelectric bounds operation speed. As applied to semi-insulating GaAs, modulating frequency about 1 kHz is required at which temperature wave length in GaAs wafer is about 100 μm. The more thick wafer could not essentially increase the "pyroelectric" response.

The occasion of ***internal absorption*** seems to be more interesting due to high operation speed. This absorption is inherent to GaAs type ***polar*** crystals and as a result they are semitransparent for infrared radiation. Thermal-to-electrical response could be got directly in the crystal lattice without any delay while MESFET is also capable to rapid operation with pulses rise of 10^{-11} s. So the inertialess is one of the advantages of new device.

The modulation frequency of IR-radiation in the III-V crystal "pyrodetector" depends on the equilibrium concentration of charge carries. In standard semi-insulating GaAs (10^{-9} $\mathrm{Ohm^{-1}m^{-1}}$conductivity) screening of pyroelectric field is overlooked at the modulation frequency 1 kHz. In some GaAs - III-V crystal solid solutions this frequency would be reduced to 20 Hz.

In GaAs and related crystals absorption and transparency may be even "resonant" in the range over 8-14 microns but an enlightenment layer is desirable in order to decrease IR reflection. The last depends on doping and its thickness can be controlled. IR radiation is absorbed in all bulk wafer while reflection gains resonant character and reflection coefficient passes trough minimum at given thickness of wafer-membrane. In the opposite case, if IR-absorbent covering is used, the only close-to-surface part of the wafer can work as transducer.

Sensor with the internal absorption could be applied for very fast IR pulses measurements. It is possible to chose such thickness of wafer at which integral reflection coefficient is very small or can be reduced. In a principle, thin-wafer detector would distinguish "IR colors".

Conclusions

Charge separation phenomena in dielectrics has always been associated with elasticity or thermally induced change of electrical polarization. It was well known that these properties have a relationship only to the crystals of 10 pyroelectric point symmetries. Nevertheless, it is originally shown that scalar thermal influence may induce pyroelectricity in all 20 piezoelectric classes of crystals if they are partially clamped.

Planar strain limitation in (111)-plates or membranes of III-V type of semi-insulating crystals opens up possibilities for new type of microelectronic sensor that would be uncooling one-crystal array. The last has advantages as over semiconductor photons arrays that need cooling so over pyroelectric ones produced by hybrid processing. Hundreds of elemental sensors on the same wafer would form matrix image processor which sensitivity increases as square root from cells number. Current status of microelectronics can guarantee identity of each cell in this one-crystal.

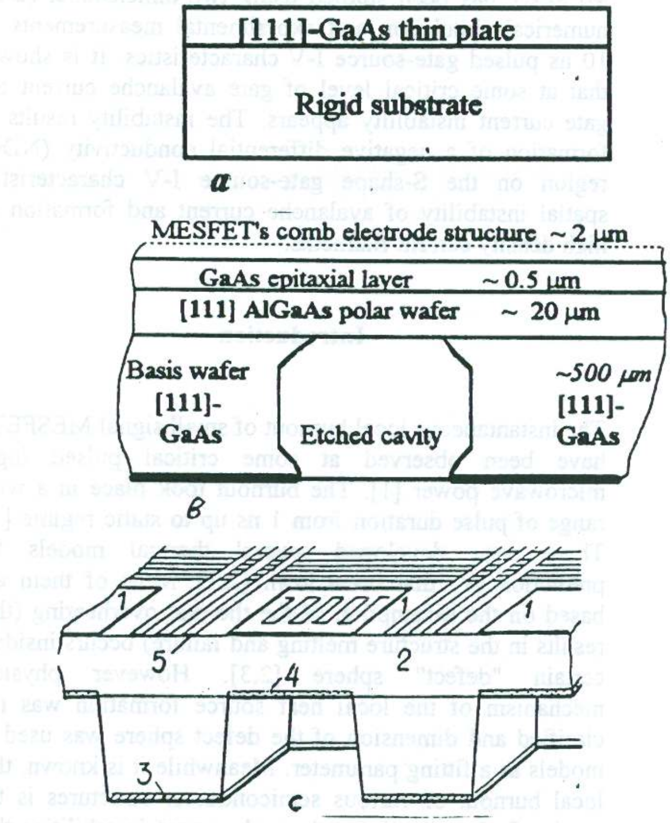

Fig.5. Awakened intrinsic polarity in GaAs type crystals and its possible application in piezo- or pyroelectric sensor devices: *a* - partial (planar) clamping by rigid substrate for strain limitation $\Delta P(T,p)$ investigations (shown on Fig.4); *b* - partial strain limitation in [111] AlGaAs membrane; *c* - possible design of smart sensor array based on GaAs: *1* - schematized MESFET, *2* - GaAs substrate, *3* - metalized ridges, *5* - read-out circuits.

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