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Novel Approach to Band-Discontinuity Determination at a Hetero-Junction Based on a Fully Computer Aided C-V Reconstruction Procedure

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We propose a novel and systematic method to determine the characteristic parameters of a hetero-junction precisely from the capacitance-voltage ($C-V$) measurement data. The band-discontinuity ΔE_c, the position of hetero-interface x_i, and the doping profile at the hetero-junction $\Gamma(x)$ are synthesized numerically based upon a fully computer aided $C_{\mathcal{W}} - V$ reconstruction procedure. In this procedure, it is shown that the capacitance should be calculated from the electrostatic energy and the conventional concept of the interface charge density is no longer needed. As a test device, the VPE grown GaInAs/InP avalanche photodiode is used.

1. Introduction

Recently, extensive studies have been worked on the determination of band-discontinuities at hetero-junctions, particularly, in GaInAs/InP and AlGaAs/GaAs material systems[1]. These values play significant roles in the simulation of the carrier injection in quantum-well lasers and the carrier transport in photodetectors.

In this paper we propose a novel and general method to determine the characteristic parameters of a hetero-junction such as the band-discontinuity ΔE_c precisely from the capacitance-voltage ($C-V$) measurement data. The parameter extraction procedure termed inverse $C_{\mathcal{W}} - V$ simulation is based on the iterative solution of the forward simulation by adjusting unknown parameters to minimize the difference between the measured $C-V$ characteristics and the simulated data. It will be emphasized that the conventional concept of the interface charge density is not necessary for the procedure if the measured capacitance is compared with the synthesized capacitance calculated from the electrostatic energy.

2. Definition of capacitance of a semiconductor diode

The small-signal capacitance of a reverse biased semiconductor diode arises from the electrostatic charge circulating within its external biasing circuits due to the change of the probing bias voltage. From the conservation of power in the diode, we obtain

$$\Psi\, i_c = \Psi \frac{dQ_{\mathcal{W}}}{dt} = \int_0^l \psi(x)\frac{\partial \rho(x)}{\partial t}dx, \tag{1}$$

where Ψ is the voltage difference between the two electrodes, i_c the AC current density flowing in the capacitance, $\psi(x)$ the voltage distribution, $\rho(x)$ the space charge density in the diode and $Q_{\mathcal{W}}$ is the charge which generates the current i_c. From the equation, we obtain

$$\Psi \delta Q_{\mathcal{W}} = \int_0^l \psi(x)\delta\rho(x)dx. \tag{2}$$

The left-hand side of this equation is exactly equal to the change in the electrostatic energy $\delta\mathcal{W}$ with the increase of the space charge density of the amount of $\delta\rho$. The capacitance $C_{\mathcal{W}}$ measured from the actual device[2] is then given by

$$C_{\mathcal{W}} = \frac{dQ_{\mathcal{W}}}{d\Psi} = \frac{1}{\Psi}\frac{d\mathcal{W}}{d\Psi}, \tag{3}$$

where $\mathcal{W}$ is the electrostatic energy defined by

$$\mathcal{W} = \frac{1}{2}\int_0^l \epsilon(x)E(x)^2dx. \tag{4}$$

On the other hand, conventionally the capacitance has often been defined from the change in the space charge density by the applied bias voltage as

$$C_{sc} = \frac{dQ_{sc}}{d\Psi}, \tag{5}$$

where $dQ_{sc} = q\int_0^l \delta n(x)dx$ and $\delta n(x)$ is the amount of depleted electron concentration due to the incremental change in the bias voltage $\delta\Psi$.

We will demonstrate the discrepancy between the energy capacitance $C_{\mathcal{W}}$ and the space charge capacitance C_{sc}, for simplicity, for a one-sided p^+n homo-junction diode with the doping concentration of N_D in the n-side. The exudation of the electrons at the depletion edge is assumed to be approximated by the exponential Debye length decay. The Debye length L_D is given by

$$L_D = \sqrt{\frac{\epsilon k_B T}{q^2 N_D}}, \tag{6}$$

and the depletion width w is given by

$$w = \sqrt{\frac{\epsilon(V_{bi} - V)}{qN_D}}. \tag{7}$$

For such a simple model, $C_{\mathcal{W}}$ and C_{sc} are represented as

$$C_{\mathcal{W}} = \frac{\epsilon}{w + L_D} \frac{1}{1 + (\frac{L_D}{w+L_D})^2}, \tag{8}$$

and

$$C_{sc} = \frac{\epsilon}{w + L_D}. \tag{9}$$

Explicitly, the energy capacitance $C_{\mathcal{W}}$ is found smaller than the space charge capacitance C_{sc} by the factor of $\left(1 + (\frac{L_D}{w+L_D})^2\right)^{-1}$. Accordingly, the change of capacitive charge $dQ_{\mathcal{W}}$ caused by the change of the depletion width dw

$$dQ_{\mathcal{W}} = qN_D dw - qN_D \frac{L_D^2}{(w + L_D)^2 + L_D^2} dw, \tag{10}$$

is smaller than $dQ_{sc} = qN_D dw$. The second term in eq. (10) arises from the incoming charge from the external measurement circuits.

On the other hand, the *apparent* carrier concentrations $\hat{n} = \frac{q\epsilon}{2} \frac{d}{d\Psi}(C^{-2})$ are represented for each definition of capacitance as

$$\hat{n}_{sc}(w) = N_D, \tag{11}$$

$$\hat{n}_{\mathcal{W}}(w) = \frac{N_D}{1 - (\frac{L_D}{w+L_D})^4}. \tag{12}$$

It is found from eq. (12) that the moment conservation theorem[1] : $\int_0^\infty n(x)dx = \int_0^\infty \hat{n}_{\mathcal{W}}(x)dx$ etc. can no longer hold because the measured *apparent* carrier density $\hat{n}_{\mathcal{W}}$ contains the extra charge correction due to the incoming charge from the external circuits. In spite of this fact, Kroemer et. al introduced the concept of the interface charge density σ_i at a hetero-junction assuming the moment conservation. Consequently, the conventional determination procedure of hetero-junction parameters[1] may lead erroneous data. In the next section, we will propose our precise determination procedure and then show its application.

3. Inverse $C_{\mathcal{W}} - V$ simulation and its application

A VPE grown GaInAs/InP avalanche photodiode shown in Fig.1 is used as a test sample. In this sample, the two depletion layers appear separately at the P-N and the hetero-interfaces until the N-InP layer between them is completely depleted by a large reverse bias voltage.

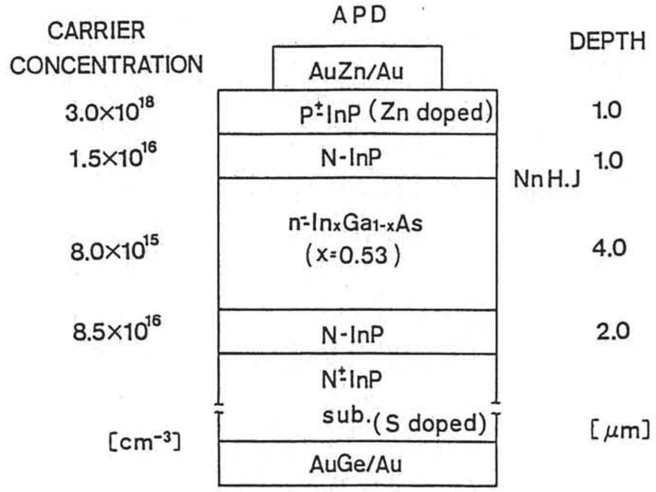

Fig. 1. Schematic structure of $Ga_{0.47}In_{0.53}As/InP$ APD under measurement.

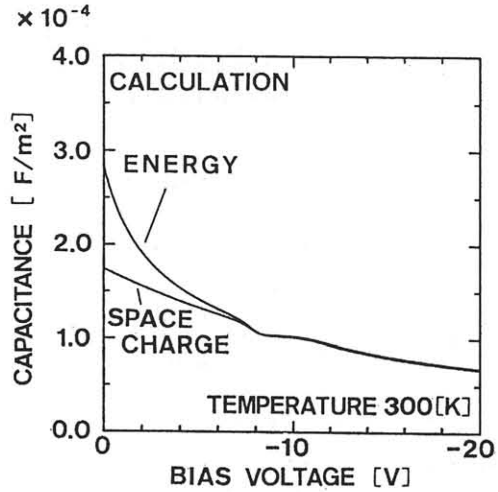

Fig. 2. Comparison between the C-V characteristics calculated by the refined procedure (ENERGY) and those by the conventional method (SPACE CHARGE).

The C-V characteristics for the device shown in Fig.1 are simulated based on the two definitions of capacitance and compared in Fig.2. A large discrepancy can be found at the reverse bias less than 8 V at which the punch-through appears to take place in the N-InP between the P-N and the hetero-interfaces. As discussed in the previous section, this discrepancy is caused by the extra charge from the external circuits.

Obviously, we can no longer apply the conventionall procedure for this case. Our novel procedure (inverse $C_{\mathcal{W}} - V$ simulation) is based on the iterative solution of our hetero-device simulator (forward simulation) to minimize the sum of the squared differences between measured and simulated data values[3]. Since the capacitance defined by the electrostatic energy $\mathcal{W}$ is used in the $C_{\mathcal{W}} - V$ reconstruction, we need not introduce the ambiguous parameters such as the interface charge density. As an iteration method for the parameter extraction, the Powell's non-linear optimization process[4] is adopted to ensure the nonsingularity of the solution. The whole parameter extraction procedure is illustrated in Fig.3. The final reconstructed data of this $Ga_{0.47}In_{0.53}P$/InP system are ΔE_c=0.17 eV, x_i=0.70 μm, and the doping profile $\Gamma(x)$ is shown in Fig.4. The residual capacitance errors for such a reconstruction are shown in Fig.5 as a function of reverse bias voltage.

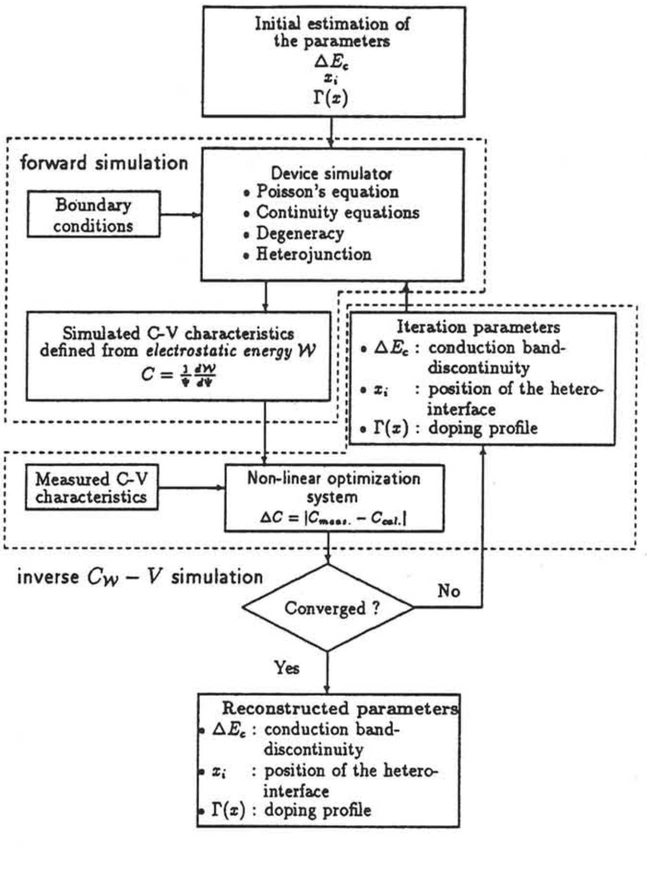

Fig. 3. Flow chart of the reconstruction procedure.

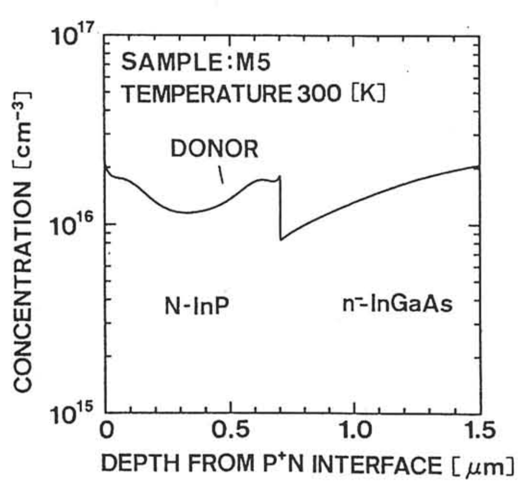

Fig. 4. Reconstructed doping profile $\Gamma(x)$ and the position of the hetero- interface x_i = 0.70 μm.

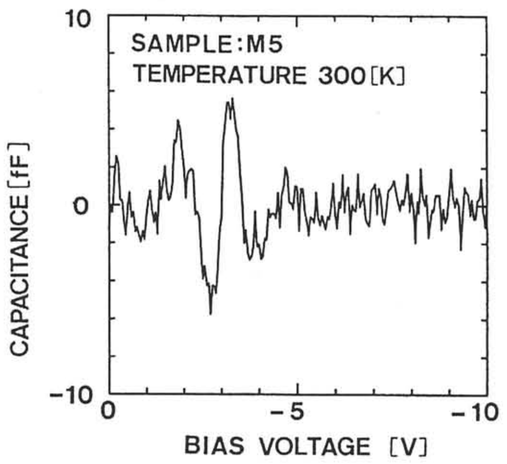

Fig. 5. Final residual errors in the present reconstruction procedure at each bias voltage.

4. Summary

In this paper we have proposed the inverse $C_{\mathcal{W}} - V$ simulation as a general and nondestructive determination procedure of physical parameters of hetero-junctions. It is stressed that since the measured capacitance corresponds to the energy capacitance $C_{\mathcal{W}}$, the energy capacitance must be used for the determination of parameters in the $C - V$ reconstruction procedure. It is also shown that in our procedure proposed the parameters can be reconstructed without introducing any ambiguous parameters such as the interface charge density.

In the application to the VPE grown $Ga_{0.47}In_{0.53}As$ /InP hetero-junction, the conduction band-discontinuity is found to be ΔE_c = 0.17 eV. The maximum error is found to be 5.8 fF which is comparable to the noise level of our measurement system.

We believe that the method proposed here is superior to the conventional C-V determination method and the PL measurement because in our procedure the self-consistent capacitance calculation and the nonlinear parameter optimization are included, and in addition, it is available to actual devices at room temperature.

References

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