PHYSICAL REVIEW B VOLUME 60, NUMBER 23 15 DECEMBER 1999-I

Effect of hydrostatic pressure on the characteristic parameters of Au/*n*-GaAs Schottky-barrier diodes

G. Çankaya, N. Uçar, E. Ayyildiz, H. Efeoğlu, A. Türüt,* S. Tüzemen, and Y. K. Yoğurtçu
Physics Department, Faculty of Arts and Sciences, Atatürk University, Erzurum, Turkey

(Received 16 November 1998; revised manuscript received 10 May 1999)

Au/*n*-GaAs Schottky barrier diodes SBDs have been fabricated. Schottky diode parameters such as the ideality factor, the series resistance, and the Schottky barrier height (SBH), Φ_b, have been measured as a function of hydrostatic pressure using the current-voltage (I-V) technique. We have seen that the SBH has a linear pressure coefficient of 11.21 meV/kbar (=112.1 meV/GPa). Also, the series resistance value increases with increasing pressure. We have concluded that the variation of the barrier height due to the applied pressure should follow precisely the variation of the semiconductor band gap, accepting that the Fermi level is a reference level which is pinned to the valance-band maximum as a function of the pressure. That is, we have concluded that the experimental results is in agreement with the model that the pressure coefficient is caused by the pressure coefficient of the direct midgap level. [S0163-1829(99)07643-2]

INTRODUCTION

The recent developments in the field of Schottky contacts have opened up interesting new possibilities for the study and application of these materials. In particular, Schottky barriers (SB's) appear to hold considerable promise for photovoltaic solar energy conversion and other device applications.[1–3] For many years, pressure has been employed as a tool in the investigation of the properties of semiconductor materials.[4] In recent years, various studies have been made on the hydrostatic press effects in Schottky diodes (SD's), and the effects were explained by the introduction of stress-sensitive generation-recombination centers, the change of band structure, and the change of minority-carrier lifetime.[5–9]

In some studies,[10,11] it has been found that the Schottky barrier height (SBH) is almost independent of the surface orientation of the substrate, preparation of surface, and the type of metal being used. So, the SBH has been measured for ideal metal/GaAs contacts by means of current-voltage (I-V) and capacitance-voltage (C-V) techniques and has been postulated models for Schottky barrier formation.[12] Recently, hydrostatic pressure has been used to explain the electronic structure of semiconductors by means of SB height measurements.[13] According to this matter, Peanasky and Drickamer[14] have showed that a pressure study of barrier height decouples the measurements of the conduction-band minimum E_c movement from the valence-band maximum E_v and creates a second frame of reference for interpreting the energy-band movement with pressure. The pressure dependence of the SB height at the Pt/GaAs interface has been determined by measuring the forward I-V characteristics of Schottky diodes using a diamond anvil cell (DAC) by Shan *et al.*[15] They have found that the SB height shifts to higher energy with a linear pressure coefficient of 11 meV/kbar and have shown that defect states are responsible for pinning the Fermi level in Schottky barriers under pressure. However, Mönch[16] and Chen *et al.*[17] have concluded that the Fermi level is pinned relative to the valance-band maximum (VBM) to explain both the temperature dependence[16,17] and externally applied pressure dependence[16] of the SBH in the Schottky contacts. Furthermore, Werner and Güttler[18] have found that the pressure coefficients of the barrier heights at type-*A* and type-*B* NiSi_2/n-Si(111) interfaces vary between values of about −2.2 and −1.1 meV/GPa.

Although an enormous amount of information on metal-semiconductor Schottky diodes has been gained, little is known about the effect of pressure on the diode parameters. The purpose of this study is to investigate the hydrostatic pressure dependence of Schottky diode parameters such as the ideality factor, barrier height, and series resistance by using the I-V characteristics.

EXPERIMENTAL METHOD

The Au/*n*-GaAs Schottky diodes used in this study were fabricated using *n*-type liquid-phase epitaxy (LPE) GaAs wafers (Te doped) with [100] orientation and 0.01-Ω cm resistivity. The wafer was rinsed by ultrasonic vibration in deionized water and was dried by high purity nitrogen. After this procedure, Ohmic contact was made evaporating Au-Ge (12% Ge) and annealing 425 °C for 3 min. The Schottky contacts were formed by evaporating Au as dots with a diameter of about 1 mm onto the mirror surfaces. All evaporation processes were carried out in a turbo molecular fitted vacuum coating unit at about 10^{-6} mbar.

The pressure was created by a piston and cylinder-type chamber apparatus as sketched in Fig. 1. A special transformer oil was used to transmit the pressure. Au/*n*-GaAs Schottky diodes were located in a pressure cell with a special designed sample holder and I-V measurements under 0–6 kbar hydrostatic pressure were made by electrical connections from cell to measuring device. The value of pressure in the pressure cell was measured with the resistance changes of the manganin wire. I-V characteristics of Schottky diodes under the pressure were performed around an HP4140B picoampermeter at room temperature. The high-pressure equipment used in this experiment has been described elsewhere.[13,14] The effect of hydrostatic pressure up to 6 kbar

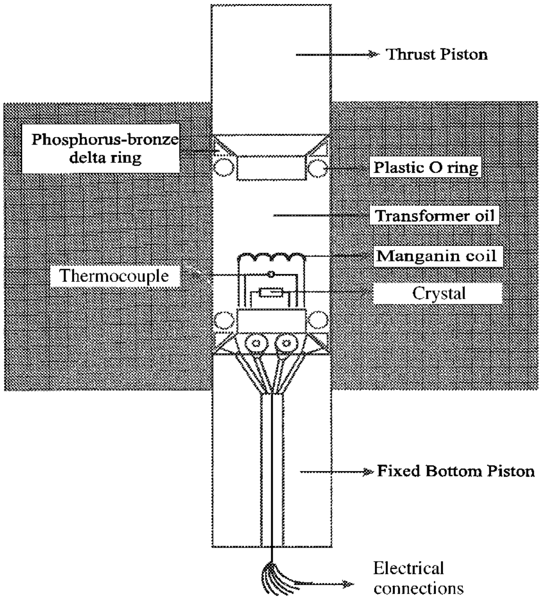

FIG. 1. Schematic drawing of a hydrostatic press cell.

at room temperature on I-V characteristics of Au/n-GaAs Schottky diodes is presented in Fig. 2. A strong dependence on pressure is evident. There are a hydrostatic pressure effect both in the forward and reverse directions. With an increase in pressure, I-V characteristics move to lower current values.

RESULTS AND DISCUSSION

The formation of a Schottky diode occurs at a metal-semiconductor interface when the work function of a metal is greater than the electron affinity of (n-type) semiconductor. It is well known that the barrier height is the potential difference between the Fermi level of metal and the conduction-band minimum at the interface. Various techniques are available for the determination of Φ_b, the most generally used is the I-V relation.[14,19,20]

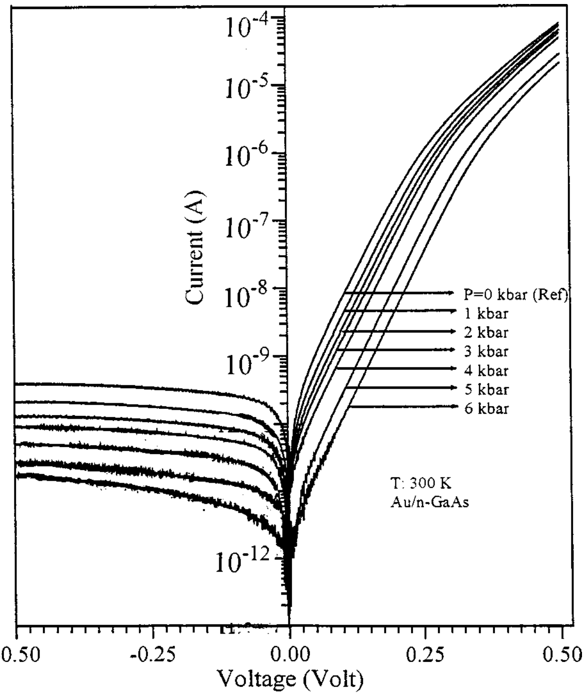

FIG. 2. The effect of hydrostatic pressure on I-V characteristics of Au/n-GaAs Schottky diodes.

TABLE I. Diode parameters obtained from I-V characteristics of the Au/n-GaAs Schottky diodes under pressure.

P (kbar)	n	Φ_b (eV)	R_s	I_0 (A)
0 (Ref.)	1.061	0.80	16.69	1.83E-11
1	1.058	0.82	17.98	9.96E-11
2	1.052	0.83	19.38	6.37E-11
3	1.055	0.84	20.56	4.50E-11
4	1.057	0.85	21.49	2.68E-11
5	1.018	0.89	23.58	6.08E-12
6	1.037	0.91	24.79	2.92E-12

The forward bias I-V characteristics due to thermionic emission of a Schottky diode with the serie resistance can be expressed as[21–23]

$$I = I_0 \exp\left(\frac{q(V-IR_S)}{nkT}\right)\left[1-\exp\left(-\frac{q(V-IR_S)}{kT}\right)\right]. \quad (1)$$

In the above, the saturation current I_0 is expressed as

$$I_0 = AA^*T^2 \exp\left(-\frac{q\Phi_b}{kT}\right), \quad (2)$$

where q is the electron charge, V is the applied voltage, A is the effective diode area, k is the Boltzman constant, T is the absolute temperature, A^* is the effective Richardson constant of 8.16 $\mathrm{A\,cm^{-2}\,K^{-2}}$ for GaAs, R_S is the series resistance and its values were calculated from the forward-bias I-V data using the method of Cheung and Cheung.[24] Φ_b is the barrier height and n is an ideality factor which can be determined accurately from the slope of the linear portion of the $\ln I/[1-\exp(-qV/kT)]$ vs V plot, and from Eq. (1). In fact, the ideality factor n can be written as

$$n = \frac{q}{kT}\left[\frac{dV}{d(\ln I)}\right]. \quad (3)$$

The values of the barrier height of Au/n-GaAs Schottky diodes were calculated with the help of Eq. (2) from the y axis intercepts of the semilogarithmic forward-bias I-V plots, and the values of n were obtained using Eq. (3) from the linear region of these plots indicating that the series resistance effect in linear region is not important (Fig. 2). These values calculated in this study are given in Table I. As can be seen in Table I, the values of Φ_b and n range from 0.80 eV and 1.061 (at $P=0$ kbar) to 0.91 eV and 1.037 (at $P=6$ kbar), respectively. Thus, the Φ_b value has increased by 0.110 to 0.91 eV at 6 kbar in the Au/n-GaAs SBD's while the ideality factor remains about unchanged up to 4 kbar. However, the ideality factor value decreases after 4 kbar, down to 1.018 at $P=5$ kbar and 1.037 at $P=6$ kbar. But series resistance increases with increasing hydrostatic pressure continuously. We can confidently assume the sample to have an almost ideal I-V characteristic due to an ideality factor value of 1.061 at $P=0$ kbar. The values of R_S range from 16.69 Ω (at $P=0$ kbar) to 24.47 Ω (at $P=6$ kbar). Fontain, Oku-

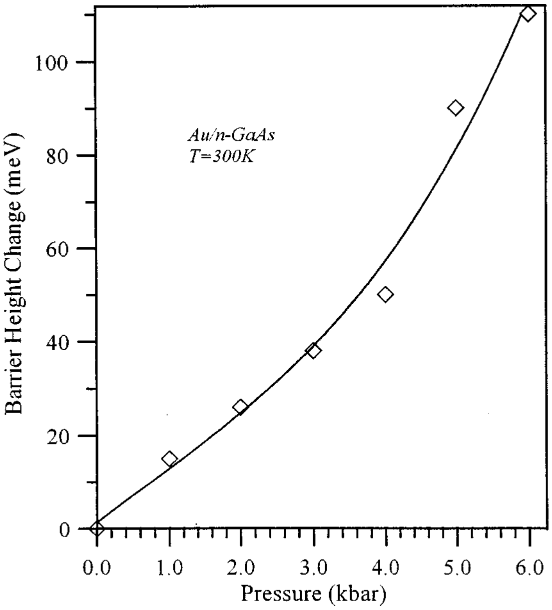

FIG. 3. Change of the SB height with hydrostatic pressure of Au/n-GaAs Schottky diodes.

mura, and Tu[25] also suggested that any damage in the interface affects the I-V behavior because defects act as recombination centers or as intermdeiate states for trap-assisted tunneling currents.

The effect of pressure up to 6 kbar at room temperature on the barrier height Φ_b of the Au/n-GaAs Schottky diodes from the intercept currents I_0, which are the saturation currents, is presented in Fig. 3. The variation in the SB height with pressure was fitted with the equation

$$e\Phi_b(P)=e\Phi_b(0)+\alpha P+\beta P^2+\gamma P^3 \tag{4}$$

with $\alpha=11.21$ meV/kbar ($=112.1$ meV/GPa), $\beta=-0.345$ meV/kbar^2 and $\gamma=0.25$ meV/kbar^3. As have been indicated by Mönch,[16] the pressure dependence of the barrier heights in the ideal Schottky contacts are determined by the pressure coefficient of the zero-charge-transfer barrier heights. In the ideal Schottky diodes, the metal-induced gap states (MIGS) may be considered to be the physical mechanism which determines the barrier heights.[16] According to the MIGS model of ideal semiconductor contacts, the charge transferred between the metal and the semiconductor varies as a function of the position of the Fermi level relative to the intrinsic charge-neutrality level (CNL) of the MIGS within the semiconductor band gap or as a function of the barrier height. No charge will be transferred across the interface when the Fermi level coincides with the intrinsic CNL of the MIGS. In this case, the barrier height measured is called the zero-charge-transfer barrier heights. Furthermore, it has been reported according to the experimental findings that the zero-charge-transfer barrier height of Schottky contacts on p-type semiconductor substrates do not change as a function of pressure.[16] Therefore, the pressure dependence of the zero-charge-transfer barrier height of Schottky contacts on n-type semiconductor substrates is determined by the respective variations of the width E_g of the bulk band gap.[15,16,26] Thus, we may say that the pressure coefficient of the band gap of the Au/n-GaAs contact has a value of 11.21 meV/kbar. Welber *et al.*[26] also showed that the pressure coefficient of the barrier height of the GaAs contacts is the same as that of the fundamental gap of GaAs. In this study, the linear pressure coefficient of 11.21 meV/kbar obtained for Au/n-GaAs Schottky diodes is in close agreement with the value of 11 meV/kbar for Pt/n-GaAs diodes reported by Shan *et al.*[15] who reported that the amphoteric native defects is responsible for Fermi-level pinning at metal GaAs interfaces. However, according to the MIGS model of ideal semiconductor contacts, the analysis of the pressure or temperature variations of the barrier heights at metal-semiconductor interface indicates the existence of a reference level which is pinned to the valance-band maximum (VBM) as a function of the pressure or temperature.[16] In case of the zero-charge-transfer barrier height, the intrinsic CNL of the MIGS or Fermi level thus is the reference level which is pinned to the VBM as a function of the pressure or temperature.[16,17] Thus, if the Fermi level is pinned relative to the VBM at the Au/n-GaAs interface as concluded also by Mönch[16] and Chen *et al.*,[17] the variation of the barrier height should follow precisely the variation of the semiconductor band gap. Briefly, according to the model of Mönch,[16] the CNL of the MIGS is identical with the direct midgap level. Thus, the direct midgap level is the reference level which is pinned to the VBM as a function of the pressure.

In addition, it is well known that the pressure coefficients are large and positive for direct transitions in the middle of the first Brillouin zone (about $+100$ meV/GPa) but negative and by a factor of approximately 10 smaller for indirect transitions from the VBM to conduction-band minima near to the X point at the Brillouin-zone boundary of the bulk band structure (-10 meV/GPa).[16] Therefore, it can be said that the pressure coefficient of the minimum gap of positive 112.1 meV/GPa obtained for own our Au/n-GaAs Schottky contact is for direct transitions in the middle of the Brillouin zone. Thus, as a function of externally applied pressure, the barrier heights of Schottky contacts increase on n-type GaAs substrates.

In conclusion, the obtained results in the present study for Au/n-GaAs Schottky diodes are in good agreement with previously published results. The behavior of ideal semiconductor contacts due to externally applied pressure may be explained by the MIGS model. We have concluded that the variation of the zero-charge-transfer barrier height due to applied pressure should follow precisely the variation of the semiconductor band gap because the intrinsic CNL of the MIGS or Fermi level has been accepted as a reference level which is pinned to the VBM as a function of the pressure.

---

[*] Author to whom correspondence should be addresed. Fax.: +442 233 1062. Electronic address: amecit@rocketmail.com, or amecit@atauni.edu.tr

[1] G. Y. Robinson, in *Physics and Chemistry of III–V Compound Semiconductor Interfaces*, edited by C. W. Wilmsen (Plenum, New York, 1985).

[2] S. P. Kowalczky, J. R. Waldrop, and R. W. Grant, Appl. Phys. Lett. **38**, 167 (1981).

[3] R. Zucca and E. J. Wood, J. Appl. Phys. **46**, 3 (1975).

[4] A. Jayaraman, in *Physics of the Solid State*, edited by S. Alakrisa, M. Krishamurthi, and B. Ramachandra Rao (Academic, New York, 1969).

[5] J. Oda and Y. Matsukura, Jpn. J. Appl. Phys. **6**, 411 (1967).

[6] L. Beji, B. El Jani, P. Gibart, J. C. Portal, and P. Basmaji, J. Appl. Phys. **83**, 10 (1998).

[7] N. Balasubramanyam and V. Kumar, Phys. Status Solidi A **101**, K29 (1987).

[8] T.-H. Shen and C. C. Matthai, J. Phys.: Condens. Matter **3**, 613 (1991).

[9] M. Yamaguchi, A. Yamamoto, and A. Shibukawa, Jpn. J. Appl. Phys. **22**, 1727 (1983).

[10] J. Van Laar and A. Huijser, J. Vac. Sci. Technol. **13**, 769 (1976).

[11] W. E. Spicer, I. Lindau, P. E. Gregory, C. M. Garner, P. Pianette, and P. W. Chye, J. Vac. Sci. Technol. **13**, 780 (1976).

[12] J. R. Waldrop, Appl. Phys. Lett. **44**, 1002 (1984).

[13] D. A. Gulino, L. R. Faulkner, and H. G. Drickamer, J. Appl. Phys. **54**, 2483 (1983).

[14] M. J. Peanasky and H. G. Drickamer, J. Appl. Phys. **56**, 3471 (1984).

[15] W. Shan, M. F. Li, Y. Yu, W. L. Hansen, and W. Walukiewicz, Appl. Phys. Lett. **53**, 974 (1988).

[16] W. Mönch, *Semiconductor Surfaces and Interfaces*, 2nd ed. (Springer, Berlin, 1995), pp. 75–84, 364, 382–387.

[17] T. P. Chen, T. C. Lee, S. Fung, and C. D. Beling, Phys. Status Solidi A **141**, K29 (1994).

[18] J. H. Werner and H. H. Gütter, J. Appl. Phys. **73**, 1315 (1993).

[19] M. O. Aboelfotoh, Solid-State Electron. **34**, 51 (1991).

[20] A. Türüt, B. Bati, A. Kökçe, M. Sağlam, and N. Yalçin, Phys. Scr. **53**, 118 (1996).

[21] S. M. Sze, *Physics of Semiconductor Devices*, 2nd ed. (Wiley, New York, 1981), p. 245.

[22] E. H. Rhoderick, *Metal-Semiconductor Contacts* (Oxford University, Oxford, 1978), p. 121.

[23] A. Ziel, *Solid State Physical Electronics*, 2nd ed. (Prentice-Hall, Englewood Cliffs, NJ, 1968).

[24] S. K. Cheung and N. W. Cheung, Appl. Phys. Lett. **49**, 85 (1986).

[25] C. Fontaine, T. Okumura, and K. N. Tu, J. Appl. Phys. **54**, 1404 (1983).

[26] B. Welber, M. Cardona, C. K. Kim, and S. Rodriguez, Phys. Rev. B **12**, 5729 (1975).