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The Gaussian distribution of barrier height in Au/n-GaAs Schottky diodes at high temperatures

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The current-voltage (I-V) characteristics of Au/n-GaAs (MS) Schottky diodes were determined in the temperature range of 300-400 K**.** The estimated zero-bias barrier height (Φ_{Bo}) and the ideality factor (n) assuming thermionic emission (TE) theory show strong temperature dependence. The barrier height for current transport decreases and the ideality factor increases with the decrease temperatures. This behavior of Φ_{Bo} and n is attributed to Schottky barrier inhomogeneities by assuming a Gaussian distribution (GD) of the barrier heights (BHs) at the metal/semiconductor interface. The Richardson plot is found to be linear in the temperature range measured, but activation energy value of 0.322 eV and Richardson constant (A^*) value of $4.12\text{x}10^{-4}$ $\text{Acm}^{-2}\text{K}^{-2}$obtained this plot are much lower than the known values. The nonlinearity in the Richardson plot and strong dependence of Schottky barrier parameters on temperature may be attributed to the spatial inhomogeneity in the interface. We attempted to draw a Φ_{Bo} versus q/2kT plot in order to obtain evidence of the GD of BHs, and the values of $\overline{\Phi}_{Bo}$ = 0.912 eV and σ_o = 0.132 V for the mean barrier height and standard deviation at a zero bias, respectively, were obtained from this plot. A modified $\ln(I_o/T^2)-q^2\sigma_o^2/2k^2T^2$ versus q/kT plot gives $\overline{\Phi}_{Bo}$ and A^* as 0.914 eV and 8.32 $\text{Acm}^{-2}\text{K}^{-2}$, respectively. This value of the Richardson constant 8.32 $\text{Acm}^{-2}\text{K}^{-2}$ is very close to the theoretical value of 8.16 $\text{Acm}^{-2}\text{K}^{-2}$ for n-type GaAs.

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1. Introduction

Schottky diodes are the basis of a number of semiconductor electronic devices, including high-electron mobility transistors (HEMTs), field-effect transistors (FETs), microwave diodes, solar cells, and photodetectors [1-4]. Due to this technological importance of the Schottky diodes, a full understanding of the nature of their electrical characteristics is of great interest.

The performance and reliability of these devices, such as metal-semiconductor (MS) Schottky diodes, particularly depend on the formation of an insulator layer and the inhomogeneities of the Schottky barrier formation at metal/semiconductor interfaces, the density of interface states distribution at insulator / semiconductor interfaces, the ideality factor, and the series resistance of the device [5-12].

The electrical characteristics of these devices do not obey the ideal Schottky theory. Usually, the thermionic emission (TE) mechanism is used to extract the main diode parameters. The current-voltage (I-V) characteristics of the real Schottky barrier diode (SBD) usually deviate from the ideal TE model. The strong dependence of both the barrier height (BH) (Φ_B) and the ideality factor (n) on temperature and the nonlinearity of the Richardson plots are the factors associated with the deviation of the TE model [13-15].

On the other hand, it is found that BH is inhomogeneous in the metal/semiconductor interface. This is also one of the mechanisms for deviating the I-V characteristics from the ideal TE model. The mechanisms responsible for producing an inhomogeneity are not yet fully understood. The BH is likely to be a function of the interface atomic structure and the inhomogeneity at a MS interface may be caused by grain boundaries, multiple phases, facets, defects, and a mixture of different phases [16-21]. The deviation in TE model observed in I-V characteristics could be quantitatively explained by assuming specific distribution of nanometer scale patches of small regions with low BH. In such cases, the current across the MS contact may be greatly influenced by the presence of interfacial patches [17-23].

In addition, analysis of the I-V characteristics of Schottky barrier heights (SBHs) based on TE theory usually reveals an abnormal decrease in the BH and an increase in the ideality factor n with a decrease in temperature which lead to non-linearity in the activation energy ln (I_o/T^2) vs 1/T plot [18-20]. Lately, the nature and origin of the decrease in the BH and increase in ideality factor with a decrease in temperature in some studies have been successfully explained on the basis of a TE mechanism with a Gaussian distribution (GD) of the barrier heights (BHs) [14,15,20,23].

In the present study, the forward bias I-V characteristics of the Au/n-GaAs (MS) Schottky diodes were measured in the wide temperature range of 300-400 K. The temperature dependent barrier characteristics of the Au/n-GaAs (MS) Schottky diodes were interpreted on the basis of the existence of a GD of the BHs around a mean value due to BH inhomogeneities prevailing between the metal and the semiconductor interface.

2. Experimental detail

The Schottky diodes have been prepared using cleaned and polished n-GaAs (as received from the manufactured) with <100> orientation and 5×10^{17} cm^{-3} carrier concentrations. Before making contacts, the n-GaAs wafer were dipped in $5H_2SO_4 + H_2O_2 + H_2O$ solution for 1.0 min to remove surface damage layer and undesirable impurities and then in H_2O + HCl solution and then followed by a rinse in de-ionized water of 18 MΩ. The wafer dried with high-purity nitrogen and inserted into the deposition chamber immediately after the etching process. Au-Ge (88% and 12%) for ohmic contacts was evaporated on the back of the wafer in a vacuum-coating unit of 10^{-6} Torr. Then low-resistance ohmic contacts were formed by thermal annealing at 450 ^oC for 3 min in flowing N_2 in a quartz tube furnace. Then, the wafer was inserted into the evaporation chamber for forming the reference Schottky contacts. The Schottky contact was formed by evaporating Au as dots with diameter of about 1 mm onto all of n-GaAs surfaces. The interfacial insulator layer thickness was estimated to be about 27 Å from high frequency (1 MHz) measurement of the interface oxide capacitance in the strong accumulation region for Au/n-GaAs (MS) Schottky diode.

The current-voltage (I-V) measurements were performed by the use of a Keithley 220 programmable constant current source, a Keithley 614 electrometer in the temperature range of 300-400 K using a temperature-controlled Janes vpf-475 cryostat, which enables us to make measurements in the temperature range of 77-450 K. The sample temperature was always monitored by using a copper-constant an thermocouple close to the sample and measured with a dmm/scanner Keithley model 199 and a Lake Shore model 321 auto-tuning temperature controllers with sensitivity better than ± 0.1 K. All measurements were carried out with the help of a microcomputer through an IEEE-488 ac/dc converter card.

3. Results and discussion

The current-voltage relationship for a MIS Schottky diode, based on the TE theory can be expressed as [1,2]

$$I = I_o \exp\left(\frac{qV}{nkT}\right)\left[1-\exp\left(-\frac{qV}{kT}\right)\right] \tag{1}$$

where I is the measured current, V is the applied voltage, q is the electronic charge, n is the ideality factor that describes departure from the ideal diode equation for reverse bias as well as forward bias, k is the Boltzmann's constant, T is the absolute temperature in Kelvin, I_o is the reverse saturation current derived from the straight-line intercept of lnI at zero bias and is given by

$$I_o = AA^*T^2\exp\left(-\frac{q\Phi_{Bo}}{kT}\right) \tag{2}$$

where A is the rectifier contact area, A^* is the effective Richardson constant and is equal to 8.16 $Acm^{-2}K^{-2}$ for n-type GaAs, and Φ_{Bo} is the apparent barrier height at zero-bias, which can be obtained from Eq. (2)

$$q\Phi_{Bo} = kT\ln(AA^*T^2/I_o) \tag{3}$$

The ideality factor and is a measure of the conformity of the diode to pure thermionic emission. The ideality factor is calculated from the slop of the linear region of the forward bias ln(I)-V plot and can be written from Eq. (1) as

$$n = \frac{q}{kT}\left[\frac{dV}{d(\ln I)}\right] \tag{4}$$

Typical forward current-voltage characteristics of Au/n-GaAs (MS) Schottky diode in the temperature range of 300-400 K are shown in Fig. 1. The saturation current I_o was obtained by extrapolating the linear intermediate voltage region of the part of the linear curve to a zero applied bias voltage for each temperature.

The experimental values of the ideality factor (n) and zero-bias barrier height (Φ_{Bo}) were determined from Eq. (3) and Eq. (4), respectively, and are reported in Table 1. As shown in Table 1, the values of the ideality factor decrease with increase in temperature and are greater than unity at each temperature. Larger ideality factors are attributed to secondary mechanisms at the interface [1,10,16,18,21-24] such as lateral inhomogeneous distribution of barrier heights may be created by interface defects. In addition, the values of the barrier height increase with the increase of temperature. That is to say the values of Φ_{Bo} and n assuming thermionic emission (TE) theory show strong temperature dependence. Such temperature dependence is an obvious disagreement with the reported negative temperature coefficient of the barrier height or forbidden band gap of a semiconductor.

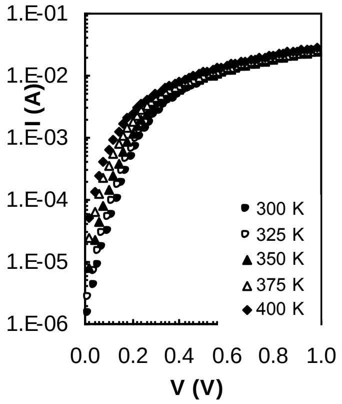

Fig. 1. The experimental forward bias I-V characteristics of Au/n - GaAs Schottky diode as a function of temperature.

Table 1. Temperature dependent values of various diode parameters determined from I-V characteristics of Au/n-GaAs Schottky diode in the temperature range of 300-400 K.

Temperature (K)	I_o (A)	n	Φ_{Bo} (eV)
300	1.437×10^{-6}	1.301	0.572
325	2.753×10^{-6}	1.254	0.606
350	8.457×10^{-6}	1.213	0.623
375	2.429×10^{-5}	1.154	0.638
400	4.928×10^{-5}	1.116	0.661

Fig. 2 shows a plot of the experimental BH versus the ideality factor for various temperatures. As can be seen from Fig. 2, there is a linear relationship between the experimental effective BHs and the ideality factors of the Schottky contact that was explained by lateral inhomogeneities of the BHs in the Schottky diodes [25-27]. The extrapolation of the experimental BHs versus ideality factors plot to n=1 has given a homogeneous BH of approximately 0.712 eV. Thus, it can be said that the significant decrease of the zero-bias BH and increase of the ideality factor are possibly caused by the BH inhomogeneities.

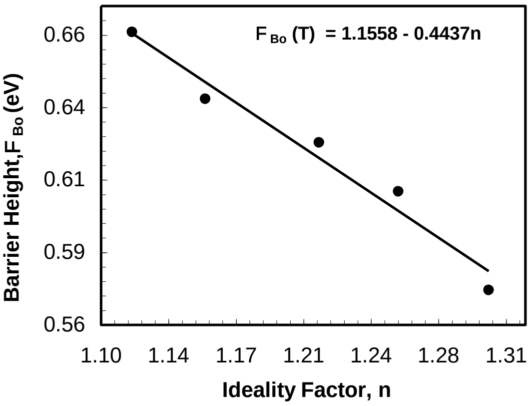

Fig. 2. Linear variation of apparent barrier height versus ideality factors at various temperatures.

For the evaluation of the barrier height, one may also make use of the Richardson plot of reverse saturation current (I_o). Eq.(2) can be written as

$$\ln\left(\frac{I_0}{T^2}\right) = \ln\left(AA^*\right) - \frac{q\Phi_{Bo}}{kT} \tag{5}$$

According to Eq. (5), the plot ln (I_o/T^2) yields a straight line with a slope given by barrier height at 0 K and the intercept is the Richardson constant. The conventional energy variation of ln (I_o/T^2) versus 1000/T plot is found to be linear in the temperature range measured as shown in Fig. 3. The value of A* obtained from the intercept of the straight line portion of the ordinate is equal to 4.12×10^{-4} Acm^{-2}K^{-2}, which is much lower than the known value of 8.16 Acm^{-2}K^{-2}. An activation energy value of 0.322 eV is obtained from the slope of the straight line. The deviation in the Richardson plot may be due to spatially inhomogeneous barrier height and potential fluctuation at the interface that consists of low and high barrier areas [13,17,19,21,28,29,] that is, the current through the diode will flow preferentially through the low barrier in the potential distribution. Furthermore, the value of the Richardson constant obtained from the I-V characteristics as a function of temperature may be affected by the lateral inhomogeneity of the barrier.

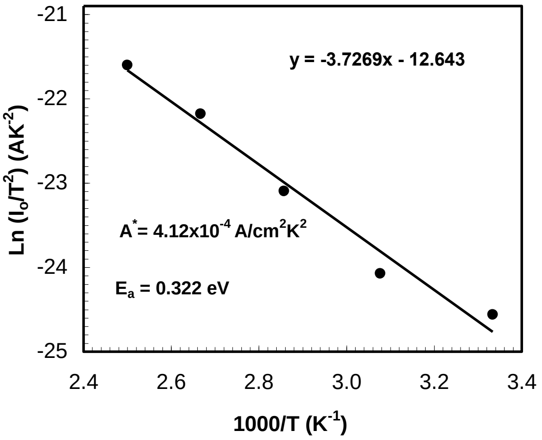

Fig. 3. Richardson plots of the ln(I_0/T^2) versus 1000/T for Au/n-GaAs Schottky diode.

To explain the commonly observed abnormal deviation from classical TE theory, some authors [10,23,27] have considered a system of discrete region of low barrier imbedded in a higher background uniform barrier. This abnormal behaviors can be explained by assuming a Gaussian distribution of the barrier height with a mean value $\overline{\Phi}_{Bo}$ and standard deviation σ_s, which can be given as [10,14,15,23,30-36]

$$P(\Phi_B) = \frac{1}{\sigma_s\sqrt{2\pi}}\exp\left[-\frac{(\Phi_B - \overline{\Phi}_B)^2}{2\sigma_s^2}\right] \tag{6}$$

where $1/\sigma_S\sqrt{2\pi}$ is the normalization constant of the Gaussian barrier height distribution. The total I(V) across a Schottky diode containing barrier inhomogeneities can be expressed as

$$I(V) = \int_{-\infty}^{+\infty} I(\Phi_B, V)P(\Phi_B)d\Phi \tag{7}$$

where I(Φ_B,V) is the current at a bias V for a barrier of height based on the ideal TED theory and P(Φ_B) is the normalized distribution function giving the probability of accuracy for barrier height.

Now, introducing I(Φ_B,V) and P(Φ_B) into Eq. (7) from Eq. (1) and Eq. (6), and performing this integration from -∞ to +∞, one can obtain the current I(V) through a Schottky barrier at a forward bias V, similar to Eq. (1) and Eq. (2) but with the modified barrier

$$I(V)=A^*T^2\exp\left[-\frac{q}{kT}\left(\bar{\Phi}-\frac{q\sigma_S^2}{2kT}\right)\right]\exp\left(\frac{qV}{n_{ap}kT}\right)\left[1-\exp\left(-\frac{qV}{kT}\right)\right] \tag{8}$$

with

$$I_o = AA^*T^2\exp\left(-\frac{q\Phi_{ap}}{kT}\right) \tag{9}$$

where Φ_{ap} and n_{ap} are the apparent barrier height and apparent ideality factor, respectively, and are given by [21,24,37]

$$\Phi_{ap} = \overline{\Phi}_{Bo}(T=0) - \frac{q\sigma_o^2}{2kT} \tag{10}$$

$$\left(\frac{1}{n_{ap}}-1\right) = \rho_2 - \frac{q\rho_3}{2kT} \tag{11}$$

It is assumed that the mean SBH $\overline{\Phi}_B$ and σ_S are linearly bias dependent on Gaussian parameters, such as $\overline{\Phi}_B = \overline{\Phi}_{Bo} + \rho_2 V$ and standard deviation $\sigma_S = \sigma_{SO} + \rho_3 V$, where ρ_2 and ρ_3 are voltage coefficients which may depend on temperature, quantifying the voltage deformation of the BH distribution [8,11,13,21,22,32].

The temperature dependence of σ_S is usually small and can be neglected [32]. It is obvious that the decrease of zero-bias barrier height is caused by the existence of the Gaussian distribution and the extent of influence is determined by the standard deviation itself. Also, the effect is particularly significant at low temperatures. Fitting of the experimental data in Eq. (2) or Eq. (9) and in Eq. (4) gives Φ_{ap} and n_{ap} at zero-bias respectively which should obey Eq. (10) and Eq. (11). Thus, the plot of Φ_{ap} versus q/2kT (as seen in Fig. 4) should be a straight line that gives $\overline{\Phi}_B$(T=0) = 0.912 eV and σ_o = 0.132 V from the intercept and slope, respectively.

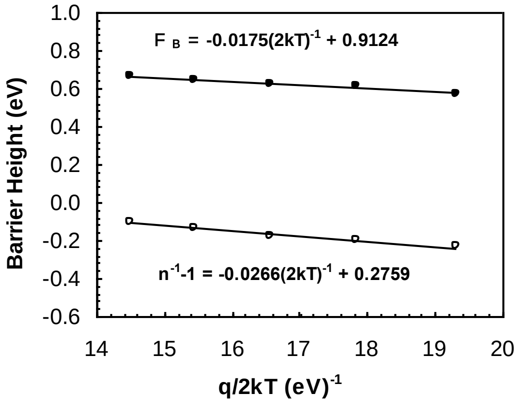

Fig. 4. Zero-bias apparent barrier height and ideality factor versus 1/T curves of Au/n-GaAs Schottky diode according to Gaussian distribution of barrier height.

The lower value of σ_O corresponds to more homogeneous BH. Clearly, the diode with the best rectifying performance presents the best barrier homogeneity with the lower value of standard deviation. It was seen that the value of σ_o = 0.132 V is not small compared to the mean value of $\overline{\Phi}_B$ = 0.912 eV, indicating the presence of the interface inhomogeneties. The temperature dependence of ideality factor can be understood on the basis of Eq. (11). Fitting showing ideality factor n in Fig. 4 is a straight line that gives voltage coefficient ρ_2 and ρ_3 from the intercept and slope of the plot where ρ_2 = 0.278 and ρ_3 = -0.027 V from the experimental data. The linear behavior of the plot shows that the ideality factor expresses the voltage deformation of the Gaussian distribution of the SBD.

In Fig. 3 the plot of $\ln(I_o/T^2)$ versus 1/T plot shows that the activation energy and Richardson constant which deviates from known value. To explain this behaviour, Eq.(7) can be rewritten by Eqs.(9) with Eq.(10) as follows,

$$\ln\left(\frac{I_0}{T^2}\right)-\left(\frac{q^2\sigma_o^2}{2k^2T^2}\right) = \ln(AA^*) - \frac{q\overline{\Phi}_{B0}}{kT} \tag{12}$$

The modified $\ln(I_o/T^2)$ - $q^2\sigma_O^2/2k^2T^2$ versus q/kT plot according to Eq. (12) should give a straight line with the slope directly yielding the mean $\overline{\Phi}_{Bo}$ and the intercept (= lnAA*) at the ordinate determining A* for a given diode area A (as seen in Fig. 5). In Fig. 5, the modified $\ln(I_0/T^2)$ - $q^2\sigma_O^2/2k^2T^2$ versus q/kT plot gives $\overline{\Phi}_{Bo}$ (T=0) and A* as 0.914 eV and 8.32 A cm^{-2} K^{-2}, respectively.

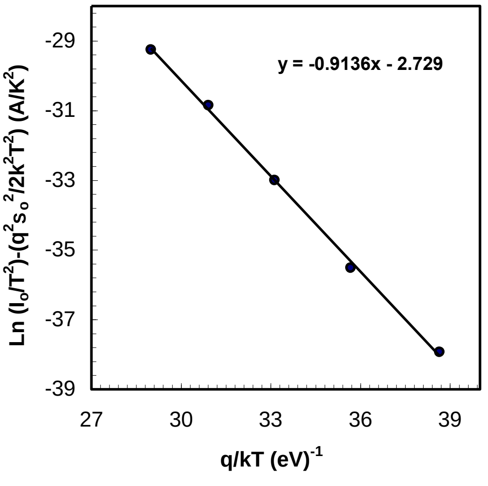

Fig. 5. Modified Richardson Ln (I_o/T^2)-$q^2\sigma^2$ /2kT^2 versus 1/T plot for Au/n-GaAs Schottky diode according to Gaussian distribution of barrier height.

4. Conclusions

The forward bias I-V characteristics of the Au/n-GaAs Schottky diodes were measured in the temperature range of 300-400 K. The experimental results reveal an increase of zero-bias barrier height (Φ_{Bo}) and a decrease of ideality factor (n) with increasing temperature. Such behavior is attributed to the Schotky barrier inhomogeneities by assuming a GD of BHs due to barrier inhomogeneities that prevails at interface. In order to obtain evidence of a GD of BHs, we have drawn a Φ_{Bo} versus q/kT plot, and the values of $\overline{\Phi}_{Bo}$ = 0.912 eV and σ_o = 0.132 V for the mean barrier height and standard deviation at a zero bias, respectively, have been obtained from this plot. Then, the values of Φ_{Bo} and A^* are obtained from a modified $\ln(I_o/T^2) - q^2\sigma_o^2/2k^2T^2$ versus q/kT plot as 0.914 eV and 8.32 $Acm^{-2}K^{-2}$, respectively. The value of the Richardson constant of 8.32 $Acm^{-2}K^{-2}$ is very close to the theoretical value of 8.16 $Acm^{-2}K^{-2}$ for electrons in n-type GaAs. Therefore, it has been concluded that the temperature dependence of the forward bias I-V characteristics of the Au/n-GaAs Schottky diode can be successfully explained on the basis of the TE mechanism with a GD of the BHs.

Acknowledgments

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References

[1] E. H. Rhoderick, R. H. Williams, Metal-Semiconductor Contacts, 2nd Ed., Clarendon Press, Oxford, 1978.
[2] S. M. Sze, K. Ng Kwok, Physics of Semiconductor Devices, 3rd Ed., Wiley, New Jersey, 2007.
[3] Z. Yu, S. J. Schablitsky, S. Y. Chou, Appl. Phys. Lett. **74**, 2381 (1999).
[4] R. L. Van Meirhaeghe, W. H. Lafl*é*re, F. Cardon, J. Appl. Phys. **76**, 403 (1994).
[5] P. Cova, A. Singh, Solid State Electron. **33**, 11 (1990).
[6] S. Ashok, J. M. Borrego, R. J. Gutmann, Solid State Electron. **22**, 621 (1979).
[7] P. Chattopadhyay, A. N. Daw, Solid State Electron. **29**, 555 (1986).
[8] K. Haraguchi, K. Hiruma, T. Katsuyama, T. Shimada, Current Appl. Phys. **6**, 10 (2006).
[9] H. C. Card, E. H. Rhoderick, J. Phys. D. **4**, 1589 (1971).
[10] S. Chand, J. Kumar, Appl. Phys. A **63**, 171 (1996).
[11] Ş. Karatas, Ş. Altındal, Mater. Sci.and Eng. B **122**, 133 (2005).
[12] A. Tataroğlu, Ş. Altındal, Microelectron. Eng. **83**, 582 (2006).
[13] O. Pakma, N. Serin, T. Serin, Ş. Altındal, J. Appl. Phys. **104**, 014501-1 (2008).
[14] J. H. Werner, H. H. Guttler, J. Appl. Phys. **69**, 1522 (1991).
[15] Y. P. Song, R. L. Van Meirhaeghe, W. H. Laflere, P. Cardon, Solid-State Electron. **29**, 633 (1986).
[16] S. Bandyopadyay, A. Battacharya, S. K. Sen, J. Appl. Phys. **85**, 3671 (1991).
[17] E. Dobrocka, J. Osvald, Appl. Phys. Lett. **65**, 575 (1994).
[18] A. A. Kumar, V. Janardhanam, V. R. Reddy, P. N. Reddy, J. Optoelectron. Adv. Mater. **9**, 3877 (2007).
[19] R. T. Tung, Phys. Rev. B **45**, 13509 (1992).
[20] J. P. Sullivan, R. T. Tung, M. R. Pinto, W. R. Graham, J. Appl. Phys. **70**, 7403 (1991).
[21] A. Gümüş, A. Türüt, N. Yalçın, J. Appl. Phys. **91**, 245 (2002).
[22] İ. Dökme**,** Ş. Altındal, İ. M. Afandiyeva, Semicond. Sci. Technol. **23**, 035003 (2008).
[23] S. Chand, J. Kumar, J. Appl. Phys. **80**, 288 (1996).
[24] Ş. Altındal, H. Kanbur, A. Tataroğlu, M. M. Bülbül, Physica B **399**, 146 (2007).
[25] J. H. Werner, H. H. Guttler, J. Appl. Phys. **73**, 1315 (1993).
[26] R. F. Schmitsdorf, T. U. Kampen, W. Mönch, Surf. Sci. **324**, 249 (1995).
[27] R. T. Tung, Mater. Sci. Eng. R **35**, 1 (2001).
[28] A. Tataroğlu, Ş. Altındal, J. Alloys Compd.**484**, 405 (2009).
[29] H. von Wenckstern, G. Biehne, R. A. Rahman, H. Hochmuth, M. Lorenz, M. Grundmann, Appl. Phys. Lett. **88**, 092102 (2006).
[30] F. R. Roccaforte, F. Lucolana, F. Giannazzo, A. Alberti, V. Raineri, Appl. Phys. Letters **89**, 022103-1 (2006).
[31] A. F. Özdemir, A. Türüt, A. Kökçe, Semicond.Sci. Technol. **21**, 298 (2006).
[32] M. K. Hudait, S. P. Venkateswarlu, S. B. Krupanidhi, Solid- State Electron. **45**, 133 (2001).
[33] A. Tataroğlu, Ş. Altındal, J. Alloys Compd. **479**, 893 (2009).
[34] S. Zhu, C. Detavernier, R. L. Van Meirhaeghe, F. Cardon, G. P. Ru, X. P. Qu, B. Z. Li, Solid-State Electron. **44**, 1807 (2000).
[35] B. H Lee, L. Kung, R. Nieh, W. J. Qi, J. C. Lee, Appl. Phys. Lett. **77**, 1926 (2000).
[36] S. Chand, S. Bala, Appl. Surf. Sci. **252**, 358 (2005).
[37] T. G. Finstad, M. A. Nicolet, Thin Solid Film **68**, 393 (1980).

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