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6. F. J. Feigl, in "VLSI Electronics," Vol. 6, N. G. Einspruch and G. B. Larrabee, Editors, Academic Press, New York (1983).

7. A. M. Goodman and J. M. Breece, This Journal, **117**, 982 (1970).

8. Y. Kamigaki and Y. Itoh, *J. Appl. Phys.*, **48**, 2891 (1977).

9. A. C. Adams, T. E. Smith, and C. C. Chang, *This Journal*, **127**, 1788 (1980).

10. S. M. Hu, *Appl. Phys. Lett.*, **42**, 872 (1983).

11. E. A. Irene, *J. Appl. Phys.*, **54**, 5416 (1983).

12. E. Harari, *ibid.*, **49**, 2478 (1978).

13. C. S. Jeng, T. R. Ranganath, C. H. Huang, H. S. Jones, and T. L. Chang, *IEDM Tech. Dig.*, Paper 165, 388 (1981).

14. F. P. Heiman, *Trans. Electron. Devices*, **ed-24**, 781 (1967).

15. M. Kuhn, *Solid-State Electron.*, **13**, 873 (1970).

16. E. H. Nicollian and J. R. Brews, "MOS Physics and Technology," p. 410, John Wiley & Sons, New York (1982).

17. F. J. Feigl, D. R. Young, D. J. DiMaria, S. Lai, and J. Calise, *J. Appl. Phys.*, **52**, 5665 (1981).

18. B. H. Vromen, *Appl. Phys. Lett.*, **27**, 152 (1975).

19. P. Solomon, *J. Appl. Phys.*, **48**, 3843 (1977).

20. M. Lenzinger and E. H. Snow, *ibid.*, **40**, 278 (1969).

21. Z. A. Weinberg, *ibid.*, **53**, 5052 (1982).

22. M. Av-Ron, M. Shatzkes, T. H. DiStefano, and R. A. Gdula, *ibid.*, **52**, 2897 (1981).

23. J. M. Gibson and D. W. Dong, *This Journal*, **127**, 2722 (1980).

24. J. S. Johannessen, W. E. Spicer, J. F. Gibbons, J. D. Plummer, and N. J. Taylor, *J. Appl. Phys.*, **49**, 4453 (1978).

25. S. A. Schwarz, R. W. Barton, C. P. Ho, and C. R. Helms, *This Journal*, **128**, 1101 (1981).

26. Y-P. Han, J. P. Mize, B. T. Moore, J. Pinto, and R. Worley, *41st Annual Dev. Res. Conf., Tech. Dig.*, Paper II-5, Chicago (1983).

27. B. T. Moore, J. P. Mize, Y-P. Han, J. Pinto, and R. Worly, *41st Annual Dev. Res. Conf., Tech. Dig.*, Paper III-3, Chicago (1983).

The Polycrystalline-Si Contact to GaAs

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ABSTRACT

Polycrystalline-Si/GaAs interfaces have been prepared by depositing hydrogenated amorphous Si (a-Si:H) onto GaAs in a silane plasma at 450°C and annealing at temperatures between 600° and 1050°C. Rutherford backscattering, secondary ion mass spectroscopy, and transmission electron microscopy analyses show that the resulting polycrystalline-Si/GaAs interface is metallurgically stable when the Si is undoped, while significant interdiffusion occurs when P or As are added to the Si. The Si diffusion into the GaAs is rapid ($D = 10^{-11}$ cm²/s at 1000°C) depends on concentration and increases with increasing P content in the Si. Ohmic contacts prepared using Si(P-4 atom percent (a/o))/GaAs (semi-insulating) annealed at 800° and 1050°C, gave contact resistance of 1.7×10^{-4} and 1.2×10^{-4} Ω cm², respectively.

A plausible equilibrium band diagram for n⁺-Si/n-GaAs is shown in Fig. 1. Incorporated in the diagram is a valence band offset of 0.05 eV, as measured with photoemission spectroscopy (1) for amorphous Si (a-Si) deposited onto (110) GaAs in ultrahigh vacuum conditions. We have also assumed that interface states pin the Fermi level to a near midgap energy level [as is the case for other lattice mismatched GaAs heterojunctions and most metal/GaAs interfaces (2)]. Since evaporated Si/GaAs interfaces are known to be metallurgically stable to temperatures as high as 1050°C (3), degenerately doped Si may therefore provide a high temperature stable Schottky contact to GaAs.

To investigate this interface, we deposited a-Si onto GaAs by plasma enhanced chemical vapor deposition, adding P or As by mixing the appropriate gas to the silane plasma. We report here on the contact properties of these interfaces after anneals to 1050°C. Instead of a stable degenerate Si/GaAs interface, high concentrations of Si diffused into the GaAs in conjunction with Ga and As out-diffusion into the Si. Schottky contacts were not obtained but, in the case of the P-Si alloys, ohmic contacts

formed with contact resistances on the order of $10^{-4}\Omega$ cm².

Experiment

Polycrystalline-Si/GaAs interfaces were prepared by depositing hydrogenated amorphous Si (a-Si:H) in a silane plasma at 450°C and annealing at temperatures between 600° and 1050°C. Arsenic or phosphorus were added to the silicon in the range 4 to 30 a/o (atom percent) by mixing
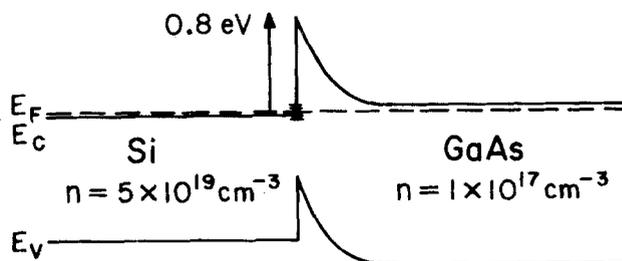
Fig. 1. Equilibrium band diagram for the n⁺-Si/n-GaAs heterojunction with interfacial states. The valence band offset $\Delta E_v = 0.05$ eV was obtained from Ref. (2).

the appropriate gas, arsine (AsH₃), or phosphine (PH₃). All depositions and experiments were run in parallel with samples from two substrate types: polished GaAs (semi-insulating, liquid encapsulated Czochralski (LEC), (100)) and thermally oxidized Si. Film thicknesses were typically 100 nm. The substrates were used as-received from the manufacturer but were cleaned in an Ar⁺ plasma *in situ* prior to the Si depositions.

Rapid thermal annealing to temperatures between 900° and 1050°C for 10s was carried out by a flash lamp system in flowing Ar/H₂. The temperature was monitored with a thermocouple attached to the Si wafer sample platform. Annealing at lower temperatures, 600°-800°C for 15 min, was carried out in a vacuum furnace (base pressure 1 × 10⁻⁷ torr). Foils for cross-sectional TEM were prepared by ion-milling 50 μm thick sections (4 keV, 40 μA). To study out-diffusion and composition, samples were analyzed using Rutherford backscattering (RBS) with 3 MeV He⁺⁺ and Auger sputter profiling. Hydrogen content was measured with He⁺⁺ recoil analysis (75° tilt angle). The total concentration of Si diffused into the GaAs was measured by secondary ion mass spectroscopy (SIMS) after plasma etching the deposited Si in SF₆. The profiles were calibrated using a Si implant standard. The sheet resistance and carrier concentration were measured with van der Pauw patterns or with a four-point probe. Contact resistances of polycrystalline-Si/GaAs, henceforth Si/GaAs, were measured using the transmission line technique. The transmission line pattern (50 μm width) was fabricated after annealing, with the diffused Si providing the doped channel in the semi-insulating GaAs substrate. Titanium metallization was used as an ohmic contact to the Si. Sputter cleaning of the Si prior to Ti deposition was found critical to the formation of Ti/Si contacts of resistance lower than the underlying Si/GaAs interface. The quality of Ti/Si contacts were checked with films deposited on the thermally oxidized Si wafers.

Results and Discussion

The films deposited on thermal SiO₂ were visibly smooth before and after annealing. With GaAs substrates, the majority of the surface area of the films was smooth, but randomly spaced bubbles, indicative of compressive stresses in the film, developed in the Si-As alloy films after annealing. However, the density of these bubbles
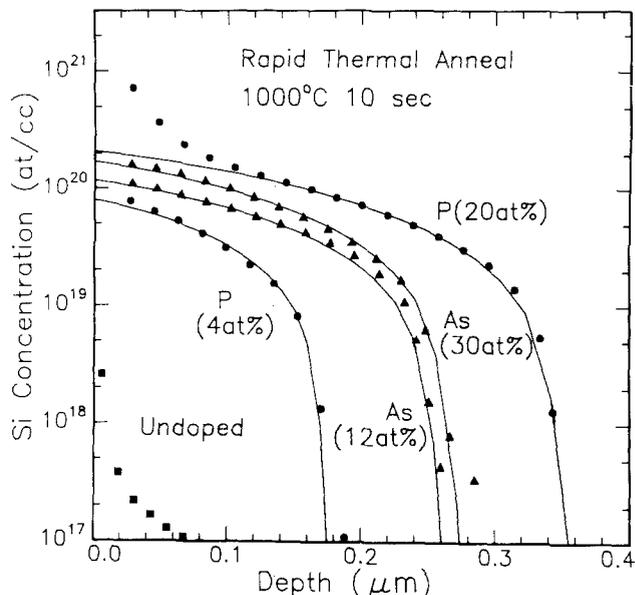
Fig. 3. SIMS profiles of Si diffusion into semi-insulating GaAs measured relative to the Si/GaAs interface, as a function of Si alloy composition. The annealing temperature was 1000°C for 10s. The solid lines are calculated profiles from the Greiner/Gibbons theory (Ref. (3)).

did not interfere with the interface analysis undertaken in this work. Cross-sectional TEM confirmed that the Si crystallized and that the interface remained planar. Examination of electron diffraction patterns of the Si did not reveal any phases other than Si. In particular, neither SiP (orthorhombic), SiAs₂ (cubic, a₀ = 6.0252Å) nor SiAs (monoclinic) were detected. GaP may have been present, but its lattice constant differs from Si by only 0.4% and consequently, its diffraction pattern could not be distinguished from Si. In the case of the Si-P samples, crystalline defects appeared in the top 200Å of the GaAs. Hydrogen content before annealing was about 5 a/o but none was detected with recoil analysis after annealing (<1 a/o).

Figure 2 shows RBS data of Ga and As out-diffusion from GaAs into the Si as a function of P content for a
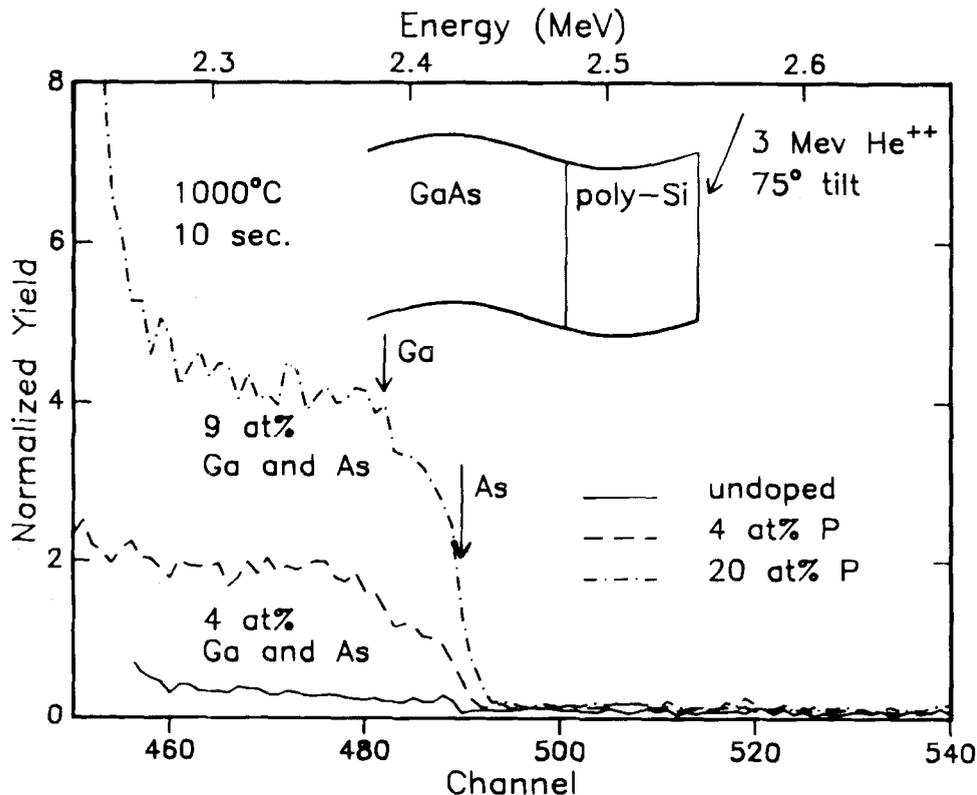
Fig. 2. RBS of Si/GaAs interfaces after rapid thermal annealing to 1000°C for 10s. The figure shows the arsenic and gallium profiles in the Si overlayer, as a function of Si phosphorus content. The element indicator arrows show the position of arsenic or gallium at the surface. The out-diffusion of arsenic and gallium into the Si were calculated by integrating the profiles.

Table I. Polycrystalline-Si/GaAs contact properties

Poly–Si Composition	Anneal Temperature	Si Pair Diff. Coeff.	Sheet Resistance	Carrier Conc.(GaAs)	Contact Resistance
	°C	cm^{2}sec^{-1}	$\Omega/\square$	atoms/cc	Ωcm^2
P (4at%)	800 15min	2.5×10^{-13}	180		1.7×10^{-4}
	1050 10sec	9.6×10^{-11}	45	4.8×10^{18}	1.2×10^{-4}
P (20at%)	750 15min		330		8×10^{-4}
	800 15min	7.6×10^{-13}	100		5×10^{-4}
	1050 10sec	1.4×10^{-10}	96	2.0×10^{18}	
As (12at%)	1000 10sec	2.6×10^{-11}	52		not ohmic
As (30at%)	1000 10sec	2.2×10^{-11}	95		not ohmic

rapid thermal anneal at 1000°C. Integration of the Ga and As surface steps indicated 4 and 9 a/o Ga plus As out-diffused into the Si in the annealed P-4 and P-20 a/o samples, respectively. Auger data indicated that the As/Ga ratios were about 4.5. Similar levels of Ga out-diffusion were observed with Auger depth profiling of the Si-As alloys (4). Figure 3 shows the corresponding diffusion of Si into the GaAs as a function of alloy composition as measured by SIMS. As with Ga and As out-diffusion into Si, Si diffusion into the GaAs increased with increasing phosphorus content in Si. Diffusion also occurred with the As alloys, though the effect of composition (over the range 12-30 a/o) was not as great as for P (4-20 a/o).

The Greiner/Gibbons theory that high concentration Si diffusion occurs via the diffusion of Si-Si pairs (3) models this data well. Theoretical profiles were calculated as described elsewhere (4), and have been overlayed with the data (solid lines in Fig. 3 and 4). Except for the near surface region of the P-Si alloys, where the Si concentration is higher, the agreement was excellent. From the fitted profiles, the diffusion coefficient of Si-Si pairs, as a function of temperature and composition, were determined. Diffusion coefficients for some alloy compositions are tabulated in Table I. Arrhenius plots of pair diffusion coefficient *vs.* reciprocal temperature has shown that the activation energy was independent of alloy composition and equal to 2.65 ± 0.25 eV. The pre-exponential factor ranged from 0.09 to 9 cm² s⁻¹ with variations in the alloy composition.

To understand the difference in out-diffusion observed between intrinsic and As or P doped plasma deposited Si, a closer look at the structure of the Si grain boundaries is required. However, we believe that the Si diffusion occurred via a flux of Ga and As vacancies formed as the GaAs out-diffused through grain boundaries in the Si.

Figure 4 shows the SIMS data for P diffusion into GaAs overlayed with the Si diffusion for the 20 a/o P-Si alloy annealed at 1000°C for 10s. The higher Si concentration in the near surface region overlays (solid line) with the diffusion of P into the GaAs. The strain introduced by the P and Si diffusion was likely responsible for the crystalline defects observed at the Si-P/GaAs interfaces. Enhanced surface concentrations of Si and interfacial defects were not seen with the As-Si/GaAs alloys.

The sheet resistance of the Si/GaAs was a function of temperature, as is shown in Fig. 5 for the P-4 a/o and As-12 a/o samples. The crystallization and dopant activation began at lower temperatures in the P samples. This conforms with the behavior reported for heavily As or P implanted polycrystalline-Si (5). Both elements segregate to grain boundaries but, at high concentrations, the pro-

cess is slower for As than for P, presumably the result of As clustering. Hall measurements show that the Si in the GaAs was activating n-type. To calculate average carrier concentrations, the depth of the doped layer was assumed equal to the depth of the SIMS data. The results from two anneals are found in Table I. Contact resistances as a function of alloy composition are found in Table I. The P-Si alloys gave ohmic contacts in the range 1.2-8 × 10⁻⁴Ω cm², depending on the anneal. The As-Si alloy contacts have, so far,[1] not been ohmic even though the Si concentration and conductivity were comparable to the ohmic P alloy contacts after the 1000°C anneal.

When GaAs is heavily implanted with Si, the free electron concentration typically obtained, after a capped furnace anneal, is no more than 2-4 × 10¹⁸ cm⁻³ (6, 7). The results obtained here by diffusion indicate the same bulk behavior. More than 98% of the Si has self-compensated, sitting on equal numbers of As and Ga substitutional

[1] Recent experiments with a Si(As-9 a/o)/GaAs interface have produced ohmic contacts (2.4 × 10⁻⁴Ω cm²) after anneals at 1000°C for 10s. A 800°C anneal of the same interface was not ohmic.
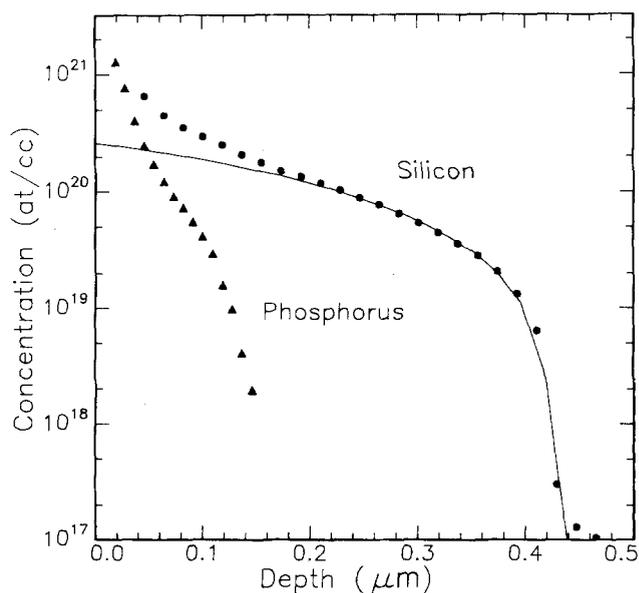
Fig. 4. Secondary ion mass spectroscopy profiles of Si and P diffusion into GaAs measured relative to the Si(P-20 a/o)/GaAs interface after rapid thermal annealing at 1020°C for 10s. The solid line is a calculated profile from the Greiner/Gibbons theory (see text).
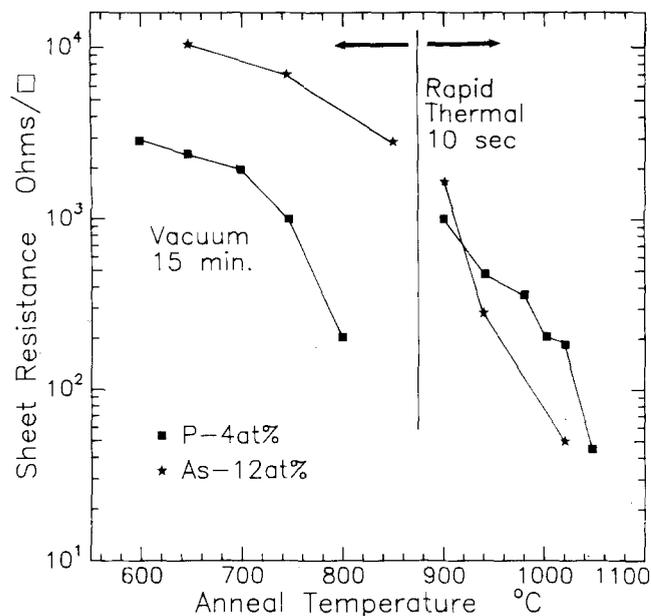
Fig. 5. Sheet resistance of Si/GaAs vs. anneal temperature for the 4 a/o P and 12 a/o As samples.

sites. Metal contacts to GaAs with a 4×10^{18} bulk carrier concentration usually produce ohmic contacts of resistance near $10^{-2}\Omega$ cm^2 or higher. Theoretical calculations of contact resistance as a function of doping for a tunneling mechanism support this result. For example, Chang *et al.* (8) predict a contact resistance of $6.3 \times 10^{-2}\Omega$ cm^2, while the more recent calculations of Boudville and McGill (9) predict a value $1.4 \times 10^{-3}\Omega$ cm^2. The contact resistance of $1.2 \times 10^{-4}\Omega$ cm^2 obtained for the Si(P) contacts indicates that the surface may have had a net donor concentration in the range $6\text{-}12 \times 10^{18}$ cm^{-3}.

A similar situation has been reported for molecular beam epitaxy (MBE) layers (10). *In situ* deposition of Ag onto heavily Si doped GaAs grown by MBE has produced contact resistances of $1.1 \times 10^{-6}\Omega$ cm^2. The bulk carrier concentration of the same material, as measured by the Hall effect, was 4×10^{18} cm^{-3}. At least in the surface region, the net donor concentration may have been as high as 1×10^{20} cm^{-3}. The explanation for this result was that the driving force for Si self-compensation is the Fermi level or the electron concentration (9). In the depletion layer at the surface, the Fermi level is pinned by surface states to 0.8 eV. In this region of lower Fermi level, the ratio of donor to acceptor sites of the Si would be closer to values obtained at lower Si concentrations. The final result: higher Si activation at the surface. If this mechanism is responsible for our results, then the effect observed here is not as significant as the results reported for the MBE layers. The higher temperatures used in our experiments or the method of Si incorporation, diffusion *vs.* layer by layer growth, may have determined the outcome. In any event, though this surface effect may apply to our data, it does not alone explain why the P samples were ohmic while the As samples were not.

Phosphorus has been reported to passivate the surface of GaAs lowering the interfacial barrier from 0.8 to 0.18 eV (11). This would clearly make it easier to form tun-

neling ohmic contacts. Alternatively, since phosphorus was seen to be diffusing into the GaAs, perhaps the ohmic contact is related to the formation of GaAsP phases. Heavy phosphorus implantation into GaAs plus annealing has been shown to produce the phase $GaAs_{0.83}P_{0.17}$ (12). The activation of Si in GaP or GaAsP may be higher.

In conclusion, Si/GaAs interfaces have been formed by plasma deposition of a-Si:H followed by anneals to temperatures of 1050°C. Large quantities of P or As (4-30 a/o) were added to the Si by mixing arsine or phosphine gases into the plasma. Undoped Si/GaAs interfaces were metallurgically stable, but high concentrations of Si diffused into the GaAs in the case of the P and As-Si alloys. The magnitude of the diffusion depended on the P composition and may also depend on the As composition. The Greiner/Gibbons theory that high concentration Si diffuses via Si-Si substitutional pairs compared well with our diffusion profiles. Ohmic contacts prepared using Si(P-4a/o)/GaAs gave contact resistances as low as $1.4 \times 10^{-4}\Omega$ cm^2. Si(As)/GaAs interfaces were not ohmic over the range of compositions and annealing temperatures studied. Phosphorus passivation at the interface or diffusion into the GaAs resulting in the formation of GaP_xAs_{1-x} at the Si interface may explain the ohmic contacts in the P-Si alloys.

REFERENCES

1. A. D. Katani, N. G. Stoffel, R. R. Daniels, Te-Xiu Zhao, and G. Margaritondo, *J. Vac. Sci. Technol. A*, **1**, 692 (1983).
2. L. J. Brillson, *Surf. Sci. Reports*, **2**, 123 (1982).
3. M. E. Greiner and J. F. Gibbons, *Appl. Phys. Lett.*, **44**, 750 (1984); and M. E. Greiner, Ph.D. Thesis, Stanford University, Stanford, CA (1984).
4. K. L. Kavanagh, J. W. Mayer, J. M. Woodall, and C. W. Magee, *Appl. Phys. Lett.*, **47**, 1208 (1985).
5. Len Mei, M. Rivier, Y. Kwark, and R. W. Dutton, *This Journal*, **129**, 1791 (1982).
6. T. C. Banwell, M. Maenpaa, M-A. Nicolet, and J. L. Tandon, *J. Phys. Chem. Solids*, **44**, 507 (1983).
7. D. V. Morgan, F. H. Eisen, and A. Ezis, *IEEE Proc. Pt.*, **128**, 109 (1981).
8. C. Y. Chang, Y. K. Gang, and S. M. Sze, *Solid-State Electron.*, **14**, 541 (1971).
9. W. J. Boudville and T. C. McGill, *J. Vac. Sci. Technol. B*, **3**, 1192 (1985).
10. P. D. Kirchner, T. N. Jackson, G. D. Pettit, and J. M. Woodall, *Appl. Phys. Lett.*, **47**, 26 (1985).
11. D. J. Olego, R. Schachter, and J. A. Baumann, *ibid.*, **45**, 1127 (1984).
12. O. Aina and K. P. Pande, *ibid.*, **44**, 544 (1984).