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High-Temperature Stability of Nb/GaAs and NbN/GaAs Interfaces

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Abstract

The interface stabilities of Nb/GaAs and NbN/GaAs contacts at temperatures up to 700°C for Nb/GaAs and 850°C for NbN/GaAs have been investigated by transmission electron microscopy and X-ray diffractometry techniques. Results reveal that a Nb/GaAs reaction takes place at temperatures above 600°C, and interdiffusion at the NbN/GaAs interface occurs at temperatures above 800°C. The correlation between the observed interface morphologies before and after annealing and previously reported electrical properties of these contacts is also discussed.

The GaAs field effect transistor(FET) has been considered as a basic element for high speed logic circuits. Various types of GaAs FET and process techniques have been proposed; among these, the self-aligned gate technique is very promising. In this processing method, the ion implanted GaAs wafer together with the gate material undergoes annealing at temperatures as high as 850°C. For this reason, a gate metallization must be used which provides a good Schottky contact with GaAs that is not degraded by the high temperature processing. Recently, increasing attention has been directed toward refractory metals, their silicides, and their nitrides because of their high temperature stabilities.^{1,2}

A recent study³ of Nb/GaAs and NbN/GaAs Schottky contacts has shown that excellent electrical characteristics can be obtained by annealing the Nb/GaAs sample at 600°C and the NbN/GaAs at 800°C, but that degradation of electrical properties was observed for Nb/GaAs annealed at 700°C and for NbN/GaAs at 850°C. In this work, a transmission electron microscopy and X-ray diffraction study of the interfacial phenomena occurring during the thermal treatment of the contacts has been undertaken in order to further investigate the high temperature stabilities of Nb/GaAs and NbN/GaAs interfaces.

Nb and NbN thin films were deposited on Si-doped (100) GaAs by dc magnetron sputtering. After the deposition, Nb/GaAs samples were annealed at 600°C and 700°C and NbN/GaAs samples were annealed at 800°C and 850°C by using an AG Associates 210 Rapid Thermal Annealing instrument. Annealing time was 10 seconds for both types of samples. Details of sample preparation and annealing procedure are described in Ref.3.

Both plan-view and cross-sectional samples were prepared by the standard techniques for transmission electron microscopy(TEM) investigation.⁴ Since niobium and niobium nitride have much stronger crystal bonding than GaAs, cross-sectional samples were carefully prepared by using the ion milling technique with a low angle(11°) to improve the uniformity of thickness at

the interface region. Observations of each sample were made in a Philips EM400 TEM and a JEOL JEM200CX TEM. A Siemens D500 X-ray diffractometer and a Seeman-Bohlin glancing angle X-ray diffractometer were also used to confirm the TEM results in macroscopic scale.

The as-deposited Nb thin film was observed to have a polycrystalline morphology by plan-view TEM which is not shown here. The cross-sectional TEM image in Fig.1a shows an abrupt interface with a thin intervening oxide layer between the deposited film and the substrate. A preferred orientation relationship between the as-deposited Nb and the substrate was also revealed by electron diffraction: $(\bar{1}10)_{Nb} \parallel (001)_{GaAs}$ and $[111]_{Nb} \parallel [110]_{GaAs}$. The presence of this preferred orientation relationship indicates that the oxide layer does not cover the substrate surface completely.

The interface morphology of the Nb/GaAs samples after annealing at 600°C and 700°C are shown in Figs. 1b and 1c. As can be seen, the Nb/GaAs interface remains sharp after annealing at 600°C while the intervening oxide has disappeared. The plan-view TEM did not show any evidence of a Nb/GaAs reaction at the interface, nor any significant change in the grain size of Nb. Annealing at 700°C resulted in a dramatic interface reaction with a laterally nonuniform morphology(Fig.1c). Two phases were formed during the annealing, yet there was still unreacted Nb, identified by electron diffraction analysis and confirmed by X-ray diffraction. The first Nb-GaAs reaction product was the tetragonal binary phase Nb_5Ga_3 and the second phase was Nb_4As_3 which has an orthorhombic unit cell. Determination of the phase distribution was difficult due to the small size of the grains, about 20nm, and high concentration of defects such as microtwins and stacking faults as shown in Fig.1c.

The plan-view micrograph in Fig.2a shows that the as-deposited niobium nitride is polycrystalline with an average grain size of about 6nm. The as-deposited phase on the GaAs substrate was identified to be tetragonal Nb_4N_3 by both the electron diffraction and X-ray diffractometry

techniques. The plan-view micrograph and electron diffraction pattern in Fig.2b reveal that a new phase, hexagonal NbN with $a=0.2968\text{nm}$ and $c=0.5548\text{nm}$, was formed in the deposited film during annealing at 800°C and comprises a majority of the film. Note that the grain size of the new phase is about ten times larger than that of the as-deposited phase. The faint rings in the diffraction pattern from Nb_4N_3 indicates that not all the as-deposited phase had transformed to NbN. Other of the rings can be assigned to pure Nb, indicating that small Nb particles were also formed during the annealing, probably as a result of the reaction $\text{Nb}_4\text{N}_3 \rightarrow 3\text{NbN} + \text{Nb}$.

The interface morphologies of NbN/GaAs samples before and after annealing are shown in cross-sectional TEM images in Fig.3. For the as-deposited sample, the interface is sharp and there exist a native oxide layer at the interface. After annealing at 800°C for 10 seconds by RTA, the interface becomes sharper and a thin intervening oxide (about 1nm) is visible at the interface as a white band (Fig.3b). It is suspected that this intervening oxide may be a result of a reaction between the free Nb and the native oxide to form Nb suboxides.⁵ No interdiffusion is observed between the NbN and GaAs at this annealing temperature.

For the sample annealed at 850°C , the cross-sectional image in Fig.3c indicates that the sample has a uniformly layered structure. The top layer is identified to be a tetragonal Nb_3N phase. The noted difference in film thickness is due to an artifact of TEM sample preparation. It is difficult to identify the interfacial phase, which appears as a white band, because it is very thin (about 3nm) and covered by a thicker Nb_3N layer. The identification of this phase is still under investigation; however, it is believed that this phase is formed due to the interdiffusion at the NbN/GaAs interface.

Present results help understanding the effects of annealing on the electrical properties of both Nb/GaAs and NbN/GaAs contacts reported previously³. In the case of Nb/GaAs, a sharp and uniform metal/GaAs interface without intervening oxide layer is obtained after 600°C RTA,

Fig.1b; which is expected to behave like an ideal Schottky barrier. This is in good agreement with the electrical measurement results where an I-V characteristic with an ideality factor of 1.03 and a Schottky barrier height of 0.78V was achieved. After 700°C RTA, the electrical properties are deteriorated as marked by the increased ideality factor (1.59) and leakage current. This appears to be due to an interfacial reaction resulting in phases with a high density of defects and nonuniform interfaces, Fig.1c.

In the case of NbN/GaAs, the intervening native oxide layer, with a thickness variation across the NbN/GaAs interface for the as-deposited sample (Fig.3a), causes the poor I-V characteristics.³ After 800°C RTA, there is an improvement of the electrical contact that may be the result of sharper interface and removal of damage caused by NbN sputtering. Furthermore, as mentioned before, the thin white band may be a suboxide of Nb. These suboxides are good conductors⁶ and may produce a more intimate electrical contact to the GaAs. This is consistent with the previously reported improvement of the ideality factor from 1.74 to 1.06 and increase of barrier height from 0.57 to 0.73V. After 850°C RTA, however, a new intervening phase is formed at the interface, Fig.3c. Because this layer is relatively thick, thermionic emission may not be the dominant carrier transport mechanism for the diode. This is supported by its poor I-V characteristics with an ideality factor of 1.51.

In summary, interface morphologies of Nb/GaAs and NbN/GaAs contacts have been investigated before and after RTA at high temperatures for 10 seconds. No reaction at the Nb/GaAs interface was observed after annealing at temperatures up to 600°C while 700°C annealing leads to the formation of two binary phases, Nb_5Ga_3 and Nb_4As_3 , with a very rough interface. By comparison, the NbN/GaAs interface remained thermally stable up to 800°C. Interdiffusion took place at the interface following a higher temperature annealing; two new phases with a layered morphology were formed at 850°C. These observed changes in interface morphology correlate

very well with the previously reported changes in electrical properties following the annealing.

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Figure captions:

- 1 Cross-section TEM images of the Nb/GaAs (a) as-deposited sample, (b) annealed at 600°C and (c) annealed at 700°C for 10 seconds.
- 2 Plan-view TEM images and corresponding electron diffraction patterns of the NbN/GaAs (a) as-deposited sample and (b) the sample annealed at 800°C.
- 3 Cross-section TEM images of the NbN/GaAs (a) as-deposited sample, (b) annealed at 800°C and (c) the sample annealed at 850°C.

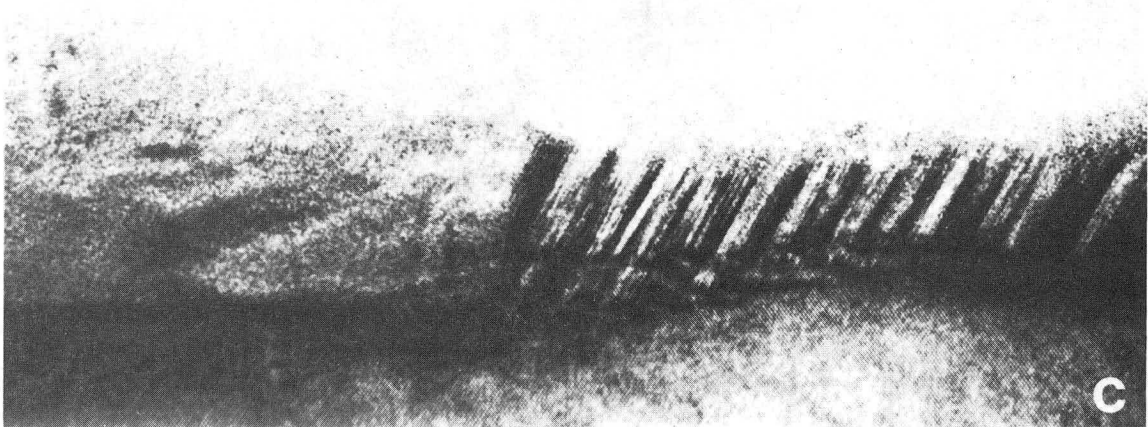
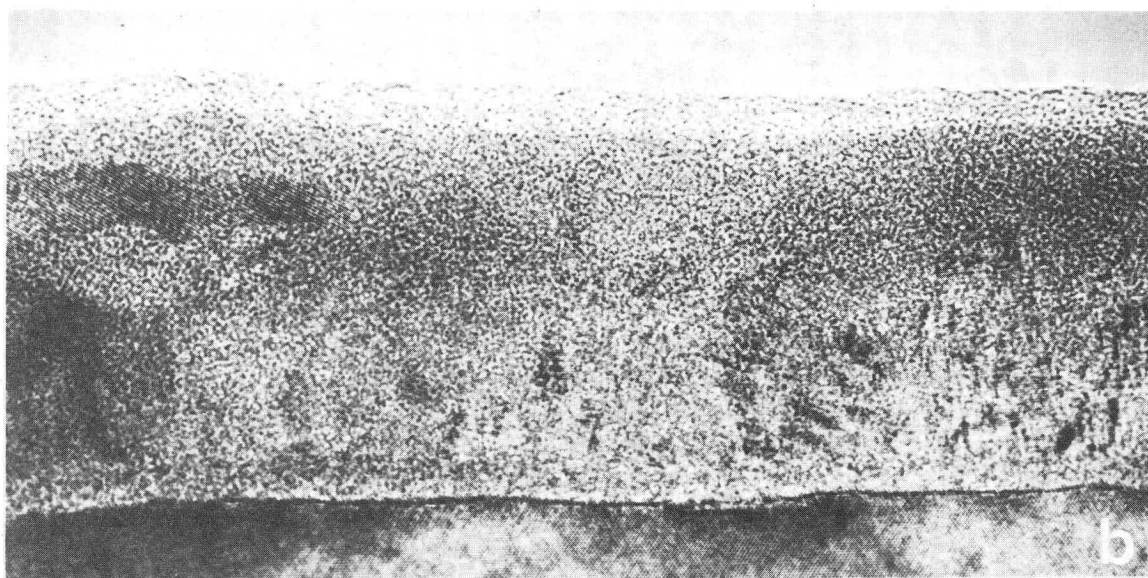
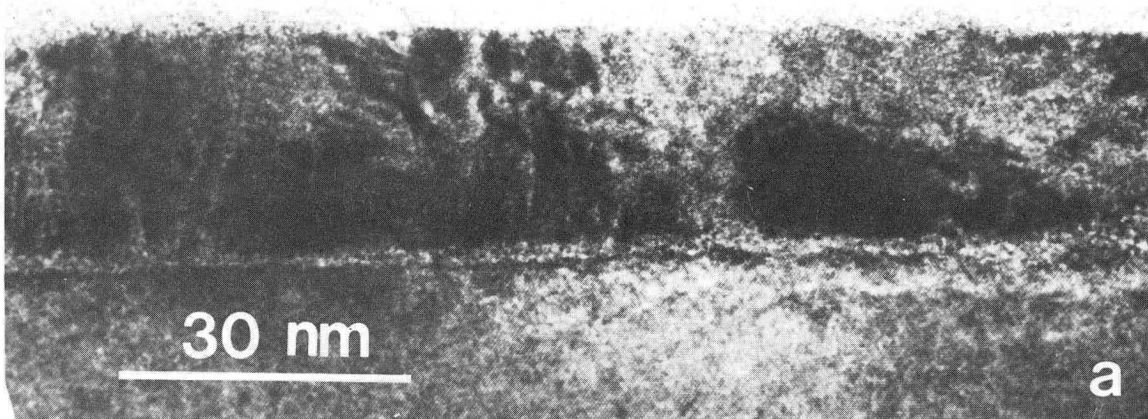


Fig. 1

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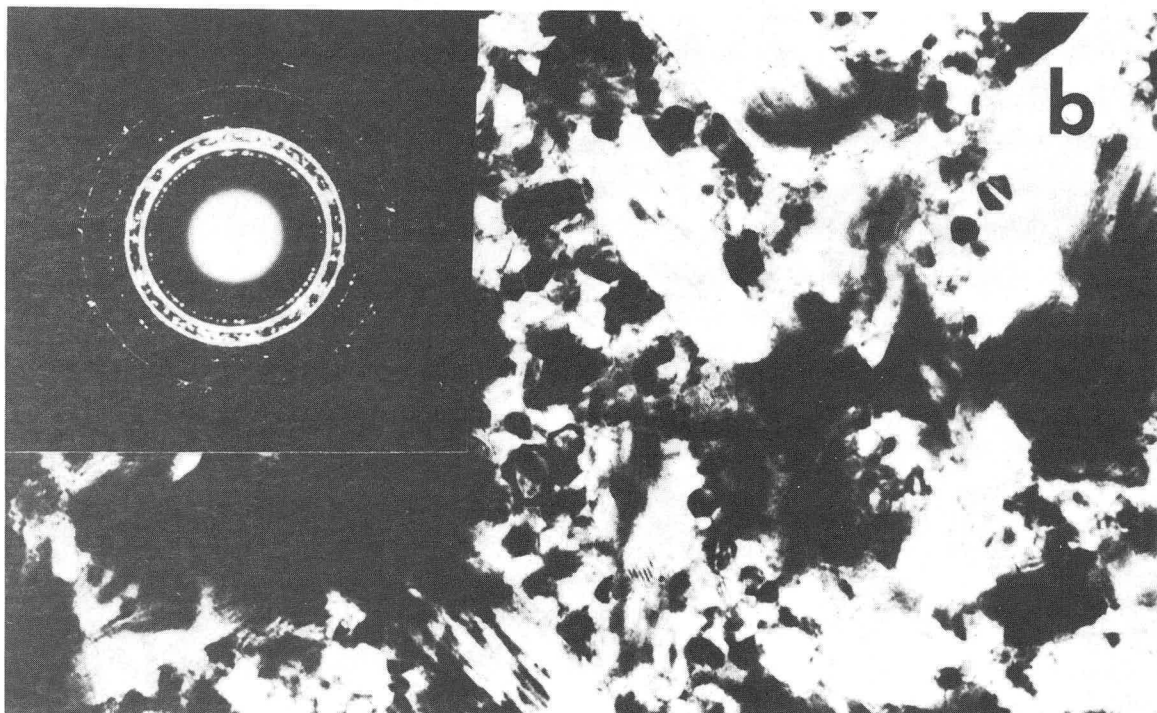
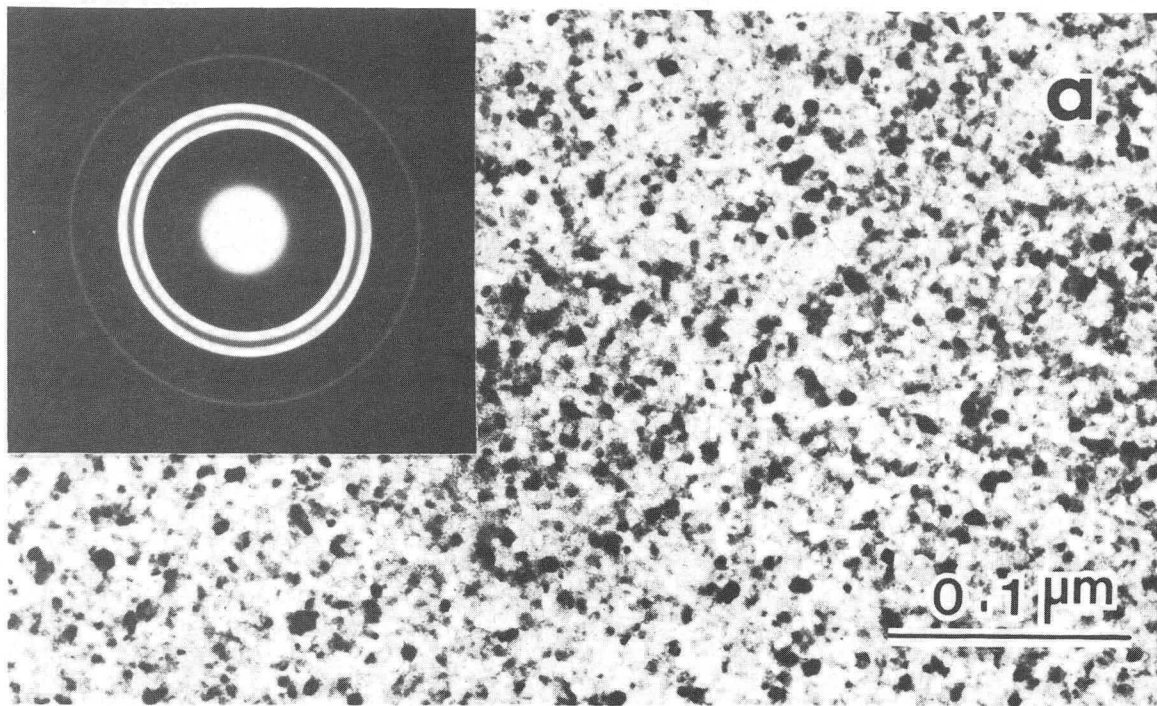


Fig. 2

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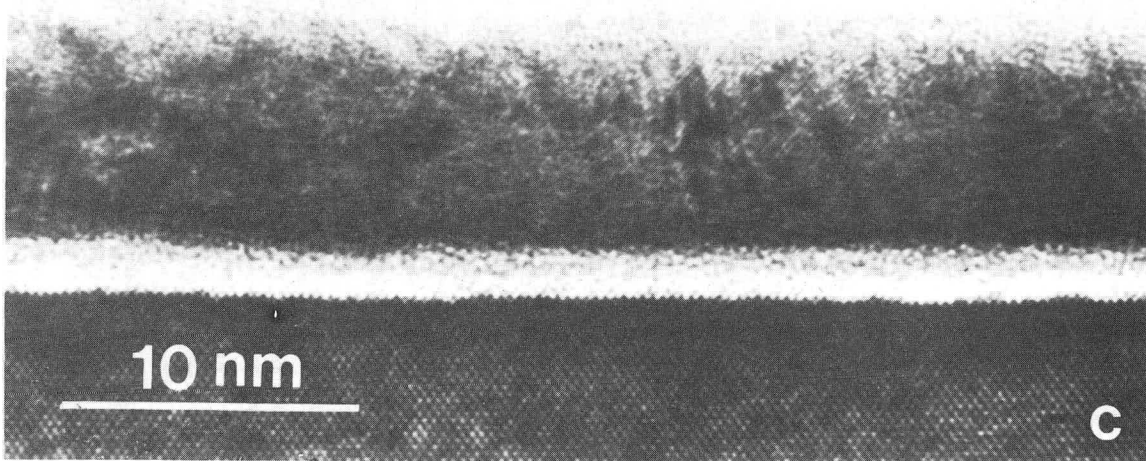
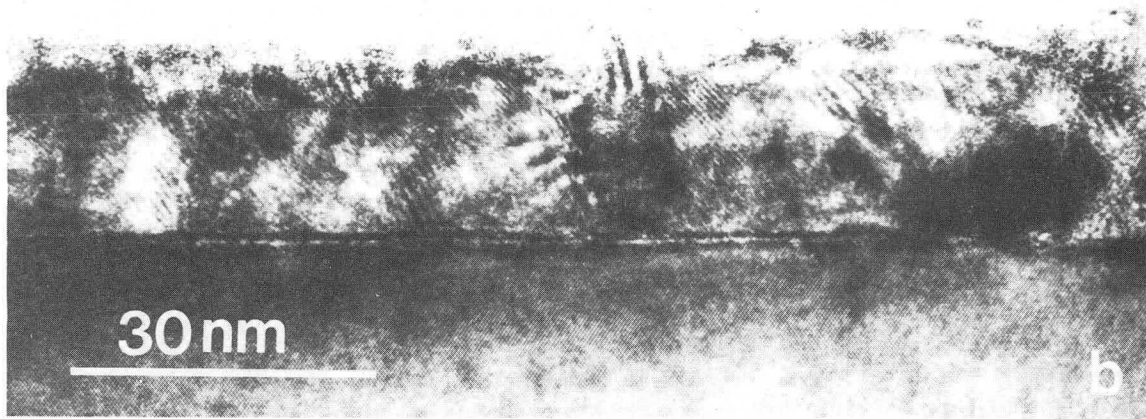
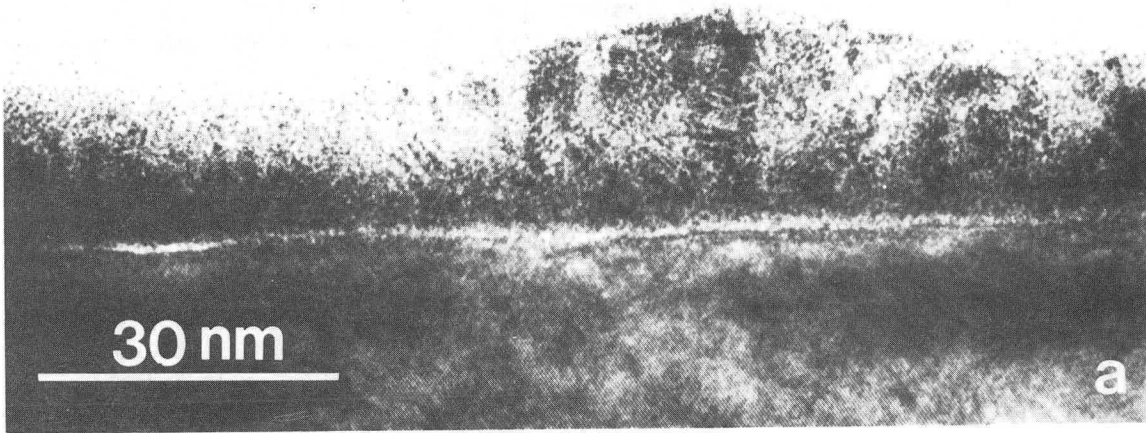


Fig. 3

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