A structural analysis of the Pd/GaN ohmic contact annealing behavior

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Abstract

For ohmic contact on p GaN, palladium is one of the best candidates showing ohmic characteristics already without annealing. To be realized in devices, it is necessary to know the behavior of the ohmic contacts at accelerated conditions, especially for high temperatures and power. We report on the structural evolution of palladium layers (30 nm) deposited on GaN (0001) by electron beam evaporation without intentional annealing. They were next cut into various pieces which were individually submitted to rapid thermal annealing at 400, 500, 600, 700 and 800°C for 10 sec. We investigate the differences in the microstructure and the location of interfacial phases and their relationships as determined by X-ray diffraction and transmission electron microscopy, we then suggest the formation mechanism based on the relationship. It is shown that the interface is disrupted at annealing above 600°C and by 800°C only very small patches of Pd are still present, however they area completely imbedded in a matrix of intermetallic phases (gallides) formed by the reaction with GaN.

Introduction

Gallium based nitrides are direct wide-band-gap semiconductors which have a large potential for high-temperature and high-power applications[1]. However, this wide-band-gap makes the device fabrication difficult for ohmic contacts, especially for p type material. Many extensive studies have been made for developing optimized ohmic contact systems.[2-4] Pd is one of the most competing candidates, showing a promising ohmic characteristics at room temperature[3]. In order for Pd to be used as a reliable metal contact on GaN, it is essential to understand the thermal stability and metallurgy of the contact. In spite of the increasing importance of Pd/GaN system, the detailed microstructure of the Pd layer and the high temperature structure are not yet understood. For device applications at high power and high temperature, it is therefore important to study the structural evolution of metal overlayers and their reactions at elevated temperatures.

In this work, we investigated the structural evolution of Pd/GaN (0001) heteroepitaxy during post annealing process. We reveal the existence of interfacial, epitaxial, Pd grains in the as-deposited Pd film that was evaporated on GaN(0001) at room temperature. During subsequent annealing up to 600°C, the grains of Pd grow and we explain the origin of the Pd epitaxy on GaN(0001) to a six-to-seven matched interface structure, wherein six-Ga atomic distances in GaN match to seven-Pd atomic distances. At high temperature annealings (~700°C), the Pd film transforms, by the Pd-Ga reaction to Ga_2Pd_5 and Ga_5Pd gallides which encapsulate the remaining Pd patches and can be in epitaxy to GaN.

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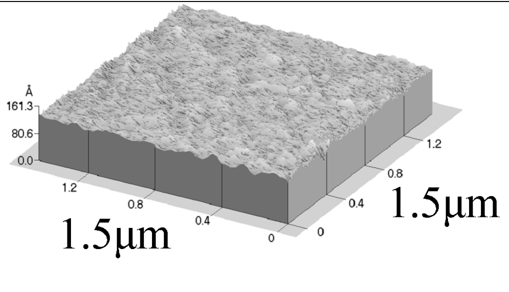
Experimental procedures

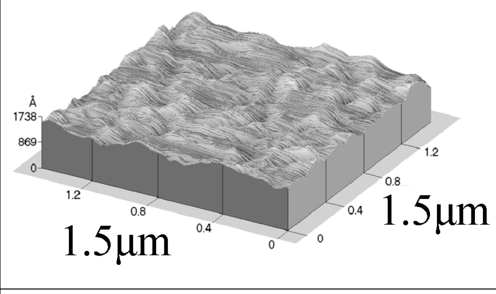
The Mg-doped p-GaN films (1.6 µm thick) were grown on sapphire (0001) substrates using metal-organic chemical vapor deposition (MOCVD). For deposition of Pd films, the GaN samples were first cleaned with organic solvents, then etched in 50 % HF and 50 % HCl, and finally loaded into an e-beam evaporation system, in which the base pressure was ~$1x10^{-7}$ Torr. Pd films were deposited to a nominal thickness of 280 Å at a rate of 2 Å/s without heating the samples. The Pd/GaN specimens were then annealed at various temperatures between 400 and 800 ºC for 30 s in a rapid thermal annealing (RTA) furnace under N_2 flowing atmosphere. The surface and the cross section of Pd/GaN films were characterized by atomic force microscopy (AFM) and high resolution electron microscopy (HREM), respectively. HREM observations were carried out along the GaN $[11\bar{2}0]$ direction on a Topcon 002B electron microscopy operating at 200 kV with a point to point resolution of 0.18nm (C_S=0.4 mm).To obtain averaged structural information, synchrotron x-ray scattering measurements were carried out at beam line 5C2 of Pohang Light Source (PLS) in Korea. The wavelength of the incident x rays was set at 1.488 Å by a double bounce Si (111) monochromator. The structural evolution of the Pd films on GaN was studied by measuring the x-ray powder diffraction profile (θ–2θ scan) and the x-ray reflectivity curve after post annealing at several temperatures. We employed a four-circle x-ray diffractometer for exploring an arbitrary momentum transfer in 3-dimensional space, which provides information about in-plane crystalline state and structural orientation.

Results and discussion

The morphological changes of the surface, as well as the metal/GaN interface under the gallide formation, were examined by atomic force microscope (AFM). For the interface, the metal overlayers were etched off using 3:1 HNO_3:HCl. The results are shown in Fig. 1. As the annealing temperature was raised from 600 ºC to 700 ºC, the root-mean-squared (RMS) roughness of the Pd surface (the Pd-interface) increased significantly from 5.2 Å (4.5 Å) to 90 Å (72 Å), respectively. The deteriorated surfacial and interfacial morphology during the formation of the gallides can be directly related with the optical scattering loss in the light emitting diode (LED) structures. Furthermore, the electrical properties of contact may be greatly changed by the formation of the gallides at the high temperature of 700 ºC.



(a)



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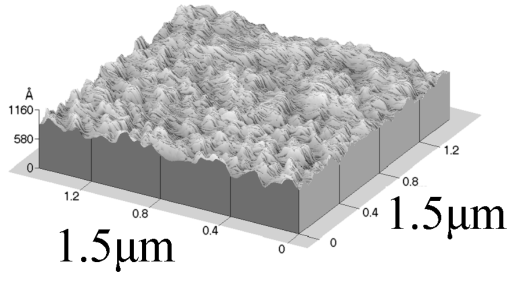

(c)

Fig. 1: Morphology of the Pd/GaN ohmic contact. a) AFM image just after the deposition, b) the surface after annealing at 700 °C, c) AFM image of the interface area after annealing at 700°C

We have used the TEM to examine the surface morphology, as can be seen in figure 2 on for the layer annealed at 400°C, the surface is flat, in agreement with the AFM observations. In this image some moiré fringes are visible at the GaN side of the interface. They may be due to interdiffusion between the metal and GaN but also could be artefacts of TEM sample preparation, although the samples were prepared by ion milling at the LN2 temperature. Further work is needed to confirm their occurrence.

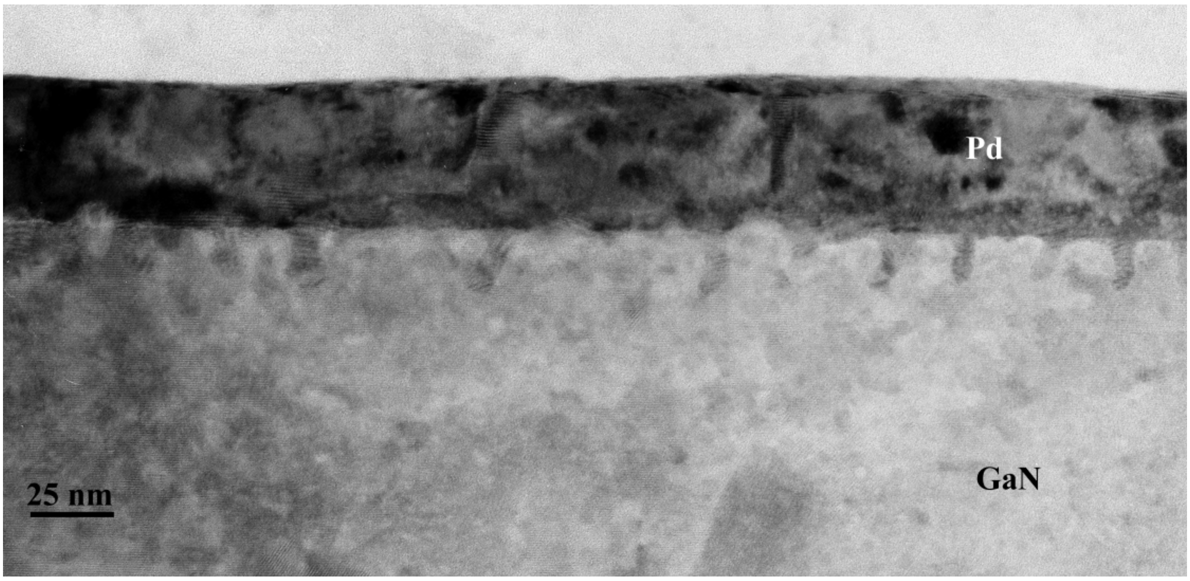

Fig. 2: The morphology of the Pd/GaN ohmic contact after annealing at 400°C

A close examination of the interface structure shows that we have a flat and abrupt interface between GaN and Pd as shown on in figure 3. The (111)Pd/(0001) epitaxial relationship is clearly seen in this figure recorded along the $[11\bar{2}0]$ zone axis of GaN.

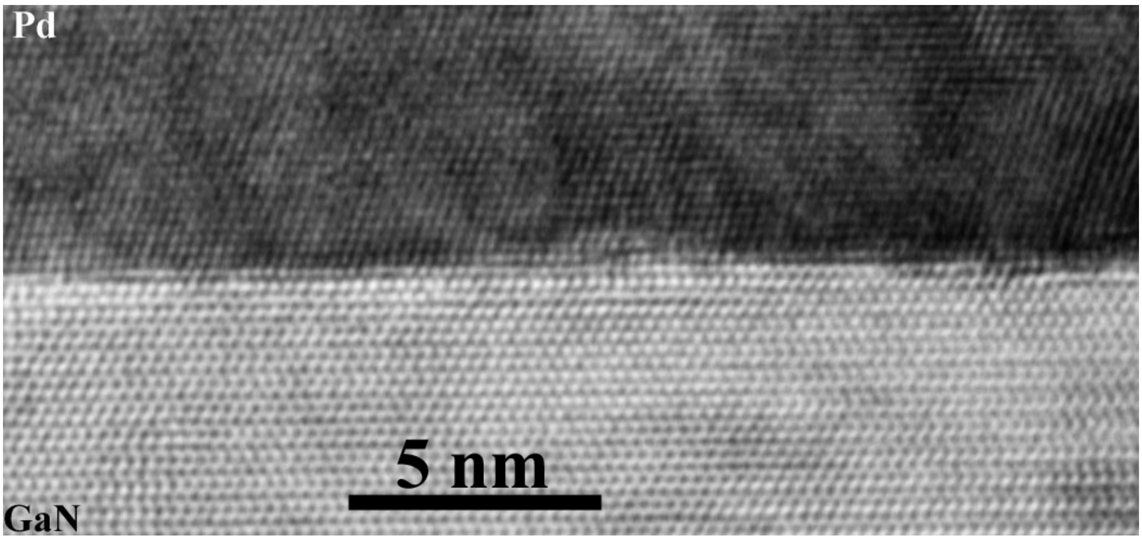

Figure 3: Interface structure and epitaxial relationship of Pd/GaN as observed in the samples after deposition, or rapid thermal annealing up to 600°C.

When the annealing temperature is increased to 700°C, the contact degrades completely. The TEM observations show that all along the surface, the Pd has peered off and also reacted strongly with GaN. Intermediate phases are visible at the interface reaction area and identified as follows by synchrotron X-ray scattering.

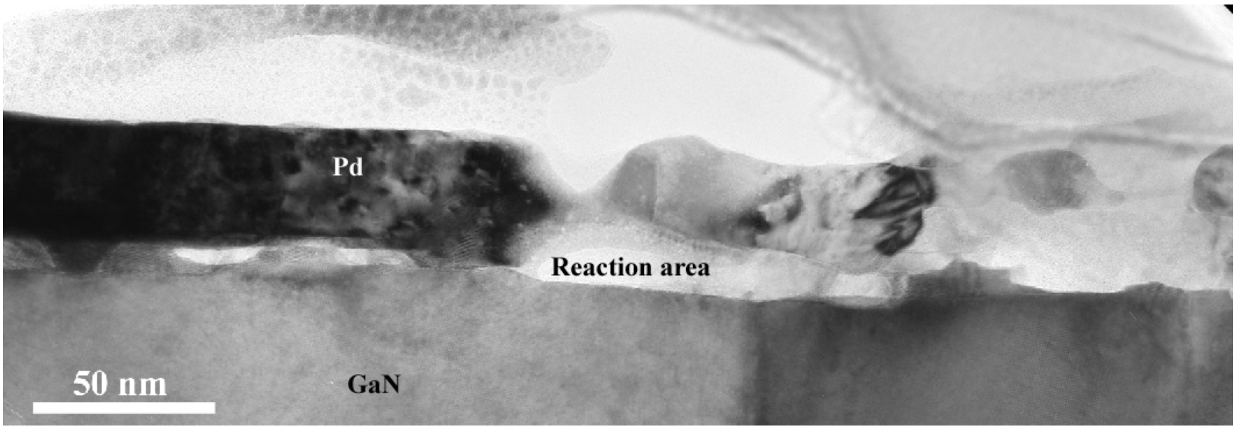

Fig. 4: The Pd/GaN ohmic contact after annealing at 700°C, the reaction area is visible at the interface, and the GaN surface has remarkably degraded.

X-ray scattering observations show that when the Pd film was annealed further to 700 ºC, interestingly, the Pd (111) reflection completely disappeared, and two new Bragg reflections at q_Z = 2.772 $Å^{-1}$ and q_Z = 2.880 $Å^{-1}$ were observed. From the in-plane orientation relationships, it turned out that the Bragg reflections at q_Z = 2.772 $Å^{-1}$ and q_Z = 2.880 $Å^{-1}$ corresponded to the Ga_2Pd_5 (201) (JCPDS 2.762 $Å^{-1}$) and Ga_5Pd (213) (JCPDS 2.878 $Å^{-1}$) reflections, respectively. Both Ga_2Pd_5 and Ga_5Pd phases were grown epitaxially on GaN(0001), which was revealed by the nonspecular Ga_2Pd_5 (221) and the Ga_5Pd (310) reflections that were located 16.1º and 47.2º away from the surface normal direction, respectively. The epitaxial relationship was investigated by observing the orientation of the non-specular reflections of the film with respect to that of the substrate on the azimuthal circles. The scattering profile along the phi scans of these non-specular gallide reflections are shown in Fig. 4.3. The well-defined peaks on the phi scans indicated that the Ga_2Pd_5 and Ga_5Pd phases were in fact grown epitaxially on GaN (0001). From the relative directions of the film and the substrate crystalline axes, we summarized the epitaxial relationships of the two gallides as follows. The Pd-rich gallide, Ga_2Pd_5 has a crystalline orientation with Ga_2Pd_5 (201) // GaN (0001) and Ga_2Pd_5 [010] // GaN $[11\bar{2}0]$. Meanwhile, the Ga-rich gallide, Ga_5Pd has a crystalline orientation with Ga_5Pd (213) // GaN (0001) in the out-of-plane direction, and Ga_5Pd [310] in the same azimuthal angle with GaN $[10\bar{1}0]$.

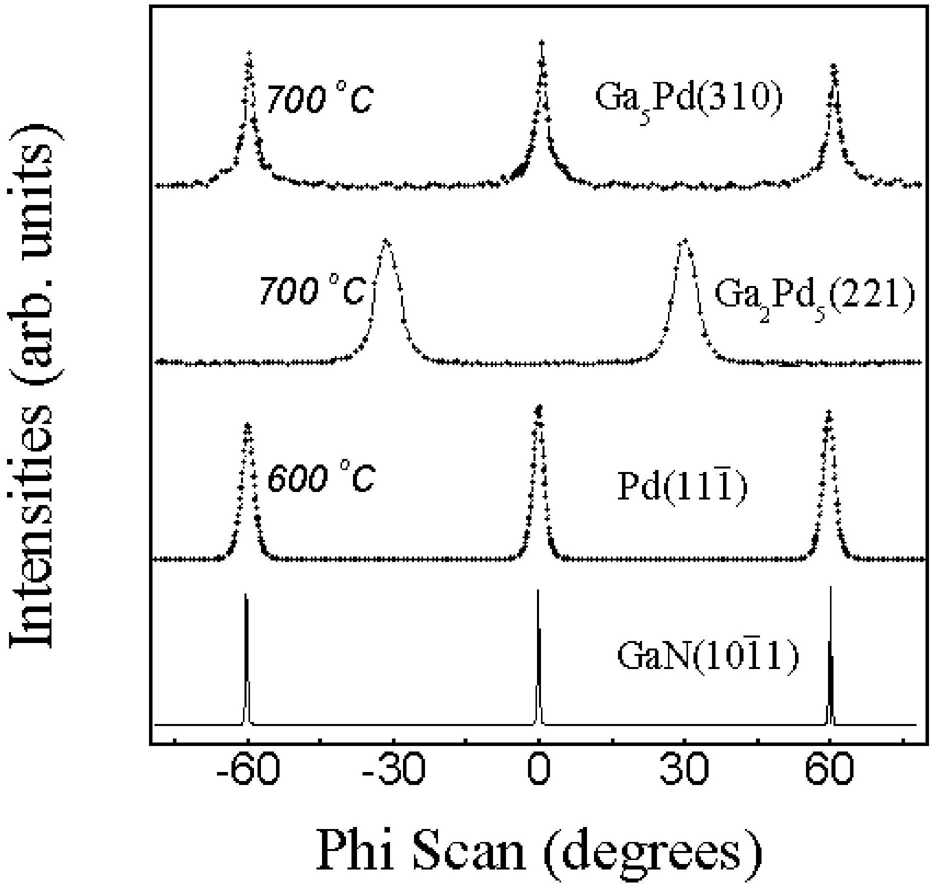

Fig.5: The typical phi scans for the GaN $(10\bar{1}1)$, Pd $(11\bar{1})$, Ga_2Pd_5 (221), and Ga_5Pd (310) nonspecular reflections along the azimuthal direction. The well defined peaks indicate that Pd and Pd gallides were grown epitaxially on GaN (000l).

At 700°C, there are still Pd/GaN patches which extend from the Pd/GaN interface to the top surface. When the annealing was done at 800°C, the metal layer has reacted much further and is covered by the gallides, at this point, no conduction through Pd would be possible. The surface is completely disrupted and very rough, but small patches of Pd can be still found on the GaN surface, although they are completely imbedded inside the gallide layer (fig. 6).

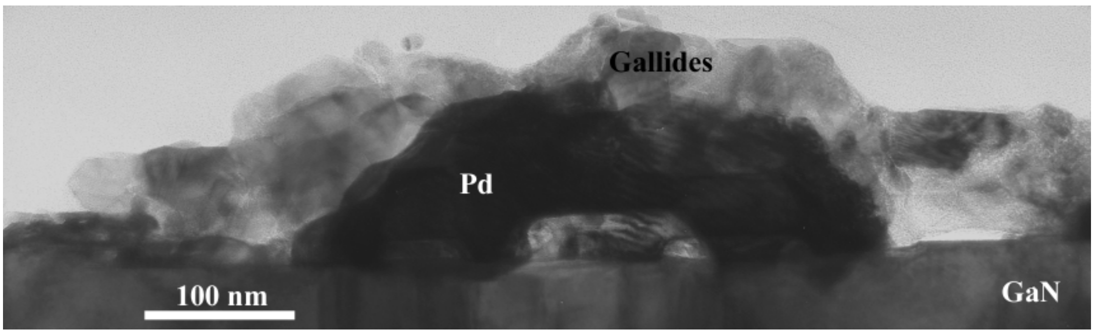

Fig. 6: The Pd/GaN contact after annealing at 800°c

The intermetallic phases can be epitaxially grown on GaN as determined by the above Xrays experiments, but as seen in figure 6, they are mostly spread all over the metallic layer. The Pd patches still have (111)Pd/(0001)GaN epitaxial relationship, but as can be seen in fig. 7, the interface does not appear to be abrupt, or atomically flat as compared to the non annealed or lower temperature annealed contacts, its extension is 1-1.5 nm.

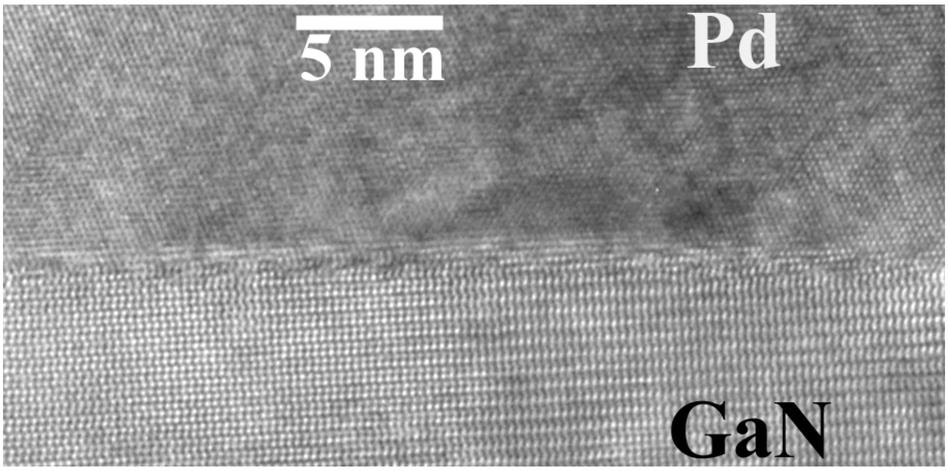

Fig. 7: Atomic scale image of the Pd/GaN interface after annealing at 800°C

In Summary

In the Pd/GaN contact, after annealing below 600°C, (Pd-Ga) intermetallic phases are not detected by X-ray diffraction[5] and HREM observations show abrupt and flat Pd/GaN interfaces. Higher temperature annealing leads to a rapid extension of these phases and they finish by embedding the remaining small Pd patches.

Acknowledgement

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