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Materials Science and Engineering B54 (1998) 207–209

MATERIALS
SCIENCE &
ENGINEERING
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Letter

Growth of gallium phosphide layers by chemical beam epitaxy on oxide patterned (001)silicon substrates

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Accepted 24 March 1998

Abstract

GaP layers grown by chemical beam epitaxy in [110] channels fabricated on oxide-patterned (001)silicon substrates have been examined in cross-section by conventional and high resolution transmission electron microscopy. Results indicate that the layers are single crystalline. For the imaging conditions used, [110] cross-sectional micrographs show that growths in contact with the oxide exhibit twinning on one edge-on variant, whereas faults or twins are observed on two such variants in the layers which nucleate on the silicon substrate. Arguments for rationalizing these observations are developed, and their implications to improve the quality of the layer by confining faults or twins by the oxide sidewall are discussed. © 1998 Elsevier Science S.A. All rights reserved.

Keywords: Gallium phosphide; Chemical beam epitaxy; Oxide patterned silicon substrates

The lattice mismatch between GaP and Si at ambient temperatures is 0.37%. Therefore, the two materials constitute a nearly ideal combination for the integration of silicon-based devices and III–V technologies. To explore this potential, a number of groups have investigated the growth of GaP layers on silicon substrates using organometallic vapor phase epitaxy (OMVPE) [1–3] and chemical beam epitaxy (CBE) [4,5]. Two significant observations emerge from these studies. First, the layer nucleates in the form of islands. Second, the islands are faceted on specific crystallographic planes. Their subsequent coalescence to form a continuous film leads to the formation of stacking faults and twins in the overgrowth. These microstructural features propagate into thicker regions of the film. One way to obviate this problem is to restrict their propagation using sidewalls of oxide-patterned substrates.

Previously, Matyi and coworkers [6,7] have deposited GaAs in channels on silicon substrates that are defined by oxide sidewalls. They have observed that the growth in contact with the oxide is polycrystalline in nature. This is attributed to the nucleation of islands on the amorphous oxide sidewall.

In the present study, we have carried out the growth of GaP layers on oxide-patterned (001)Si substrates to resolve two issues. First, whether or not patterning can restrict the growth of faults or twins in the layer. Second, whether one can grow single crystalline GaP layers on patterned substrates. The results of this study constitute the present paper.

To fabricate patterned silicon substrates, (001)Si wafers were cleaned using an RCA clean. This consisted of a 10-min dip in a 1:1:5 solution of NH_4OH, H_2O_2 and DI water maintained at 75°C, a 5-min rinse in DI water, a 10-min dip in a 1:1:5 solution of HCl, H_2O_2 and DI water also kept at 75°C and a final rinse in DI water. After cleaning, 250-nm-thick thermal ox-

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PII S0921-5107(98)00169-X

ides were grown on the substrates. Subsequently, channels oriented along the [110] direction and having different widths were opened in the oxide films using HF.

The patterned substrates were loaded into the growth chamber of a CBE system. During the heat up period to the growth temperature of 350°C, tertiary butyl phosphine (TBP) and hydrogen were introduced into the chamber to ensure transition from hydrogen to phosphorus termination of the (001)Si surface [4]. Triethylgallium (TEG) and TBP pulses were used for heteroepitaxial GaP layer growth [5]. The growth was monitored in real-time by parallel polarized reflectance spectroscopy [8].

We performed the structural evaluation of as-grown layers using conventional and high resolution transmission electron microscopy (HRTEM). The cross-sectional samples were prepared using standard procedures. Thinned samples were examined in microscopes operating at 120 and 400 keV.

Fig. 1 shows a [110] cross-sectional micrograph obtained from a 200-nm-thick GaP layer. The micrograph depicts a dark-field image that was obtained using a $(2\bar{2}0)$ reflection. Two significant observations emerge: (i) the layer in contact with the oxide is single crystalline and contains a high density of twins on one set of edge-on {111} planes, and (ii) the layer in contact with the silicon surface is also defective.

We have further characterized the Si/GaP and oxide/GaP interfaces using HRTEM, and these results are reproduced in Figs. 2 and 3. We show an example of the Si/GaP interface in Fig. 2. Stacking faults or twins on two variants appear to originate from the Si/GaP interface, whereas the oxide/GaP interface shown in Fig. 3 has a high density of twins on only one variant, a result consistent with Fig. 1. The GaP growth conforms to the topology of the underlying oxide and delamination or voiding is not observed at the interface.

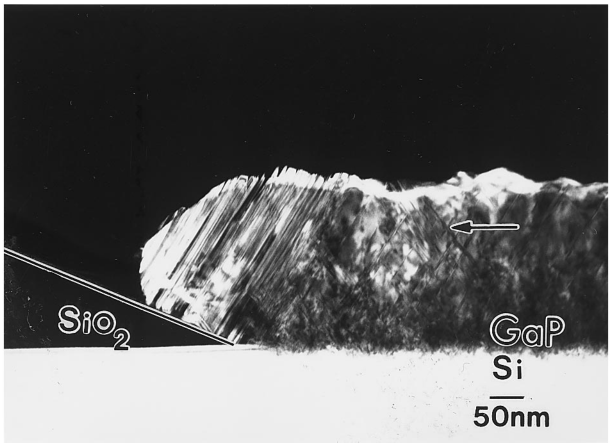

Fig. 1. A dark field electron micrograph observed from a GaP layer grown on an oxide-patterned (001)Si substrate; $(2\bar{2}0)$ reflection was used to form the image. The layer adjacent to the sidewalls exhibits a high density of twins and is single crystalline.

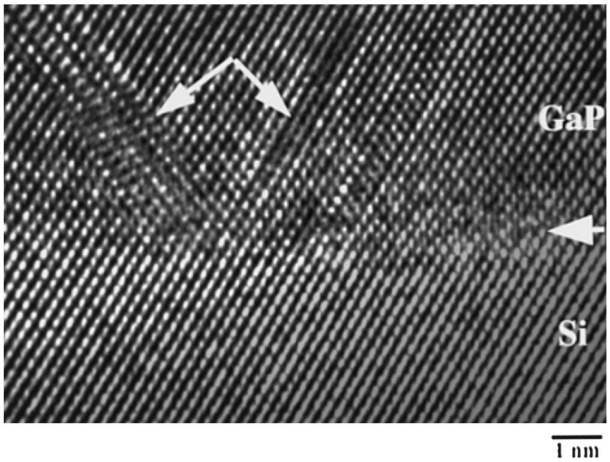

Fig. 2. A cross-sectional [110] high resolution electron micrograph of a Si/GaP interface indicating the presence of two edge-on {111} twin variants.

Two significant observations emerge from the preceding study. First, the [110] cross-section of the GaP growth on (001)Si shows faults or twins on two edge-on {111} variants. Second, the GaP growth in contact with the amorphous silicon dioxide is single crystalline. This growth contains a high density of twins on one edge-on variant and conforms to the topology of the underlying oxide.

Ernst and Pirouz [2,3] have shown that the growth of GaP on silicon nucleates in the form of faceted islands. We show this situation schematically in Fig. 4(a). Only those edge-on {111} facets are shown whose line of intersection with the (001) surface is parallel to the channel length. For the sake of conciseness, we show only two GaP islands within an oxide defined channel. During growth, faults or twins may form on the exposed facets [2,3]. The higher the growth rate of the layer, the higher the probability of forming these features.

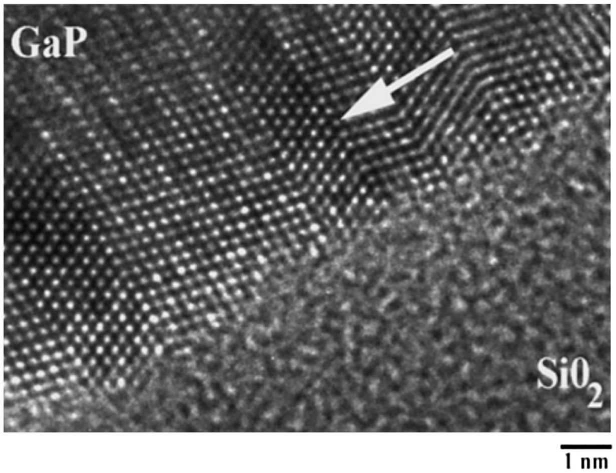

Fig. 3. A cross-sectional [110] high resolution electron micrograph showing the high density of twins in the GaP epilayer adjacent to the oxide sidewall. Only one {111} twin variant is observed.

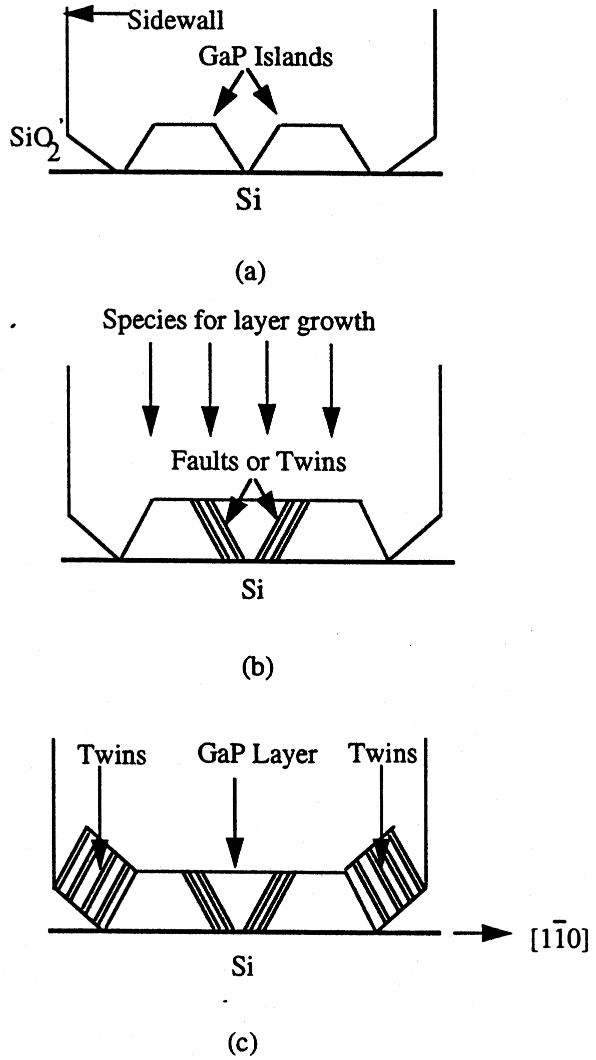

Fig. 4. Schematic illustrating the formation of faults and twins due to the growth on faceted GaP islands: (a) two faceted GaP islands that have nucleated on the silicon substrate; only those edge-on {111} variants are shown whose line of intersection with the (001) surface is parallel to the channel length in the oxide; (b) growth on facets leading to the coalescence of islands and faults and twins; and (c) growth on an exposed facet, contiguous to the oxide sidewall, leading to the formation of faults and twins in the GaP layer in contact with the oxide.

When the two islands coalesce to form a continuous film as shown in Fig. 4(b), the layer may contain faults or twins on two variants, an assessment consistent with the observations of Fig. 2.

As indicated earlier, Matyi et al. [6,7] have investigated the growth of GaAs on oxide-patterned silicon substrates. They observed polycrystalline GaAs in contact with the oxide. They attribute this to the nucleation of GaAs on the oxide surface. We, on the other hand, see single crystalline regions in contact with the oxide, implying that the layer does not nucleate on the oxide. We can rationalize this assessment in terms of the results of Li et al. [9]. They have shown that GaP and SiO$_2$ surfaces exhibit a considerable differential with regard to the pyrolysis of TBP. This is attributed to the absence of surface sites for complex bonding of TBP molecules on an SiO$_2$ surface. Even though we have not investigated this aspect with respect to Si, the presence of a single crystalline film contiguous to the oxide sidewall indicates that the TBP decomposition occurs much more readily on a Si surface than on an SiO$_2$ surface. We envisage that the observed growth contiguous to the oxide is seeded from a faceted GaP island that nucleates on the silicon surface and is close to the oxide wall. We depict this situation in Fig. 4(c). It is apparent that growth on the facet can lead to a single crystalline, highly faulted layer that is in contact with the oxide. It is emphasized that the presence of {111} facets whose line of intersection with the (001) surface is normal to the channel length cannot seed growth on the oxide. Therefore, we have ignored their existence in the above discussion.

Results indicate that the presence of sloping oxide sidewalls tend to impair the quality of the layer by the formation of additional faults or twins. We may be able to circumvent this problem by having vertical sidewalls, a situation that is difficult to achieve using wet etching. Alternately, we could negate the effects of the sloping sidewalls by growing thicker layers. We are currently examining both these issues.

In summary, we have demonstrated the growth of GaP layers by CBE on the oxide-patterned (001)Si substrates. The layers are single crystalline, but their overall quality is not improved by patterning. This could be due the fact that the growth observed in contact with the oxide sidewalls is seeded from faceted GaP islands lying close to the oxide sidewalls, resulting in a high density of faults and twins in the layer.

Acknowledgements

The authors gratefully acknowledge the support of this work by DOD-MURI grant F49620-95-1-0447.

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