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Controllable antiphase domain density in dilute nitride GaPN/GaP heterostructures on silicon

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Abstract. Formation and propagation of the antiphase domains in dilute nitride GaPN/GaP epitaxial heterostructures grown on Si (001) by plasma assisted molecular beam epitaxy (PA-MBE) on silicon is studied. Role of the layer composition, substrate orientation and growth conditions are discussed. Composition of the dilute nitride film was studied by X-ray diffraction (XRD) while the effect of the antiphase disorder in GaP buffer layer on GaPN epilayer structural properties was studied by transmission electron (TEM) and scanning electron microscopy (SEM). Controllable transition between antiphase disordered and monodomain film depending on the concentration of incorporated nitrogen is demonstrated – transition to the monodomain film occurs in dilute nitride GaPN layers starting low with 0.4% of incorporated nitrogen. Control of the antiphase disorder allows to tune mean film polarity and second order nonlinear optical response of III-phosphide heterostructures.

1. Introduction

Gallium phosphide is an indirect III-V semiconductor (E_g = 2.26 eV) with a broad transparency in visible and IR range (0.6-11 μm), high second-order nonlinear optical susceptibility and small lattice mismatch with Si (Δa/a~0.37%) which allows its epitaxial integration with silicon devices [1]. Due to these features in the last decades it has attracted an interest as an optoelectronic and photonic material for frequency conversion. Incorporation of nitrogen atoms into in GaP leads to decrease of the lattice parameter and significantly alters its electronic structure leading to bandgap shrinking (~100 meV/%) and indirect to direct bandgap transition at the N concentration higher than 0.4% [2] extending its application possibilities to the light emitting devices and solar cells [1].

However, synthesis of thin-film III–phosphide-based heterostructures on silicon faces the problem of surface energy mismatch leading to the 3D island growth and problem of polar-on-nonpolar nucleation leading to the formation of antiphase domains (APDs) growing out of phase in terms of lattice occupation with group-III and -V elements [3]. Both problems can be avoided by use of special seeding and buffer layers, such as migration enhanced epitaxy (MEE). However, since the elements of the second order optical susceptibility tensor χ(2) in APDs change its sign [4] the later mentioned problem provides the unique opportunity to tune second order nonlinear optical response of III-phosphide films by spatially and density controlled nucleation of the APDs [5].

Thus, this report aims to study formation of APDs in dilute nitride GaPN/GaP heterostructures depending on the Si (001) substrate orientation and growth regime and demonstrates controllable transition between antiphase disordered and monodomain film depending on the concentration of incorporated nitrogen.

2. Experimental

Dilute nitride phosphide heterostructures were grown with solid source Veeco GEN-III PA-MBE system equipped with valved phosphorus cracker source and Riber RF-plasma nitrogen source (13.56 MHz). Two staged GaP/Si (001) buffer layers were grown by two-staged technique with use of migration enhanced epitaxy (MEE) [6] seeding layer grown by alternate exposure to the group-III and group-V elements followed by the conventional high-temperature MBE growth at 680 ˚C. Amount of the incorporated nitrogen turns out to be sensitive both to the growth temperature and V/III ratio, thus depending on the sample during the dilute nitride layer growth temperature was reduced by 40-100 ˚C, while V/III ratio was reduced down to stoichiometric value. To prevent GaPN exposure on air GaPN / GaP / Si (001) structures were later overgrown with a thin GaP layer. Concentrations of the incorporated nitrogen in the GaPN layer were calculated according to Vegard's law basing on the Θ-2Θ X-Ray diffraction data and lies in the range of 0.4-2.1% depending on the growth condition.

2.1. Role of the silicon substrate miscut

Dimer rows presenting on the Si (001) presents barriers for surface diffusion across the dimer rows and thus highly affects nucleation and growth rate of GaP antiphase domains [7] (see Fig. 1). The usual approach to obtained single domain III-V film is to use vicinal Si (001) with 2-6˚ offcut in <110> direction [8] (see Fig. 1 a). This approach based on special annealing procedures promoting bunching and formation of bilayer of the Si surface steps resulting in anisotropic Si surface which morphology is highly sensitive to the miscut angle and orientation.

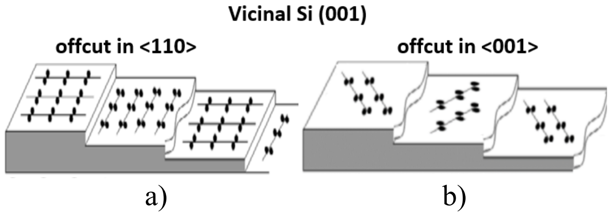

Figure. 1 Schematic representation of Si (001) surface dimers depending on the miscut orientation

In contrast to abovementioned approach we intentionally induce antiphase disorder in GaP buffer layers on Si(001), by using vicinal Si(001) substrates with a 4˚ offcut in <100> direction which corresponds to the dimer rows orientation aligned by ±45˚ relative to the surface step edges (see Fig. 1 b). Both dimer directions on the resulting Si (001) surface is equivalent and thus APDs formation cannot be restricted.

2.2. Dilute nitride heterostructures

On the Fig. 2 one can find SEM image of the surface morphology and corresponding dark-field transmission electron microscopy (DF-TEM) images of the heterostructure cross-sections obtained for the the GaP / Si (001) buffer layer and GaP / GaPN / GaP / Si(001) structure with 0.4% of incorporated nitrogen. To provide contrast between APDs DF-TEM images were taken along the <110> direction using **g**=(002) reflection of GaP [6], [9].

As can be seen from the SEM images surface of both films are formed by the grains surrounded by the sharp surface trenches, however despite lower growth temperature which was chosen for the dilute nitride growth, GaP / GaPN / GaP / Si(001) heterostructure (Fig. 2 b)) demonstrates at least five times larger mean lateral grain size in compare to the GaP/Si buffer layer (Fig. 2 a)). Moreover, for the dilute nitride heterostructure it is possible to distinguish film domain with the predominant orientation occupying a larger surface area and visible with a brighter contrast on the Fig. 2 b).

Mosaic structure of the GaP/Si(001) buffer with an average lateral grain size of 50 nm is clearly seen on the cross-section DF-TEM images on Fig. 2 b). Similar contrast is also visible in the buffer layer region of dilute nitride heterostructure on Fig. 2 d). In addition, in the III-V region of GaP/Si heterointerface region for both samples one can find irregular contrast on smaller-scale (10-15nm) marked by arrows on Fig.2 c). Above mentioned contrast features are visible only under dark-field conditions and thus they indicate presence of APDs. Lateral size of the observed film grains are several times larger than expected surface step size for the given substrate miscut. More likely, that growth of small GaP antiphase islands incoherently nucleated on adjacent Si steps turns out to be mostly suppressed in the beginning at the MEE growth stage – they are visible as a contrast on a small-scale on Fig. 2 b). However use of Si(001) with a 4˚ miscut in <100> direction does not define the predominant GaP orientation and thus inevitably leads to antiphase disordered growth but with a larger size of APD which depends on the growth condition. Resulting antiphase boundaries (APBs) of the APD in the GaP buffer tend to lie vertically close to {110} planes and protrude to the sample surface.

A much lower density of APB is observed in dilute nitride layer and layer grown above for the GaP / GaPN / GaP / Si(001) heterostructure in comparison with GaP / Si(001) (Fig. 2 b) and d)). Thus, one can conclude that APBs kink and self-annihilate in dilute nitride heterostructure at GaPN / GaP interface during their transition into dilute nitride layer. Characteristic lateral grain size on the sample cross-section is consistent with the SEM observation presented in Fig.2 and proves that surface morphology is directly related with presence of the antiphase domain structure in III-V layer. As can be seen APB density is in the GaP buffer layers for both samples are comparable, however number of APBs is decreased dramatically in the GaPN layer.

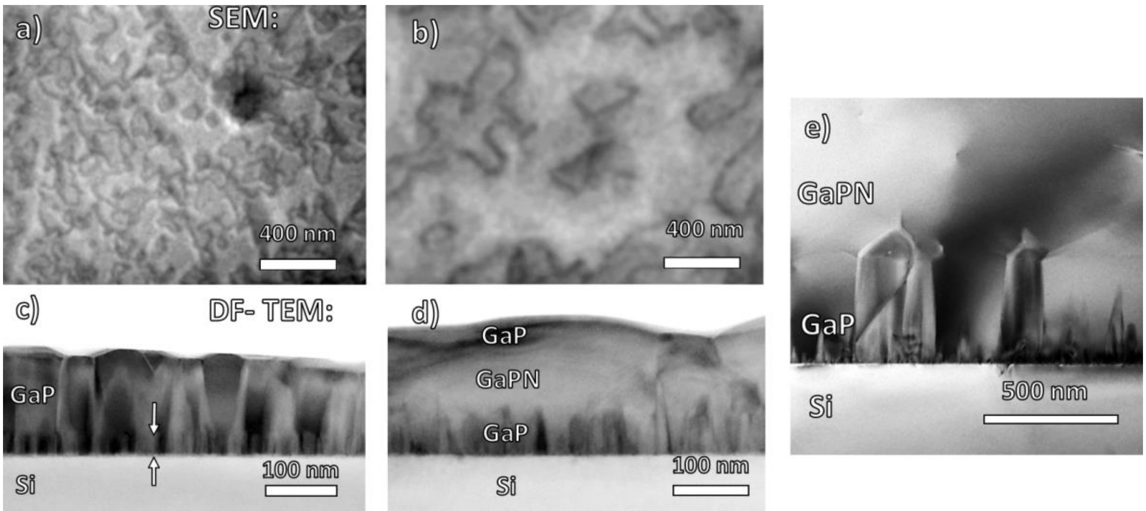

Figure. 2 Corresponding SEM (plane-view on the sample surface) and dark-field TEM (cross-section) images of the III-phosphide/Si heterostructures a)-b) GaP/Si (001), c)-d) GaP/GaPN/GaP/Si heterostructure. e) dark-field TEM image for the GaP/GaPN/GaP/Si heterostructure with 2% of N.

Effectiveness of the APB annihilation turns out to be sensitive to the nitrogen concentration. Thus, dilute nitride and GaP capping layer in the GaP/GaPN/GaP/Si heterostructure with nitrogen content of 1.92% turns out to be completely APD free – see Fig. 2 e). APBs kink and change their orientation from vertical {110} to inclined planes. APBs in the dilute nitride are lying at an angles of 53-55° and 34-36° relative to the (001) indicating their {111} and {112} orientation correspondingly. As a result, APBs are effectively self-annihilate on the distance comparable with lateral size of APD. APB reorientation process can be driven by the difference in formation energy between {111}, {112} and {110} APB planes which changes with addition of N in III-phosphide material - transition to the {112} oriented APBs can be caused by reduction of the kinetic barrier for the APB kinking in dilute nitride layer [9], while the transition to the {111} planes can be related with the observed earlier tendency to the {111} faceted growth of dilute nitrides with high nitrogen content [10].

3. Conclusion

Dilute nitride GaPN/GaP heterostructures with a nitrogen concentration up to the 2.1% have been grown on Si (001) by plasma assisted molecular beam epitaxy (PA-MBE). It is demonstrated that choosing of <001> direction for the Si (001) substrate miscut results in antiphase disordered GaP layer while lateral size of antiphase domain is dependent on the growth condition, not on the miscut angle. By means of transmission electron microscopy (TEM) and scanning electron microscopy (SEM) it was found that density of APDs is dependent on layer composition – transition to the monodomain film starts in dilute nitride GaPN layers even with low nitrogen content of 0.5%. For the GaPN film with 2% of incorporated nitrogen APBs are effectively self-annihilate on the distance comparable with lateral size of APD. GaP capping layers grown above the dilute nitride layer also becomes APD-free. Use of dilute nitride heterostructures allows us to tune antiphase disorder and mean film polarity and thus tune the second order nonlinear optical response by density-controlled arrangement of the APDs in the heterostructure. This result is also very promising for direct integration of high crystalline quality direct band gap GaPN alloys on Si for photovoltaics and light emitting devices.

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