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# Influence of the substrate on the solid-state reaction of ultra-thin Ni film with a $In_{0.53}Ga_{0.47}As$ under-layer by means of Full 3D Reciprocal Space Mapping

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***Abstract*—We studied the solid-state reaction of Ni thin films with InGaAs layers grown on InP or Si substrates. The intermetallics obtained carried an hexagonal structure, but yielded a difference in orientation regarding either the substrates or the annealing temperature.**

## I. Introduction

Among the hot topics driving the developments of new devices, the III-V materials (especially InGaAs alloys) represent serious candidates to replace silicon in elaborating sub 10 nm MOSFET [1]. It was demonstrated that such components exhibit a significant raise of electron mobility throughout the channel and limit the band-to-band tunnel leakage [2]. However, for cost efficiency and manufacturability reasons, these materials must be implemented on 12 inches silicon wafers rather than conventional III-V substrates (for instance InP which diameter does not exceed 4 inches). Consequently, III-V epitaxial layer grown onto silicon wafer is part of the main challenges due to the large unit cell parameter mismatch. In parallel, several processes, such as gate stack, source and drain contacts..., must be taken into account and separately developed.

Thus, an ultra-low contact resistivity ($10^{-9}$ $\Omega.cm^2$) is mandatory to reach entire device performances and will be therefore one of the key challenges for advanced node CMOS development. Historically, the developments of low-resistive contact have been a fine mechanism understanding in order to control the solid-state reaction (SSR) of a metal film with the Si substrate and finally the process and its related contact resistivity. There have been also intense investigations on silicide technology (e.g. $TiSi_2$, $CoSi_2$ and NiSi) [3] over more than 25 years, leading to fundamental understanding on the peculiar microstructure observed for these compounds obtained by SSR [4], [5]. On the contrary, the knowledge turns out to be limited when it comes to ohmic metal contacts on III-V materials for MOSFET applications. For such alloys, salicide-like technology has been recently developed and it have been found that Ni-$In_xGa_{1-x}As$ alloy is a promising material for self-aligned metal source/drain (S/D) of $In_xGa_{1-x}As$ n-MOSFETs [6], [7].

Thus, this paper aims to report the study carried out from the solid state reactions of Ni with InGaAs epitaxially grown on various substrates. We then focus on phase formation and the exhibited texture of these Ni-InGaAs intermetallic layers. We finally point out the influence of InGaAs crystalline quality when directly performed on silicon wafer and refer to the layer obtained on InP.

## II. Experimental part

The samples were prepared by RF-PVD of Ni on $In_{0.53}Ga_{0.47}As$ grown on InP or Si substrates. The metallic layers are capped with a TiN thin film to prevent atmosphere contamination. Full description of the samples is given in figure 1. The samples were annealed at different temperatures during 60 s and under $N_2$ flow using Rapid Thermal Annealing (typically 250 °C, 350 °C, 450 °C and 550 °C).

Fig. 1. Scheme of the as-deposited stacks of the prepared samples: (a) TiN/Ni/InGaAs/InP, (b) TiN/Ni/InGaAs/GaAs/Si.

X-ray diffraction experiments have been performed on the BM02 beamline at ESRF. They were done at an energy of 9 keV using a 6-circles goniometer. We will refer in this abstract to the $\chi$, $\phi$, and $2\theta$ angles as the angles of a conventional 4-circles diffractometer. A 2D pixel detector was used to collect the diffracted beams. Such detector allows collecting data over a relatively wide range of the reciprocal space at one time and data treatment was performed with the homemade DEVA software [8]. The setup of the diffractometer and detector was such that we were capable of measuring, at a given tilt angle of the sample ($\phi$), a range of 30° of $2\theta$ during a one-shot-measurement. Two values of $\chi$ tilt were chosen to cover a range going from 0° to about 70° depending on the $2\theta$ position, and multiple measure steps were added by rotating the sample around it's normal ($\phi$) to obtain full pole figures over 360°.

## III. Results

The reaction of Ni on GaAs have been described by Guivarch et al. [7], showing the formation of the intermetallic

TABLE I. SUMMARY OF THE ORIENTATIONS OBSERVED FOR NI/INGAAS/INP AND NI/INGAAS/SI. EACH SYMBOL CORRESPOND TO AN ORIENTATION IN FIGURE 3.

| Symbol | N° | Orientation |
|---|---|---|
| ○ | 1 | $(1\,0\,0)_{\mathrm{NiInGaAs}}\|\|(0\,0\,1)_{\mathrm{InGaAs}}$ ; $[0\,0\,1]_{\mathrm{NiInGaAs}}\|\|[0\,1\,\bar{1}]_{\mathrm{InGaAs}}$ |
| ● | 2 | $(1\,0\,0)_{\mathrm{NiInGaAs}}\|\|(0\,0\,1)_{\mathrm{InGaAs}}$ ; $[0\,0\,1]_{\mathrm{NiInGaAs}}\|\|[0\,\bar{1}\,\bar{1}]_{\mathrm{InGaAs}}$ |
| ▲ | 3 | $(1\,0\,1)_{\mathrm{NiInGaAs}}\|\|(0\,0\,1)_{\mathrm{InGaAs}}$ ; $[\bar{2}\,\bar{1}\,2]_{\mathrm{NiInGaAs}}\|\|[0\,\bar{1}\,\bar{1}]_{\mathrm{InGaAs}}$ |
| △ | 4 | $(1\,0\,1)_{\mathrm{NiInGaAs}}\|\|(0\,0\,1)_{\mathrm{InGaAs}}$ ; $[\bar{2}\,\bar{1}\,2]_{\mathrm{NiInGaAs}}\|\|[0\,1\,\bar{1}]_{\mathrm{InGaAs}}$ |

with an hexagonal structure, in coherence with the well-known NiAs structure. In case of Ni/InGaAs SSR, the chemical composition and texture of the intermetallic has been discussed in only few papers. For instance, Ivana et al. and P. Shekhter et al [9], [10] describe the hexagonal structure of the NiInGaAs with the 4:1:1:2 relative composition. Zhang et al. [11] found a similar composition ratio of 51:12:14:23. P. Shekhter et al [10] also found the following orientation for the intermetallic NiInGaAs : $(1\,0\,0)_{\mathrm{NiInGaAs}}||(0\,0\,1)_{\mathrm{InGaAs}}$ ; $[0\,0\,1]_{\mathrm{NiInGaAs}}||[0\,1\,\bar{1}]_{\mathrm{InGaAs}}$ (defined as orientation 1 in Table I). From the multiple 2D datasets we measured by XRD, two kinds of information have been extracted: i) De-textured 2theta diffractograms (not shown here) were obtained by summing over $\chi$ and $\phi$ the Debye rings of all the 2D snapshots; ii) pole figures (see for instance figures 3, 4 and 5) were reconstructed for several hkl reflections (or $2\theta$ angles). From the indexation of these diffractograms and from the symmetry of the pole figures, we identified clearly the intermetallic phases that appear during SSR with an hexagonal structure. However, our results exhibit some discrepancies with the works cited previously, especially concerning the texture of the intermetallic, as shown hereafter.

### A. Ni on InGaAs on Si substrate

For the Ni/InGaAs/Si, no reaction occurs up to 250 °C annealing temperature. At 350 °C, the intermetallic phase is appearing and the Ni is fully consumed. This phase is still observed at 450 °C with similar pole figures at both temperatures. In agreement with the results published by P. Shekhter et al. [10] and thanks to these pole figures, we identify the occurrence of an hexagonal structure. Thus far, we identify two out-of-plane orientations of the hexagonal phase instead of one in [10] and also variants of in-plane orientations for each out-of-plane orientation instead of one compared to the previous reference. All the observed orientations of the hexagonal structure is given in Table I and a stereographic projection with the corresponding orientation for each pole is given in Figure 2.

Actually, in the case of Ni deposited on InGaAs/Si we observe multiple poles for the pole figure at $2\theta$= 29.75° (Figure 3). Poles at $\chi$=33° and $\chi$=65° correspond to the projection of $(1\,0\,1)$ plane of the intermetallic phase on the $(1\,0\,0)$ plane along two in-plane directions (see orientation 1 and 2 in Table I) and the poles at $\chi$=49° and $\chi$=67° correspond to the projection of $(1\,0\,1)$ on the $(1\,0\,1)$ planes along two in-plane directions of the hexagonal structure (orientation 3 and 4). The fact that there are 2 sets of poles situated at $\chi$=33° and $\chi$=65° but at a different $\phi$ angle implies that they correspond to the same $(1\,0\,0)$ orientation of the intermetallic hexagonal structure but with the existence of a second in-plane orientation along the $[0\,\bar{1}\,\bar{1}]$ direction of InGaAs.The same goes for the out-of-plane orientations (3 and 4), where the intermetallic hexagonal structure is aligned along two equivalent directions

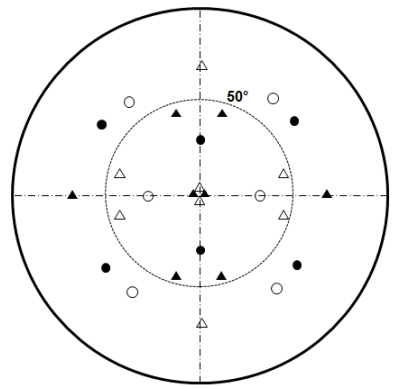


Fig. 2. Stereographic projection of the $(1\,0\,1)$ planes of the intermetallic hexagonal structure for the different orientations given in Table I.

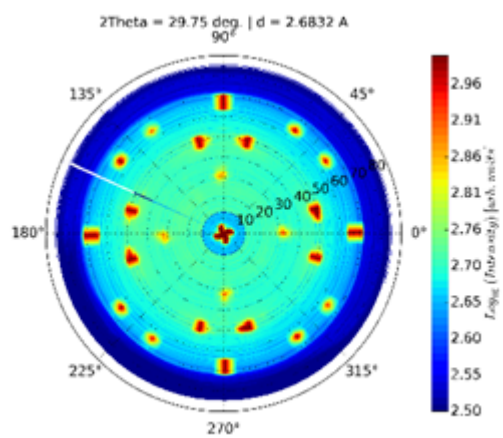


Fig. 3. X-ray diffraction pole figures of Ni/InGaAs/Si sample (after a 450 °C RTA annealing). The fixed $2\theta$ angle was 29.75° corresponding to the intermetallic $(1\,0\,1)$ reflection. The concentric dashed circles correspond to the $\chi$ angle landmarks with a 10° step.

$[0\,1\,\bar{1}]$ and $[0\,\bar{1}\,\bar{1}]$. In summary, for the Ni/InGaAs/Si substrates, the intermetallic shows the 4 orientations described in Table I and it keeps these orientations even at higher temperatures.

### B. Ni on InGaAs on InP substrate

For Ni/InGaAs/InP, the presence of such orientation was expected providing that $[0\,1\,\bar{1}]$ and $[0\,\bar{1}\,\bar{1}]$ are equivalent directions in the zinc blende system of InGaAs. But we observed different result (Figure 4); since only 3 orientations are identified (orientation 1, 3 and 4 in Table I). The second $(1\,0\,0)$ in-plane orientation did not show up during the annealing and growth of the intermetallic.

When the sample is annealed at 550 °C, further orientation change occurs. The hexagonal structure loses one of its

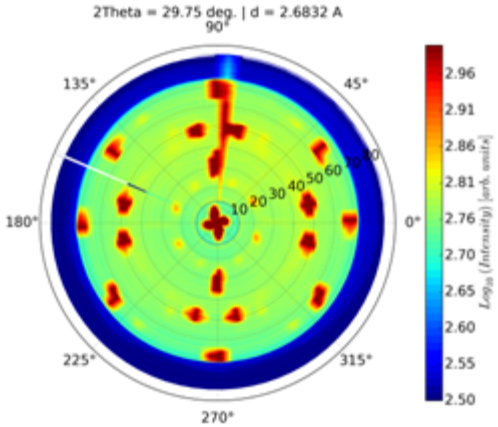


Fig. 4. X-ray diffraction pole figures of Ni/InGaAs/InP sample (after a 450 °C RTA annealing). The fixed $2\theta$ angle was 29.75° corresponding to the intermetallic $(1\,0\,1)$ reflection. The concentric dashed circles correspond to the $\chi$ angle landmarks with a 10° step.

out-of-plane orientations (orientation 1) and another in-plane orientation (orientation 4). Thus, the so-formed intermetallic yields only one orientation at 550 °C which is orientation 3 (Figure 5).

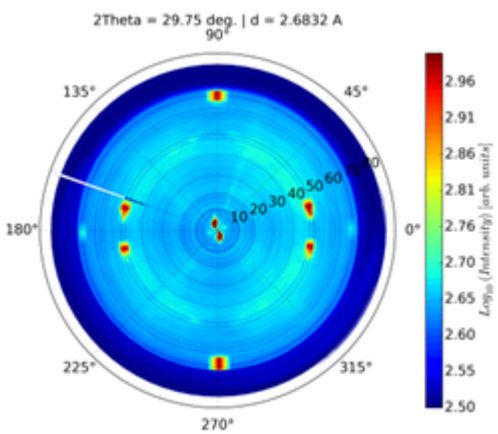


Fig. 5. X-ray diffraction pole figures of Ni/InGaAs/InP sample (after a 550 °C RTA annealing). The fixed $2\theta$ angle was 29.75° corresponding to the intermetallic $(1\,0\,1)$ reflection. The concentric dashed circles correspond to the $\chi$ angle landmarks with a 10° step.

## IV. Discussion

We demonstrate that the intermetallic obtained by SSR of a Ni layer with a InGaAs/InP substrate exhibits an hexagonal structures with two out-of-plane orientations. Yet, there are two equivalent directions along InGaAs,$[0\,1\,\bar{1}]$ and $[0\,\bar{1}\,\bar{1}]$. These directions are thermodynamically equivalent, so it is expected that the intermetallic would grow along these two directions, which is not the case as no corresponding poles appear on the pole figure. Further, we demonstrated that the intermetallic formed on InGaAs/Si yields the four orientations along in-plane and out-of-plane directions. This particular evolution of the pole figure may be explained as the following : the InP substrates might yield a low angle miscut that prevents $(1\,0\,0)$ planes from being completely parallel to the sample. Thus the substrate, and the deposited InGaAs layer, loose their four-fold symmetry and may lead to the formation of the intermetallic along some preferred directions that could be explained by epitaxial or axiotaxial relationship [5] . This point will need to be further discussed.

## V. Conclusion

We have observed that the Ni-InGaAs intermetallic compound can yield multiple orientations in-plane and out-of-the-plane. These orientations depend not only on the substrate but also on the temperature of annealing (e.g. intermetallic agglomeration, etc.). Such difference of orientations may have impact on the electrical properties of these compounds. Other investigations concerning X-Ray Diffraction in-situ studies of the intermetallic and chemical composition determination using Atomic Probe Tomography are currently under progress along with a novel study on another intermetallic compound formed by SSR of Ni-based-alloy on InGaAs.

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