



# Epitaxial formation and electrical properties of Ni germanide/Ge(110) contacts

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## ARTICLE INFO

Available online 11 October 2013

### Keywords:

Germanide  
Nickel  
Epitaxial growth  
Orientation  
Schottky barrier height  
Contact

## ABSTRACT

We have investigated the epitaxial formation and electrical properties of Ni germanide/Ge(110) contacts. X-ray diffraction and transmission electron microscopy measurements have revealed that  $\text{Ni}_5\text{Ge}_3$  and NiGe layers are epitaxially formed on a Ge(110) substrate after annealing at 200–350 °C. An epitaxial  $\text{Ni}_5\text{Ge}_3$  layer is formed after annealing with the relationships  $\text{Ni}_5\text{Ge}_3(001)//\text{Ge}(110)$  and  $\text{Ni}_5\text{Ge}_3[311]//\text{Ge}[001]$ . We found that the orientation relationship between an epitaxial NiGe layer and Ge(110) substrate depends on the annealing temperature. When annealed at 300–350 °C, the orientation relationship is  $\text{NiGe}(100)//\text{Ge}(110)$  and  $\text{NiGe}[001]//\text{Ge}[001]$ , while at 200–230 °C, the relationship is  $\text{NiGe}(102)//\text{Ge}(110)$  and  $\text{NiGe}[010]//\text{Ge}[001]$ . We demonstrate that the Schottky barrier height of the epitaxial NiGe(100)/Ge(110) contact is as low as 0.44 eV, as estimated from the current density–voltage characteristics, while that of polycrystalline NiGe/Ge(001) is 0.55 eV.

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## 1. Introduction

As integrated circuits are scaled down, the 3-dimensional (3-D) fin structure is an increasingly promising candidate for future highly scaled metal-oxide-semiconductor field effect transistors (MOSFETs) due to its excellent robustness to the short-channel effect and high carrier mobility [1]. Meanwhile, germanium (Ge), as one of the most attractive channel materials, has a higher mobility for both electrons and holes than silicon [2]. Therefore, combining the advantages of the 3-D fin structure and Ge channels, Ge FinFETs are expected to be applicable for future ultra-large-scale integrated circuits. Nevertheless, there are various challenges for the adoption of Ge FinFETs into sub-22-nm technology generations or beyond. One important issue is the development of metal/Ge contacts for crystalline orientations other than Ge(001).

Among the leading germanide contact layers, nickel monogermanide (NiGe) is of great interest because of its low resistivity (approximately 22  $\mu\Omega\cdot\text{cm}$ ), low formation temperature (approximately 350 °C), the final phase in Ni–Ge binary alloy system, and low Ge consumption for germanide formation [3]. These advantages satisfy the requirements of Ge planar MOSFETs as well as Ge FinFETs. However, the strong anisotropic properties of NiGe, with a primitive orthorhombic MnP-type structure ( $a = 5.381 \text{ \AA}$ ,  $b = 3.428 \text{ \AA}$ ,  $c = 5.811 \text{ \AA}$ ), suggest that it is difficult to form a uniform crystalline structure of NiGe on various orientations of Ge for practical application in Ge FinFETs. Most of the previous works related to NiGe have focused on amorphous Ge [4], Ge(001) [5], and Ge(111) [6]. Peng et al. have investigated the evolution of the sheet resistance

and strain of NiGe films on Ge(110) as a function of annealing temperature [7]. However, few works have studied the crystalline structure and interface electrical properties of the Ni germanide/Ge(110) contact. Therefore, the crystalline structure of NiGe formed on Ge(110) substrates other than Ge(001) requires clarification.

To reduce the contact resistivity in MOSFET, it is necessary to lower the Schottky barrier height (SBH) of the metal/semiconductor interface. However, in metal/n-Ge contacts, the SBH is high (above 0.5 eV) regardless of the metal due to the Fermi level pinning phenomenon [8]. In fact, the SBH of polycrystalline NiGe/Ge(001) contacts is generally as high as 0.61 eV [9], although there are few reports of the electrical properties of Ni germanide/Ge(110) contacts.

In this study, we investigated the details of the formation and crystalline structure of Ni germanides on a Ge(110) substrate. We also investigated the electrical properties of NiGe/Ge(110) contacts. Our results reveal that the orientation of epitaxial NiGe could be controlled by the annealing temperature. Furthermore, the epitaxial NiGe/Ge(110) contact has a lower SBH than the polycrystalline NiGe/Ge(001) contact.

## 2. Experiment

The substrates used were n-type Ge(110) and Ge(001) wafers with a resistivity of 0.1–10  $\Omega\cdot\text{cm}$ . The Ge wafers were cleaned by five repetitions of dipping into a diluted HF solution and rinsing in deionized water to remove contaminants and the surface oxide layer. After wet chemical cleaning, the Ge wafer was introduced into an ultra-high vacuum chamber with a base pressure below  $2.5 \times 10^{-5} \text{ Pa}$ , and thermal cleaning was performed at 500 °C for 30 min in the chamber. A 20- or 50-nm-thick-Ni layer was deposited by e-beam evaporation at room

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temperature. Next, samples were exposed to the atmosphere and annealed in a furnace chamber at 200–550 °C for 30 s to 120 min in  $N_2$  ambient. To investigate the electrical properties, the top Al electrode was deposited in a conventional chamber by resistance heating to prepare Schottky diodes, and the mesa structure was then formed by etching in acid solution ( $H_3PO_4:CH_3COOH:HNO_3 = 92:7:1$ ) for 5 min. Lastly, a backside Al electrode was formed as well as the top electrode.

Grazing-angle X-ray diffraction (XRD) ( $2\theta$  scan,  $\omega = 1.626^\circ$ ), and out-of-plane XRD ( $2\theta/\omega$  scan) using a Cu  $K\alpha$  source were performed to observe the crystalline structure of the Ni germanide layers. Cross-sectional transmission electron microscopy (XTEM) and transmission electron diffraction (TED) using a JEM2010F apparatus (JEOL) were conducted to reveal the morphology and crystalline structure of the Ni germanide layers with respect to the Ge substrate. The operating voltage of TEM observation was 200 kV. Samples for the TEM observation were prepared by using Ar ion milling. Combined with XRD, a standard four-point probe was used to identify the formation of the first phase. The current density–voltage (J–V) characteristics of Ni germanide/Ge Schottky diodes were measured to estimate the SBH of the Ni germanide/Ge interfaces.

### 3. Results and discussion

#### 3.1. Crystalline structure of Ni germanides formed on Ge(110)

We examined various annealing temperatures for the germanidation of Ni on Ge(110) substrates. Fig. 1(a) shows the typical results for the grazing-angle XRD ( $2\theta$ -scan) measurements of the Ni(50 nm)/Ge(110)

samples annealed at 200–550 °C for 30 s–75 min. For the samples annealed at 450 °C and 550 °C (*not shown*), only the diffraction peaks related to NiGe were observed, which is consistent with the results reported by Peng et al.[7]. These peaks can be assigned to the lattice planes of NiGe(111), (210), (112), (211), (103), (020), (013), (121), (311), (122), and (123). This result indicates the formation of a polycrystalline phase of NiGe. On the other hand, for samples annealed at temperatures below 350 °C (only ~350 °C data shown), we can observe no diffraction peaks related to the lattice planes of NiGe (112), (103), (020), (013), (122), and (123), and the peaks related to the reaction products are weaker than those of the samples annealed at temperatures above 450 °C. Considering that XRD  $2\theta$  measurements generally enable us to detect powder-like polycrystalline structures with random orientations, it is suggested that a highly oriented Ni germanide layer forms after annealing at 350 °C for 30 s.

Regarding the sample annealed at a lower temperature of 200–230 °C (only the ~220 °C data are shown unless specified otherwise), only three diffraction peaks are related to NiGe(111), (210), and (211), and the relative intensities are also weak, similar to the sample annealed at 350 °C. This result strongly suggests that the NiGe layer is also preferentially oriented.

To investigate the orientation of the NiGe layers formed under various annealing conditions, out-of-plane XRD ( $2\theta/\omega$ -scan) was also conducted to determine the lattice planes of Ni germanides parallel to the Ge(110) surface, as shown in Fig. 1(b). We found that the orientation of the NiGe layer strongly depends on the annealing temperature. For the samples annealed at 450 °C and 550 °C, various lattice planes of NiGe(200), (111), (112), (103), and (122) are observed. However, only the lattice planes parallel to the Ge(110) surface, NiGe(400) and NiGe(02), are observed for samples annealed at 200–230 °C and 350 °C, respectively. The NiGe(111), (112), (103), and (122) planes are restricted.

The TED patterns shown in Fig. 2(a) and (b) reveal the detailed orientation relationship between Ni germanide and the Ge(110) substrate. In the case of annealing at 200–230 °C, the orientation relationship of the NiGe layer is NiGe(102)//Ge(110), NiGe[010]//Ge[001], and NiGe[201]//Ge[110], while in the case of annealing at 300–350 °C, this relationship is NiGe(100)//Ge(110), NiGe[001]//Ge[001], and NiGe[010]//Ge[110]. It should be noted that we confirmed the independence of the orientation relationship on the thickness of the as-deposited Ni layer when annealing at 300–350 °C. Thus, the differences in the orientation relationships depending on annealing temperature should be related to the phase transformation mechanisms, as discussed later.

Before discussing the phase transformation mechanisms for annealing below 350 °C, we describe the formation and orientation of the precursor phase  $Ni_5Ge_3$ . The sheet resistance of Ni germanide on Ge(110) as a function of the annealing time is shown in Fig. 3. The annealing temperature was 220 °C. Although there is a complex peak overlap between Ni (PDF#65-2865),  $Ni_5Ge_3$  (PDF#24-0449), and NiGe (PDF#65-1478) in the XRD results for the 220 °C-annealed sample, the existence of  $Ni_5Ge_3$  is proven by the increase in the sheet resistance of germanide, as  $Ni_5Ge_3$  has a higher resistivity than Ni and NiGe [10]. Additionally, we do not observe other diffraction peaks corresponding to  $Ni_5Ge_3$  in Fig. 1(a) except the peak at 44.7°, which suggests that a  $Ni_5Ge_3$  layer is grown epitaxially or in a highly oriented manner on Ge(110). The out-of-plane XRD (Fig. 1(b)) and TED (Fig. 2(a)) results further indicate that the orientation relationship between  $Ni_5Ge_3$  and the Ge(110) substrate is  $Ni_5Ge_3(001)//Ge(110)$ ,  $Ni_5Ge_3[311]//Ge[001]$ , and  $Ni_5Ge_3[3\bar{3}1]//Ge[110]$ . Additionally, we found that the first-phase  $Ni_5Ge_3$  of the sample annealed at 350 °C is epitaxially grown, and the orientation relationship is same as that of 220 °C-annealed samples (*not shown*).

On the other hand, we observed the simultaneous formation of  $Ni_5Ge_3$  and NiGe in the Ni/Ge(110) system after annealing at 200–230 °C, which is consistent with the results for Ni/amorphous-Ge [4] and Ni/polycrystalline-Ge [11] systems. In the cross-sectional TEM images of Ni/Ge(110) samples annealed at 220 °C, Fig. 4(a) shows that there are three layers after annealing for 10 min. These three layers

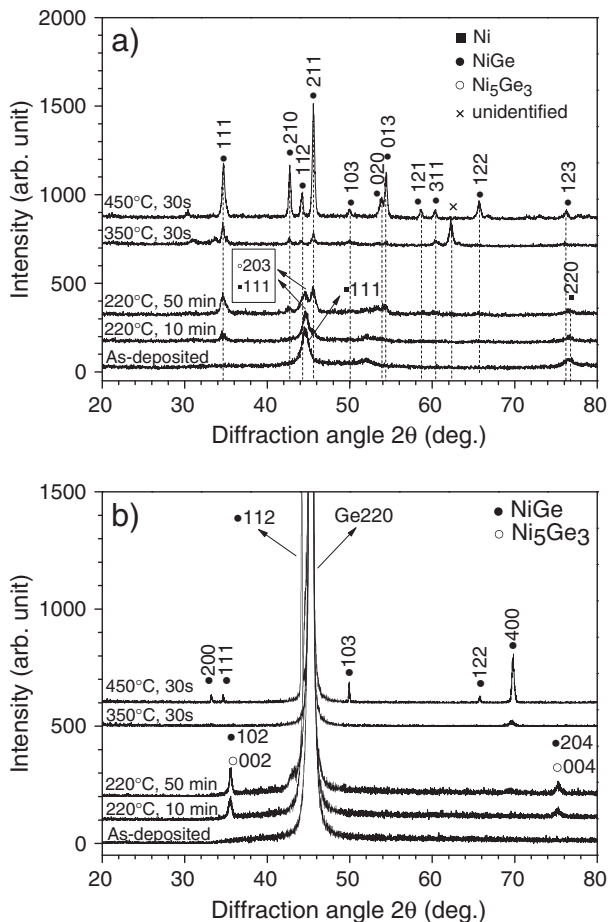


Fig. 1. XRD profiles of the Ni/Ge(110) system annealed at 200–550 °C for 30 s–50 min: (a) grazing-angle XRD ( $2\theta$  scan,  $\omega = 1.626^\circ$ ) and (b) out-of-plane XRD ( $2\theta/\omega$  scan).

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