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主　論　文　の　要　旨

論文題目 Control of Crystalline Structures and Electrical Properties of Metal Germanide/Ge Contact
（金属ジャーマナイド/Ge接合における結晶学的構造および電気的特性の制御）

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論　文　内　容　の　要　旨

We have investigated the epitaxial formation and electrical properties of Ni germanide/Ge contacts for the application of future highly scaled germanium-based metal-oxide-semiconductor field effect transistor (Ge-based MOSFET). Epitaxial NiGe layers with atomically flat and uniform interface have been explored not only on Ge(001) substrate but also on Ge(110) substrate. Those epitaxial NiGe layers exhibit a potential application in the highly scaled Ge-based MOSFET because of their promising thermal stability and morphology stability. On the other hand, we have successfully demonstrated the alleviation of Fermi level pinning (FLP) by controlling the crystalline structures of NiGe layers. Those works give rise to a new hint that controlling the crystalline structure of metal layers enables one to control the Schottky barrier height (SBH) of metal/Ge contacts, and the origin of FLP is not due to an intrinsic factor, e.g., metal induced gap states, but due to extrinsic factors such as dangling bonds and disorders at the metal/Ge interfaces.

In chapter 3, we focus on the epitaxial formation of NiGe layers on Ge(110) substrate. A partially epitaxial NiGe layer has been formed by solid phase reaction. Of interesting, the orientation relationship of the epitaxial NiGe domain with Ge(110) substrate could be modulated by the surface condition of Ge substrate before Ni deposition. For the samples with a clean surface, the Ni deposition is conducted on a clean Ge substrate without any contaminations or native oxide layer, the orientation relationships are NiGe(100) // Ge(110)

and NiGe[001] // Ge[001], while those are NiGe(102) // Ge(110) and NiGe[010] // Ge[001] for the samples with an ultra-thin native oxide interlayer between the as-deposited Ni layer and Ge(110) substrate.

We also found that the growths of epitaxial and polycrystalline NiGe domains depend on the annealing temperature. For the samples with clean surface, the growth of the epitaxial domain is coincident with that of the polycrystalline domain. The growths of polycrystalline and epitaxial domains are restrained at an annealing temperature lower than 250 °C, and they grow together at an annealing temperature higher than 300 °C. For the samples with an ultra-thin native oxide interlayer, a low annealing temperature of 200 °C favors the epitaxial growth, which is replaced by polycrystalline growth at a high annealing temperature of above 275 °C.

Chapter 4 is concerned with the epitaxial formation of NiGe layer on Ge(001) substrate. An epitaxial NiGe layer with an atomically flat and uniform interface is achieved by a 2-steps deposition method (reactive deposition + subsequent room temperature deposition), assisted with solid phase reaction method. And the orientation relationship between the epitaxial NiGe layer and Ge(001) substrate is NiGe(111) // Ge(001) and NiGe[$0\bar{1}1$] // Ge[110].

We also discussed this epitaxial formation in detail. For reactive deposition method only, an epitaxial NiGe layer could be formed, but the thickness of the epitaxial layer is limited to below 22 nm. Once over this critical thickness, the polycrystalline NiGe formation occurs. Moreover, the interface between the epitaxial NiGe layer and Ge(001) substrate is a little rough. Those issues have been solved by the 2-steps deposition plus solid phase reaction as mentioned in the last paragraph.

Here, we demonstrate the promotion of epitaxial formation by the 2-steps deposition in detail. At first, a thin epitaxial NiGe layer is formed by reactive deposition. Then, an additional Ni layer is deposited on the initially formed epitaxial NiGe layer at room temperature. Subsequently, the complete germanidation is performed by post annealing, during the germanidation, the initially formed epitaxial NiGe layer plays a role of single crystal seed to enhance the epitaxial formation.

The reason why the polycrystalline formation is suppressed by the 2-steps deposition is also clarified. At first, we describe the polycrystalline formation when the thickness of reactive deposited NiGe is over the limitation of epitaxial formation. Ge atoms are found to be the dominant diffusion species during the reactive deposition, it means that the crystallization

front is on the surface of the formed NiGe layer, rather than the interface between the formed NiGe layer and Ge(001) substrate. On the other hand, the 2-Dimensional growth would transform to 3-Dimensional growth with increase in the thickness of the reactively deposited NiGe layer, and the surface would become rough. Relying on this rough surface, the heterogeneous nucleation is easy to happen, thus the polycrystalline formation is induced.

However, for the 2-steps deposition sample, during the subsequent germanidation process, the dominant diffusion species are changed to be Ni atoms, and the crystallization front is also changed to the interface of NiGe/Ge. In this situation, the heterogeneous nucleation does not happen, and the initially formed epitaxial NiGe plays a role of single crystal seeds to induce the epitaxial formation, thus an epitaxial NiGe layer with high crystalline quality is achieved.

Chapter 5 reveals the electrical properties of various NiGe/n-type Ge contacts with different crystalline structures, and a summary of the effect of crystalline structure on the electrical properties is given. We found that the SBH of NiGe/Ge contact could be modulated by controlling the crystalline structures of NiGe layer. Compared with the polycrystalline NiGe/n-type Ge contacts, the SBH is reduced by as large as 0.15 eV for the epitaxial NiGe(100)/n-type Ge(110) contact. However, for an epitaxial NiGe(111)/n-type Ge(001) contact, the estimated SBH has no difference from that of polycrystalline NiGe/n-type Ge contact, even though the epitaxial NiGe layer with good crystalline quality is formed. This distinctive modulation of SBH could not only be explained by MIGS model. We consider this modulation of SBHs is a consequence of the variation of the density of the interface states induced by the extrinsic factors, such as the dangling bonds and defects. And our results give us a hint that the modulation of the SBH by controlling the crystalline structures is possible. To realize further low SBH, a completely atomic matching is required.