Microstructure characterization of Cu_3Ge/n-type GaAs ohmic contacts

M. O. Aboelfotoh, S. Oktyabrsky, and J. Narayan
Department of Materials Science and Engineering, North Carolina State University, Raleigh, North Carolina 27695-7916

J. M. Woodall
School of Electrical Engineering, Purdue University, West Lafayette, Indiana 47907-1285

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We have systematically investigated the microstructure and interface structure of ϵ_1-Cu_3Ge films on n-type (001)GaAs substrates using high-resolution transmission electron microscopy (HRTEM). The copper-germanium alloy forms ohmic contacts on n-type GaAs over a wide range of Ge concentrations from 5 to 40 at. % with a minimum contact resistivity of 6.5×10^{-7} Ω cm^2 on (001) GaAs (doping concentration $\sim1.0\times10^{17}$ cm^{-3} in the Ge concentration range 25–30 at. %). The cross-sectional HRTEM results show that a low-resistivity ϵ_1-Cu_3Ge phase is formed at 25 at. % Ge concentration, and above this concentration excess Ge precipitates out between the ϵ_1-Cu_3Ge grains and the GaAs substrate. Ge grows epitaxially with the GaAs substrate, but it is not present as a continuous interfacial layer. The interface between ϵ_1-Cu_3Ge and GaAs is quite sharp, with no secondary phases. The secondary ion mass spectrometry results indicate interdiffusion between Ge and Ga, which results in highly doped regions by the incorporation of Ge atoms into the GaAs on the Ga sites. The current transport by the tunneling of the carriers through this doped region provides the low-resistance ohmic behavior of the contact. From correlations between the microstructure and the properties of the heterostructure we deduce the optimum concentration of Ge to be 30 at. % for formation of low-resistance ohmic contacts.

INTRODUCTION

The eutectic-based AuGeNi contacts are commonly used as ohmic contacts to n-type GaAs with a specific contact resistivity, ρ_c, in the 10^{-6} Ω cm^2 range.[1] However, these alloyed contacts are generally electrically unstable when annealed at high temperatures (>400 °C) due to the morphological and metallurgical changes at the interface.[2,3] To overcome these problems, nonalloyed low-resistance ohmic contacts of Ge/Pd/n-type GaAs have been proposed.[4] This contact scheme involves the deposition of a metal layer, Pd, onto which a layer of amorphous Ge is then deposited. It was shown that, after annealing at 325 °C for 30 min, the entire layer of Pd is consumed in the formation of a palladium germanide layer through which excess Ge is transported to grow epitaxially on the GaAs substrate. However, annealing the Ge/Pd contacts at temperatures higher than 325 °C after contact formation was always found to result in an increase in specific contact resistivity.[5]

Recently, we have found[6] that the ϵ_1-Cu_3Ge compound forms an ohmic contact to n-type GaAs with a specific contact resistivity of $\rho_c=6.5\times10^{-7}$ Ω cm^2 at room temperature, considerably lower than that reported for AuGeNi[1] and Ge/Pd[5] contacts on n-type GaAs with similar doping concentrations (1×10^{17} cm^{-3}) and for molecular-beam epitaxially grown Ge($n=8\times10^{19}$ cm^{-3})/GaAs(1×10^{17} cm^{-3}) contacts ($\rho_c=3\times10^{-6}$ Ω cm^2).[7] We have also found[6] that the ϵ_1-Cu_3Ge contacts are electrically stable during annealing at temperatures up to 450 °C after contact formation, in contrast to the Ge/Pd contacts,[5] and that n-channel GaAs metal-semiconductor field-effect transistors using the ϵ_1-Cu_3Ge ohmic contacts exhibit a considerably higher transconductance (145 mS/mm) compared to devices with AuGeNi and Ge/Pd contacts. In an attempt to understand the ohmic contact formation mechanism in the Ge/Cu/n-type GaAs system, we have examined the microstructure and the morphology of the interfaces between contacts formed with Ge thickness just equal to and in excess of that required for ϵ_1-Cu_3Ge formation on the GaAs substrate using high-resolution transmission electron microscopy; in this article we report results of such a study.

EXPERIMENT

The Cu_3Ge contacts were formed by a sequential deposition of Cu (122 nm) and Ge (78 nm) layers on 1-μm-thick n-type GaAs epitaxial layers (doped with Si to a concentration of 1×10^{17} cm^{-3}) at room temperature, followed by an anneal. The epitaxial layers were grown by molecular-beam epitaxy on semi-insulating (001)GaAs substrates. The substrates were chemically cleaned in a solution of HCl:H_2O (1:1 by volume) until they were completely hydrophobic. The substrates were inserted into the deposition chamber immediately after chemical cleaning. The Cu and Ge layers were deposited using electron-beam evaporation in a vacuum 10^{-7} Torr at a rate of 1 nm/s. In order to investigate the effect of the presence of excess Ge, contact layers with Ge concentration in a range up to 40 at. % were also prepared by the sequential deposition of Cu and Ge layers at room temperature with a subsequent anneal. For a given Ge concentration the thickness of the Cu and Ge layers was determined by assuming a bulk density for Cu and Ge. Annealing at 400 °C for 30 min was carried out *in situ* in the deposition chamber at a pressure of 5×10^{-7} Torr. The Ge/Cu contacts were found to remain ohmic over a wide range of Ge concentration extending from 15 to 40 at. %. The value of a specific

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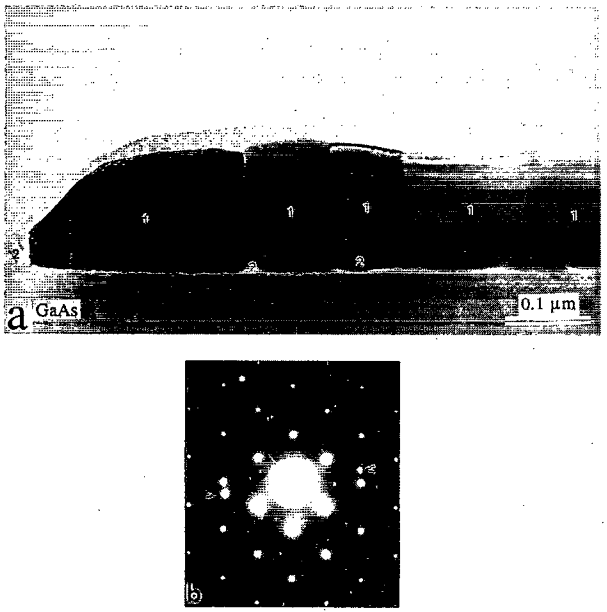

FIG. 1. (a) Cross-sectional TEM micrograph showing the general microstructure of the Cu_3Ge film on a (001)GaAs substrate. ϵ_1-Cu_3Ge and Ge grains are denoted by 1 and 2, respectively. (b) Corresponding SAD pattern showing the [110] zone axis pattern of GaAs and the strongest {111}-type spots of a ϵ_1-Cu_3Ge grain (denoted by arrows).

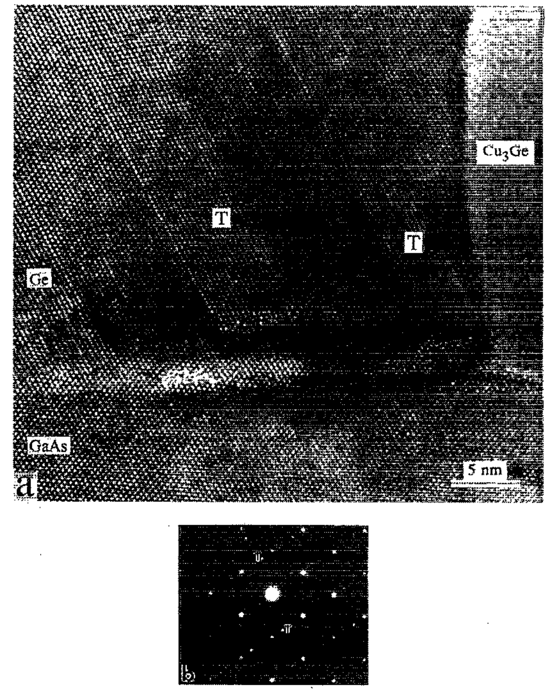

FIG. 2. (a) High-resolution TEM image showing the interface between a large epitaxial Ge grain and the GaAs substrate. Typical twin lamella are denoted by T. Arrow indicates an amorphous pocket at the interface. (b) Corresponding SAD pattern showing the [110] zone axis pattern of GaAs and Ge (unresolved) with typical twin spots (denoted by T).

contact resistivity, $\rho_c=6.5\times10^{-7}\ \Omega\ cm^2$, was measured by a transmission line method for the ϵ_1-Cu_3Ge contact (30 at. % of Ge) on n-GaAs($1\times10^{17}\ cm^{-3}$).[6] Therefore, this alloy provides low-resistance reliable ohmic contacts to n-type GaAs. The microstructure and the morphology of the interfaces were examined by cross-sectional high-resolution transmission electron microscopy (HRTEM) with a 200 kV Akashi 002B electron microscope. Secondary ion mass spectrometry (SIMS) was also used to monitor the formation of Cu_3Ge and the reaction with the GaAs substrate.

RESULTS AND DISCUSSION

Figure 1(a) shows a cross-sectional image at relatively low magnification of the 150-nm-thick Cu-Ge film on the (001)GaAs substrate which is projected in the ⟨110⟩ orientation. The film is polycrystalline, containing both Cu_3Ge (large) and pure Ge (small) grains, denoted as 1 and 2, respectively. The majority of the film consists of grains of the ϵ_1-Cu_3Ge phase having an orthorhombic (probably with slight monoclinic distortion–$\beta=89.68°$) symmetry with lattice parameters $a_0=0.528$, $b_0=0.420$, and $c_0=0.457$ nm.[8] The ϵ_1-Cu_3Ge grains have a wide distribution size with an average size of 150 nm. Most of the Cu_3Ge grains have grown through the entire thickness of the film, providing only vertical boundaries between the grains that can lead to a reduced value of bulk resistivity of the contact material.

Usually the Ge grains were small and surrounded by large ϵ_1-Cu_3Ge grains. It is interesting to note that the interface is much sharper as compared to that of AuGeNi contacts on GaAs.[9,10] The selected area diffraction (SAD) pattern in Fig. 1(b) contains ⟨110⟩ GaAs diffraction spots and ϵ_1-Cu_3Ge spots of the {111} type denoted by arrows. Figure 2(a) is an HRTEM of the Ge grain on the GaAs substrate showing a complete epitaxial relationship between the two. The SAD pattern [Fig. 2(b)] from the Ge grain shows ⟨110⟩ Ge spots along with twins at (1/3,1/3,1/3). The twin formation in Ge is characteristic of recrystallization at low temperatures <400 °C. The interface between Ge and GaAs is atomically sharp, with the occasional presence of an amorphous (contamination) region, as indicated by an arrow in the micrograph. The Ge grains were usually small, as shown in Fig. 3.

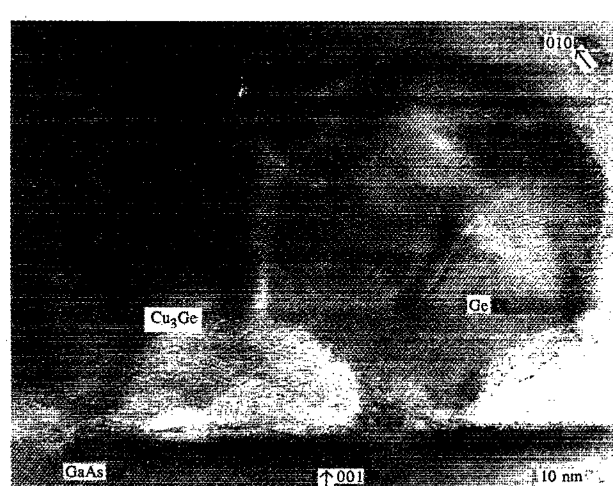

FIG. 3. High-resolution TEM image showing Ω-shaped Ge grain epitaxially grown on GaAs embedded into the ϵ_1-Cu_3Ge matrix.

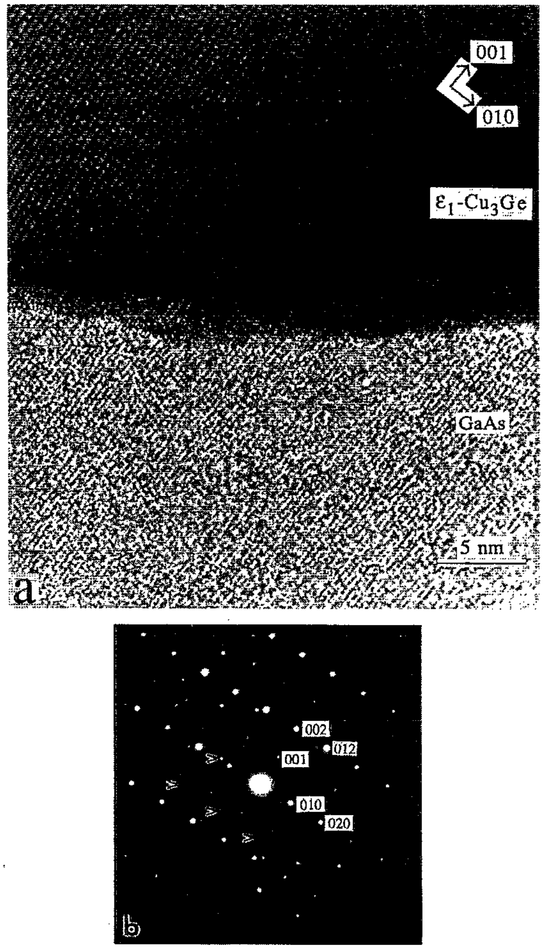

FIG. 4. (a) High-resolution TEM image of ϵ_1-Cu_3Ge/GaAs interface. The specimen is tilted into the [100] zone axis of the Cu_3Ge phase, and GaAs is 5°–8° out of the [110] zone axis. (b) Corresponding SAD pattern. Spots of [100]-oriented ϵ_1-Cu_3Ge are indexed. Arrows aim at the GaAs spots. Reflexes denoted by asterisks correspond to a neighboring ϵ_1-Cu_3Ge grain.

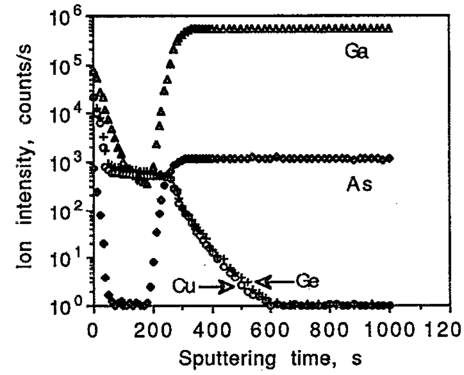

FIG. 5. SIMS profiles of an ϵ_1-Cu_3Ge/GaAs contact formed at 400 °C for 30 min. Note that only Ga has diffused into the ϵ_1-phase alloy. The As signal in the ϵ_1-phase alloy is at the background level.

Here, in the HRTEM, we observe epitaxial growth of Ω-shaped Ge grain on GaAs. The Ge grain is surrounded by the ϵ_1-Cu_3Ge phase where one can observe the lattice fringes of (010) planes with a spacing of 0.42 nm. However, it is important to note that the Ge phase does not continue along the interface.

The specimen was tilted so as to bring a ϵ_1-Cu_3Ge grain in the ⟨100⟩ orientation, and Fig. 4 shows the ⟨100⟩ ϵ_1-Cu_3Ge grain oriented close to the ⟨110⟩ GaAs substrate. The {111} planes of GaAs with 0.326 nm spacing are close to alignment with the {010} planes of ϵ_1-Cu_3Ge (spacing 0.42 nm). There is also no evidence of epitaxial Ge along the interface. The SAD pattern contains spots corresponding to a ⟨100⟩ orientation of the grain shown, as well as weaker spots of the GaAs substrate (arrows) and neighboring Cu_3Ge grain (asterisks).

TEM results clearly show that ϵ_1-Cu_3Ge contacts do not exhibit epitaxial layers of Ge on the GaAs substrate. Also, contacts formed with Ge in excess of that required for ϵ_1-Cu_3Ge formation (30 at. %) do not produce epitaxial layers of Ge on the GaAs substrate, but rather produce grains of ϵ_1-Cu_3Ge in contact with the GaAs substrate and a small portion of Ge grains that are epitaxial in nature. These contacts displayed a room-temperature contact resistivity comparable to that of ϵ_1-Cu_3Ge contacts. The ϵ_1-Cu_3Ge contacts exhibit planar and structurally abrupt interfaces to within atomic scale. Also, the contacts do not suffer from lateral spreading during high temperature annealing. These features make the ϵ_1-Cu_3Ge contacts suitable for devices with shallow junctions.

The SIMS profiles displayed in Fig. 5 for the Cu_3Ge/GaAs structure show that Ga has diffused into the ϵ_1-Cu_3Ge, indicating that the chemical potential of Ga in the ϵ_1-Cu_3Ge is lower than that in the GaAs compound. We suggest, therefore, that the ohmic behavior is due to the presence of a highly doped surface region created by the incorporation of Ge atoms into the GaAs on Ga vacant sites.

From these results we conclude that the presence of a Ge/GaAs heterojunction is not the primary factor in causing the ohmic behavior. However, for contacts formed with 30 at. % Ge layers, the heterojunction may help the current transport across the interface because of a small energy barrier. The ohmic behavior is not due to the contacting of the ϵ_1-Cu_3Ge alone since this alloy phase is known to form Schottky barrier contacts.[11] We envisage that the tunneling of carriers across a highly doped surface region results in the low-resistance ohmic behavior of the contact. This also explains the formation of an ohmic contact over a wide range of Ge concentration from 5 to 40 at. %. It should be pointed out that the specific resistivity of the Cu-Ge alloy increases from 2 to 50 $\mu\Omega$ cm as Ge concentration increases from 5 to 15 at. %, and then it decreases to 6 $\mu\Omega$ cm at 25 at. % of Ge. Thus, the optimum composition to form a low-resistance ohmic contact is in the 25–35 at. % Ge range, preferably at around 30 at. %, which produces both the low-resistivity ϵ_1-Cu_3Ge phase and the excess Ge phase to facilitate the transport of current because of a small interfacial energy barrier. Thus, the Cu-Ge alloy offers stable and reliable low-resistance ohmic contacts for advanced GaAs semiconductor devices.

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