Section 4. Physics

https://doi.org/10.29013/AJT-22-9.10-26-30

Ataubayeva Akkumis Berisbayevna,
Berdah Karakalpak State University, Nukus, Uzbekistan

ON BEHAVIOR OF INTERPHASE INTERACTIONS IN SILICON CONTACT STRUCTURES DUE TO QUICK THERMAL TREATMENT

Abstract. The author has studied how an ohmic contact between TiB_x and heavily doped silicon is shaped. As it has been shown, a low-resistance Au-Ti-TiBx-Ti-n+-Si ohmic contact is conventionally formed by its deposition on an n+-Si-substrate heated to 150 °C. The experiment reveals that quick thermal treatment (QTT) at T = 400 °C does not practically affect properties of Au-Ti-TiB_x-Ti-n^+-Si ohmic contacts, whereas QTT at T = 600 °C helps shape a kind of a $TiSi_2$– phase and leads to an increase in the value of ρ_c in comparison with both the original sample and thermally heated (at T = = 400 °C) sample. Diffusion barriers based on Ti and TiB_x appear heat-resistant in the range of temperatures to 600 °C.

Keywords: ohmic contact, boride of titan, diffusion barrier, rapid thermal annealing.

Introduction

As more and more microelectronics devices over lately are designed to operate in ultra-high frequency band applications, thus the role of stable metal-semiconductor ohmic contacts becomes immense in ensuring their reliable and effective operation.

To slow down or eliminate altogether degradation processes stemming from mixing in the contact-forming layer as well as contact metallization in general, diffusion barriers are used in contact metallization, consisting either of layers of refractory metals or of interstitial phases that do not interact with surrounding metal and semiconductor layers [1].

In silicon electronics, contact layers are usually formed by silicides [2]. It turns out that depending on a variety of factors (such as surface processing, thermal treatment regimes, quality of initially evaporated metal layers, etc.), even at sufficiently optimal thermal treatment conditions (as it would seem at first sight), across the entire area of metal-Si interface, several silicide phases (previously well-known to researchers) are usually formed, each characterized by its own electron work function φ_m, [3], while, plethora of unknown silicide phases are shaped as well. This in turn implies that along the process, substantial metal-semiconductor interfacial inhomogeneity in terms of electrical properties appears that does not contribute to improving its reliability. In the present research paper, we investigate how ohmic contacts to *n+-Si* based on titanium silicide phases and *Ti*- and TiB_x-film diffusion barriers, are shaped.

Techniques of measurement and samples

The authors in the present investigation applied two types of samples, i.e., trial samples for measurement of ρ_c by applying Transmission Line Method (TLM) as well as trial samples with metallization layers for measurement of distribution profiles of components by method of Auger spectroscopy in ohmic contact before and after quick thermal treatment during 60 seconds at temperatures of 400 and 600 °C.

Single crystalline *Si* (111) doped with phosphorus ~$2 \cdot 10^{19}$ cm^{-3}, obtained by CZ technique was used as an initial sample. On preliminarily cleaned surface of *Si* that was heated to 150 °C, *Ti* (60 nm), TiB_x(100 nm), *Ti* (60 nm) and *Au* (100 nm) layers were sequentially deposited by applying the technique of thermal evaporation of metals in vacuum. The first deposited layer of *Ti* was the contact-forming layer, the second one TiB_x – is the diffusion barrier, and the following *Ti* layer is the diffusion barrier and adhesive layer at the same time that in turn ensures reliable contact of *Au*.

For measurement of ρ_c we have used the previously mentioned reference method [4]. Distribution profiles of components in contact metallization layer were measured by applying Auger electron spectroscopy LAS-2000.

Experimental and discussion

The schematic diagram of *Au-Ti-*TiB_2*-Ti-n-Si* is shown on (Fig. 1). The TiB_2 – based diffusion barrier ensures high thermal stability of contact systems in the temperature range of 700 °C in QTT temperature mode. This takes place due to peculiarities of chemical bonds prevalent in TiB_2, characterized by high thermal stability, chemical inertia and melting temperature that is more characteristic of metals. Additional layer of *Ti* also serves as a diffusion barrier and ensures better adhesion of TiB_2 and *Au*.

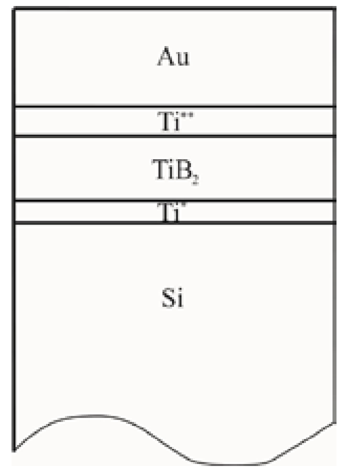

Figure 1. *Au-Ti-*TiB_2*-Ti-n-Si*-type *contact system structure*

Si – silicon sample doped with phosphorus;
*Ti** – contact-forming layer of titanium;
TiB_2 – diffusion barrier layer;
*Ti*** – additional diffusion barrier layer;
Au – outer contact layer of aurum

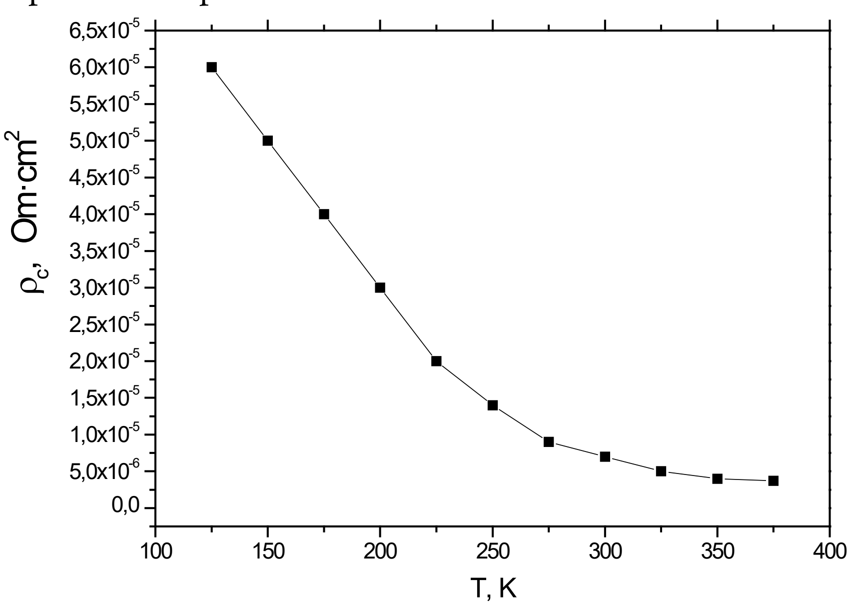

Figure 2. Temperature dependence of ρ_c In *Au-Ti-*TiB_x*-Ti-*n^+*-Si*-type ohmic contact

The (Fig. 2) shows a temperature curve of dependence of ρ_c of the initial sample (metals were applied on a sample surface heated up to 150 °C). As is shown in this figure in the measurement range from 125K to 375K, ρ_c rather decreases. Such dependence of ρ_c(T) manifests thermal field charge transfer behavior in ohmic contact [5].

As it is well known, majority of low power Si based microelectronics devices operate in the temperature range that does not exceed 100 °C. In this regard, we have measured the $\rho_c(T)$ dependence in the temperature range of 300–375 K before and after QTT.

The experimental results shown in (Fig. 3) reveal that the dependence of $\rho_c(T)$ before and after QTT at T = 400 °C does not virtually change at all, whereas the behavior of ρ_c(T) curve before and after QTT at T = 600 °C in the measurement temperature range, had significantly increased.

The experiment reveals that the ohmic contact is formed along the process of deposition of metals on the surface of heated sample. The electron work function φ_m for Ti is 3,95 eV, whereas for phases $TiSi$, Ti_5Si_3 and $TiSi_2$ it is 3,99 eV, 3,71 eV and 4,17 eV, respectively [3; 6]. These are data for the above phases that are shaped during the deposition process or QTT. These work functions are substantially lower in comparison with that of Si (4,8 eV) that allow forming ohmic contact even without having to carry out high temperature treatment.

Meanwhile, the existence in the contact-forming layer of comparatively low-temperature phases of $TiSi$ и Ti_5Si_3 along with pure Ti characterized by slightly varying electron work functions allows forming relatively evenly distributed contact, evidenced by experiments (curves 1 and 2 on Fig. 3).

While the temperature of QTT increases to 600 °C, as the paper [7] reveals, an intensive formation of $TiSi_2$ phase takes place characterized with electron work function of ~ 4,18 eV, which in the existence of other silicide phases leads to shaping of unevenly distributed contact and an increase in the value of ρ_c (curve 3 in Fig. 3).

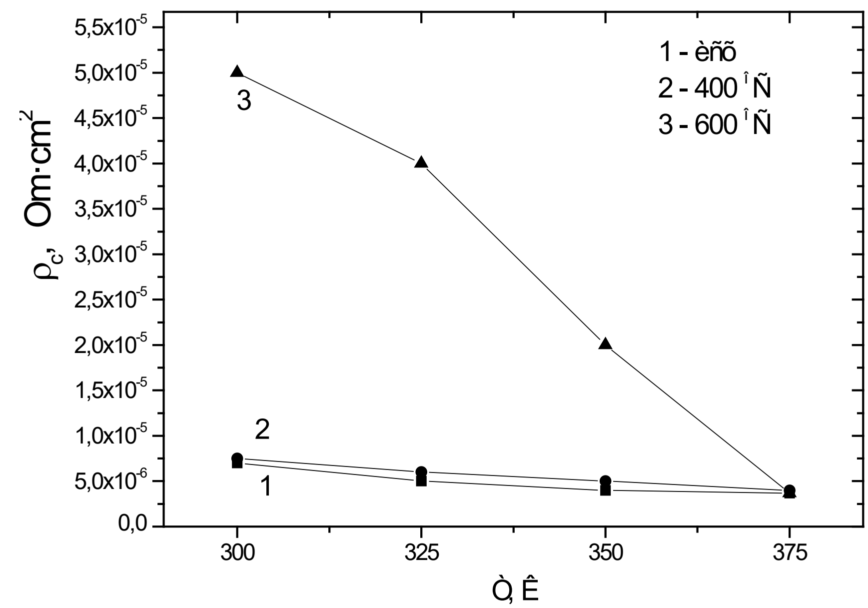

Figure 3. Dependence *of* ρ_c on temperature before and after *QTT* at T = 400 and 600 °C

The experimental dependence curves of $\rho_c(T)$ before and after QTT well correlate with distribution profiles of components in contact metallization layers (Fig. 4). As is evident from (Fig. 4 a, b), the results of profile distribution of initial sample and that of a sample that had undergone quick heat treatment at 400 °C

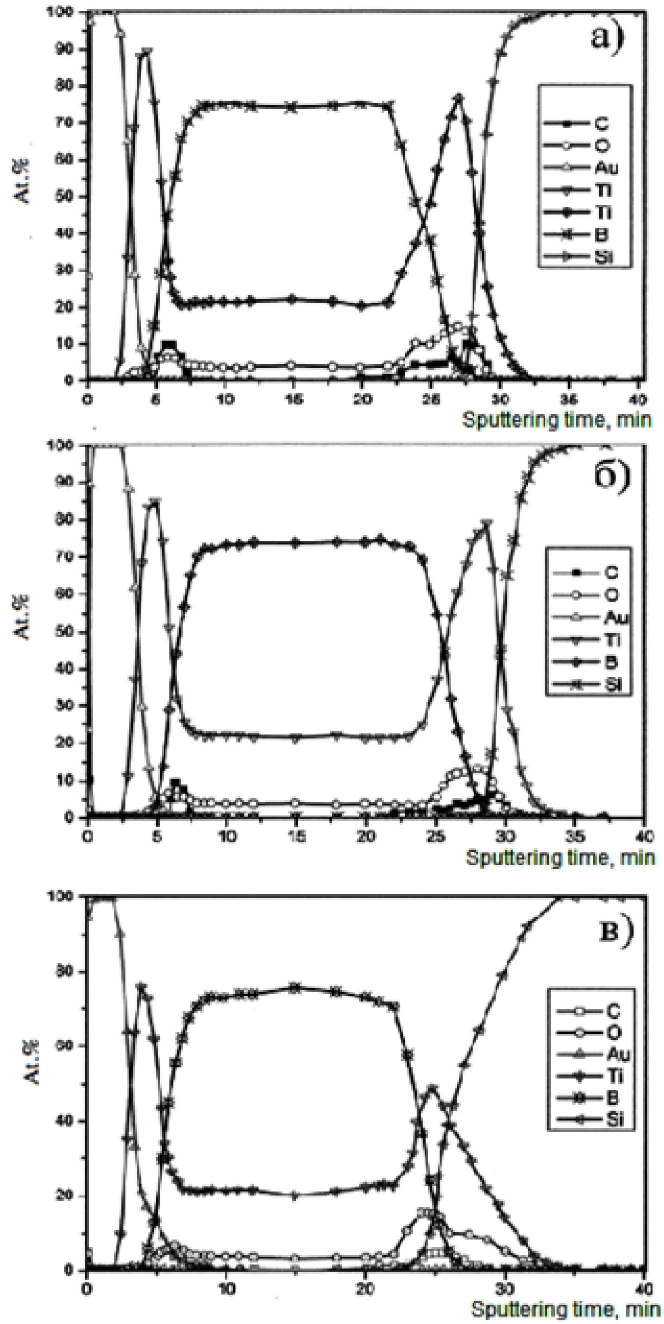

Figure 4. Profiles of distribution of components in Au-Ti-TiB_x-Ti-n^+-Si contact before (a) and after quick heat treatment at 400 °C (b) and 600 °C (c) during 60 seconds

are almost identical, whereas in the sample annealed at T = 600 °C (Fig. 3, c) one can witness intensive mass transfer of Si towards contact shaping silicide layer.

This in turn, according to the data in [8] leads to shaping of $TiSi_2$ phase, thus in our case conditioning appearance of uneven contact and the increase in the value of specific contact resistance.

Judging by the profiles of distribution of components in Au-Ti-TiB_x-Ti-n^+-Si before and after QTT at 400–600 °C during 60 seconds, one can conclude that comparatively high quality of *Ti* and TiB_x diffusion barriers precondition stability of interface *"contact forming layer – n^+-Si"* layers.

Conclusion

The experimental results indicate that a low-resistance Au-Ti-TiB_x-Ti-n^+-Si ohmic contact is formed in the course of deposition of metallization layer on a thermally heated (to 150 °C) n^+-Si substrate without having to additionally heat it afterwards in QTT regime. QTT at T = 400 °C has practically no effect on distribution profile of the metallization layer components and the value of ρ_c in comparison with the initial sample obtained by deposition of metals on a *Si* substrate heated to 150 °C. QTT at T = 600 °C contributes to forming of $TiSi_2$ phase and, as a result, leads to occurrence of an inhomogeneous ohmic contact with a value of ρ_c larger than ρ_c of the initial sample and the one that had undergone heat treatment (QTT) at T = 400 °C.

Ti and TiB_x diffusion barriers manifest heat resistance after QTT at T=400 and 600 °C.

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