WEB OF SCIENTIST: INTERNATIONAL SCIENTIFIC RESEARCH JOURNAL
ISSN: 2776-0979, Volume 4, Issue 5, May, 2023

PROPERTIES OF IRON SILICIDES IN SINGLE-CRYSTAL SILICON

Daliev Khojakbar Sultanovich[1],
Khusanov Zafarjon Murodovich[2]
[1]Branch of the Federal State Budgetary Educational Institution of Higher Education "National Research University MPEI", dalievkhs@yandex.ru
[2]Institute of Semiconductor Physics and Microelectronics at NUUz (Tashkent), Uzbekistan
zafarjonxusanov@umail.uz

Abstract

This paper presents the properties of iron silicide compounds in n-type silicon. The iron layer was formed with a thickness of 1 ÷ 2 µm by magnetron sputtering onto the surface of silicon grown by the n-type Czochralski method in an atmosphere of pure inert argon gas. The properties of iron silicide and the formation of complexes of iron silicides in the volume of silicon have been studied.

Keywords: silicides, morphology, vacancy, spectrum, temperature, diffusion, composition, surface.

Introduction

Iron is one of the most common and harmful metal impurities in silicon. Generation-recombination centers associated with dissolved iron and its complexes increase leakage currents in any reverse biased junction, which increases energy consumption and heat generation. In crystalline and polycrystalline photovoltaic devices, iron contamination leads to the creation of recombination centers that reduce the diffusion length of minority charge carriers and hence the efficiency of the solar cell [1]. As device sizes continue to shrink, device performance becomes more susceptible to defects and contamination [2,3]. Since ultrapure technology to reduce surface iron contamination to below 1010–1011 cm–2 is extremely expensive, understanding the mechanisms of iron contamination, the detrimental role of iron in silicon devices, and the allowable limits of iron contamination for each specific process is becoming increasingly important. This requirement aroused great interest in the physics of iron in silicon.

The main obstacle in establishing a consistent experimental picture of 3d - transition metals in silicon and, in particular, iron, arises from the high diffusivity of these elements. Iron remains mobile at room temperature and can diffuse rapidly at temperatures above 100 ^{0}C. Because interstitial iron is positively charged in p-Si at room and slightly elevated temperatures, it readily pairs with negatively charged defects such as shallow acceptors. The diffusion coefficients of transition metals in silicon depend on the charge state of the metal, since the ionic radii of neutral and ionized particles are different, as well as the degree of overlap of the electron density of diffusing atoms with the surrounding silicon matrix. The migration enthalpies and preexponential factors of the largest of the 3d ions can be calculated with amazing accuracy as the difference in elastic energies at tetrahedral and hexagonal interstices using the hard sphere model, as proposed by U [4].

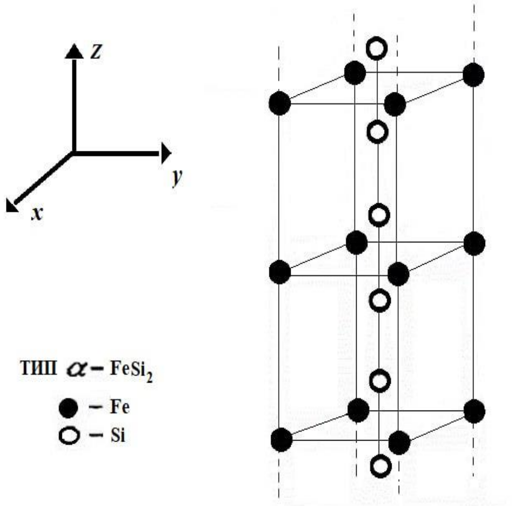
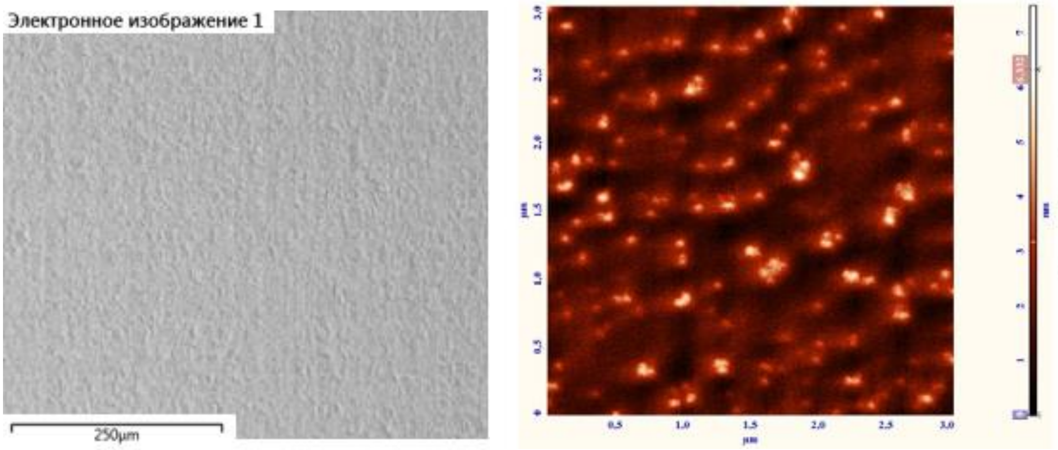


Fig. 1. Compound of iron silicide $FeSi_2$ have the same cubic crystal structure.

Experiment

Single-crystal silicon samples 0.7x14x15 mm in size with ρ = 50 Ohm·cm of n-type with a surface layer of iron were annealed in an electric muffle furnace of the KSI-1075-1 brand in the temperature range of 900-1250 °C for 10-12 hours. As a source of diffusion, iron was used, deposited by the method of magnetron ion sputtering with a thickness of 1.5-2 μm in an argon atmosphere on cold silicon substrates on the polished surface of a silicon sample with carborundum powder M-14, M-10, M-7.

Fig. 2. shows the surface of silicon before and after the deposition of pure iron by magnetron ion sputtering in an argon atmosphere [5]. Since sputtering is a low-temperature process, it can be used to obtain films of metals (including refractory), alloys (including multicomponent composition), semiconductors and semiconductor compounds.



(a) (b)

Fig.2. AFM image of the silicon surface before (a) and after the deposition of pure iron (b) by magnetron ion sputtering in an argon atmosphere at room temperature of the substrate.

The Raman spectrometer makes it possible to measure Raman spectra (RS) and combine spatially resolved molecular information with high-quality microscopic images. Using a BRUKER SENTERRA II Raman spectrometer, the elemental composition of the initial single-crystal silicon (Fig. 3) and iron-doped silicon was determined.

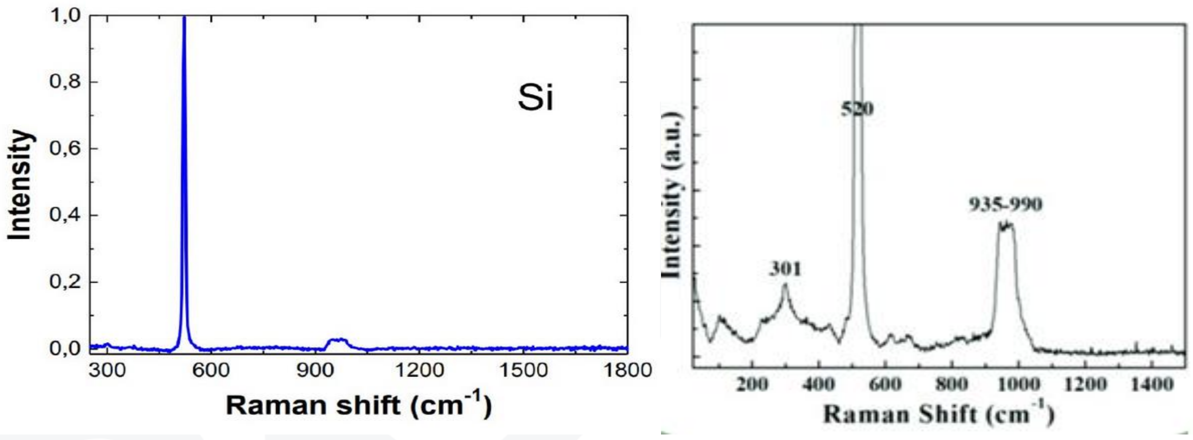


Fig.3. Raman spectrum of original(a) and iron-doped silicon.

Discussion of results. As shown by these studies, on the surfaces of single-crystal silicon of the Si(100)2x1 and Si(111)7x7 orientations, the formation of various non-magnetic silicides is detected at the Si/Fe interface, which worsens the spin injection into silicon. In this case, the formation of films strongly depends on the degree of crystallinity of the surface and its roughness. In addition, the formation processes turn out to be nonidentical for the Si/Fe and Fe/Si interfaces. Understanding this difference is important in the process of creating multilayer films (Fe/Si) n-model systems for elements of non-volatile memory and sensors. In the "iron-silicon" system, there are a number of stable and metastable phases of iron silicides. The phases stable at room temperature in the case of bulk samples include iron disilicides β-$FeSi_2$, ε-FeSi, Fe_3Si [4]. The first of them is a direct-gap semiconductor with a band gap of 0.85 eV and is stable up to a temperature of 920°C. Above this temperature, β-$FeSi_2$ transforms into α-$FeSi_2$ metal silicide. Monosilicide ε-FeSi is a semimetal (the forbidden energy interval at the Fermi level is 0.05 eV). The Fe_3Si compound, which is the most iron-rich in comparison with other silicides, is a ferromagnetic metal with low conductivity.

Conclusions

The Fe_3Si compound crystallizes in a cubic lattice with a lattice constant of 5.656 Å. Silicide ε-FeSi is formed in a simple cubic lattice B-20 (a=4.488 Å). Silicide α-$FeSi_2$ has a tetragonal lattice with constants a=9.86 Å, b=7.79 Å, c=5.128 Å. Metastable phases include α-$FeSi_2$, γ-$FeSi_2$ and $FeSi_{1+x}$ solid solutions at ($0 \leq x \leq 1$) [3]. Iron disilicide γ-$FeSi_2$ has a face-centered cubic lattice of the CaF2 type and with a defect structure of the same type. According to [6], the silicide γ-$FeSi_2$ has ferromagnetic properties. There are also reports on the preparation of a metastable phase that decomposes into FeSi and Fe_3Si below 825°C [7], such as Fe_5Si_3, in the form of nanowires and nanogranules in a silicon matrix.

Literature:

1. Boltaks B.I., Bakhadyrkhanov M.K., Gorodetsky S.M., Kulikov G.S. Compensated silicon. - L. Nauka, 1972. 122 p.
2. P. He, Z. You: Phys. Status Solidi A 125, K31 (1991)
3. Dulov E.N. Studies of thin magnetic films obtained by Implantation of iron ions into silicon /E.N.Dulov, D.M.Khripunov// Abstracts of the IV scientific-practical conference of young scientists and specialists RT-2001.-Kazan2001, P.29.
4. J. Utzig: J. Appl. physical 65, 3868 (1989)
5. Muzafarova. S.A. Method for manufacturing a photosensitive device. 11.05. approved -2008. Patent No. IAP 03702.
6. Bendik N.T., Milevsky L.S.: Dokl. acad. AN SSSR 195, 107 (1970)
7. Z.M. Khusanov, M.K. Khusanova, A.A. Akbarov Properties of silicon doped with iron atoms // Proceedings of the international scientific and scientific-technical conference "Prospects for the development of condensed matter physics" Karshi State University. October 14-15, 2022 vs. 2022. St. 151-155.