Study of the profiles of the distribution of atoms of the contacting material over the depth of pure and ion-doped silicon

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Abstract. Auger electron spectroscopy combined with ion etching was used to study the effect of ion doping on the distribution profiles of atoms in silicon in contact with its surface. It has been established that preliminary implantation of Ba^+ ions with E_0=0.5-1 keV leads to a sharp decrease (by a factor of 10-12) in the diffusion length of oxygen and nickel atoms.

1 Introduction

Currently, research is underway to create materials with desired properties used in many areas [1,2], including microelectronics, where special attention is paid to the study of interfacial phenomena of multilayer structures [3,4], a necessary condition is to reduce to an acceptable value the concentration and penetration depth of impurities that penetrate into the matrix during various operations (heating, exposure to air, spraying of the contacting metal, etc.).

One of the most important operations is obtaining stable ohmic contacts. Considering good conductivity and low cost, Al, Cu, and Ni are often used as contact materials. However, for example in the case of silicon, the noticeable diffusion of atoms of these metals in the matrix sometimes limits their application. Its reduction can be achieved by preliminary deposition of Au or Pt atoms on the surface. One of the reasons for this, apparently, is the formation of silicides of these metals [5].

The formation of chemical bonds in Si is also observed during high-dose implantation of ions of active elements [6-9]. The composition, structure, and properties of near-surface layers of ion-doped samples have been studied quite well by now. The results of such studies are very promising for the creation of thin-film structures with desired controlled properties.

At present, the composition, structure, and properties of films of various thicknesses obtained by various methods are well studied [10-12]. In this case, homogeneous silicon dioxide nanofilms, as in the case of metal silicides [13-15], were obtained by low-energy

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ion implantation in combination with subsequent annealing [12]. The presence of impurity atoms or silicon clusters in thin films of silicon dioxide and metal silicides leads to a significant change in their physical properties [16-19]. In the case of thin SiO_2/Si films (d ≤ 10 nm), Si atoms can diffuse into the SiO_2 film.

However, until now, the possibilities of creating a diffusion barrier (protective layer) for non-indegenous impurities using ion implantation have been little studied. In this connection, in this work, we studied the effect of high-dose implantation of Ba^+ ions on the distribution of atoms penetrating into the near-surface layers of silicon from air and metal (nickel) deposited on the surface.

2 Methods

Purification of silicon, implantation of ions, control of the composition and structure of the surface was carried out in a multi-chamber device under high vacuum conditions (~$5\cdot10^{-7}$ Pa). The experimental device and experimental technique are described in [20]. Silicon was degassed and purified by heating at T=1200 K for 8–10 h and at T=1500 K for 10-15 min. Such a cleaning regime made it possible to obtain Si, surfaces free of contaminants (at the sensitivity level of an Auger spectrometer). Ba^+ ions were implanted with energy E_0=0.5-5 keV at saturation dose D=$6\cdot10^{16}$ cm^{-2}. At such a dose, the surface layers of silicon are completely disordered, and a further increase in its value does not lead to a noticeable change in the concentration profiles of the distribution of barium over the depth of silicon. The samples under study were contacted with air by holding them in air for 10–12 h. Ni atoms were deposited on the surface of the targets under study at a vacuum of no less than 10^{-3} Pa. Before deposition, the nickel plates were degassed at T=1400 K. Implantation of ions, exposure of samples to air, deposition of Ni, and all measurements were carried out at room temperature of the target.

The concentration profiles of the distribution of the main and impurity atoms over the depth of the matrix were determined by Auger electron spectroscopy (AES) in combination with ion etching on a standard LAS-2200 setup. The etching was carried out by a beam of Ar^+ ions with an energy of 3 keV, directed at an angle of 15° to the surface. Etching rate 4 Å/min. The concentration of various atoms was calculated by the method of elemental Auger sensitivity coefficients [21]. In this case, the high-energy Auger peaks of the elements Si (1618 eV), O (508 eV), C (272 eV), Ba (584 eV), Ni (848 eV) were mainly used.

3 Results and discussion

To control the presence of non-indegenous impurities before contact with air, the composition of the surface and near-surface layers of pure and ion-doped Si was preliminarily studied under high vacuum conditions in the same device where silicon purification and ion implantation were performed. On figure1 shows survey Auger spectra of the surface of pure silicon and implanted with Ba^+ ions with E_0=0.5 keV and D=$6\cdot10^{16}$ cm^{-2}. It can be seen that after ion implantation in the spectrum, along with the appearance of intense peaks of barium (E=54, 68, 71, 582, 591 eV), the main low-energy Si$L_{23}VV$ peak splits into two (E=90 and 94 eV). The change in the shape of the Si$L_{23}VV$ peak is associated with the formation of chemical compounds such as BaSi and $BaSi_2$. The formation of barium silicides also leads to a shift in the position of the high-energy silicon peak E=1618 eV by 4-5 eV. At high implantation doses, regardless of the ion energy, a weak peak E = 506-508 eV, characteristic of oxygen, appears in the spectra. Its concentration in the surface layer (up to a depth of 100-150 Å) of pure and ion-doped Si, kept for 10-12 hours in a high ($P=5\cdot10^{-7}$ Pa) vacuum, did not exceed 1-2 at.%.

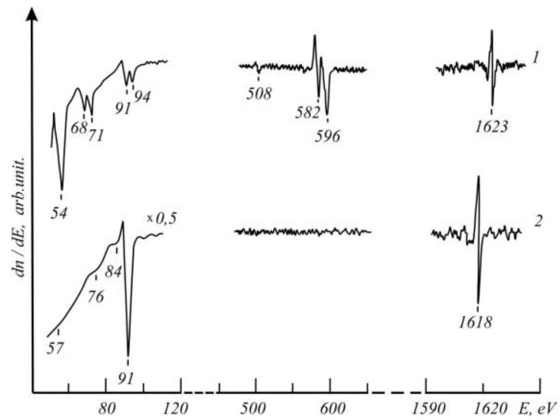

Fig. 1. Auger spectra of pure and ion-doped Si; 1 – $Ba^+ \rightarrow$ Si, 2 – Si(111); E_0=0.5 keV; D=$6\cdot10^{16}$ cm^{-2}.

The main components of non-indegenous impurities introduced into the near-surface layers of the test sample upon its contact with air were carbon and oxygen atoms. In this case, the distribution profiles of the main (Si, Ba) and impurity (O, C) atoms depended significantly on the energy during ion doping.

As an example, in figure 2 shows the distribution of oxygen atoms over the depth of Si samples doped with Ba^+ ions with different energies after contact with air. It can be seen that the surface of both pure and ion-doped samples has a significant amount of oxygen atoms (up to 30–35 at.%). In all cases, as *d* increases, the oxygen concentration decreases. However, this decrease in the case of ion-doped samples is much smaller than in the case of pure Si, i.e. ion implantation leads to a sharp decrease in the concentration of impurity atoms and their penetration depth into the surface layers of the sample. The most efficient diffusion barrier was created at low ion energies (E_0=0.5-1 keV). Similar data were also obtained for impurity carbon atoms.

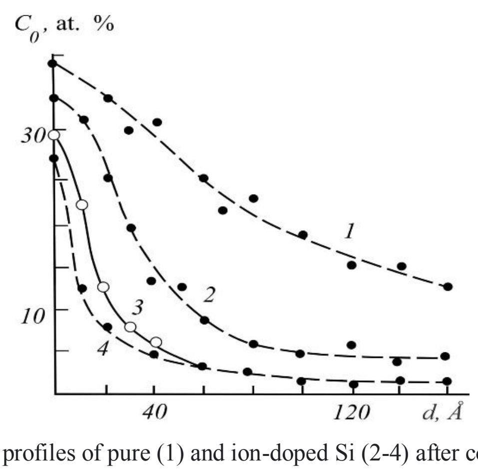

Fig. 2. Depth distribution profiles of pure (1) and ion-doped Si (2-4) after contact with air; E_0=5.1 and 0.5 keV (2-4 respectively).

On Fig. 3 shows the dependences $C_{Ba}(d)$ for ion-doped Si crystals obtained before and after contact with air. It can be seen that the presence of C and O impurity atoms leads to a noticeable redistribution of barium atoms only near the surface. A comprehensive analysis of the Auger electron spectroscopy results shows that in this case, the relative concentration of barium mainly changes, while its absolute concentration does not change significantly.

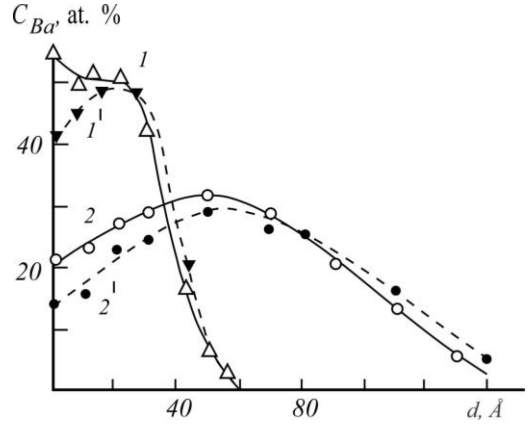

Fig. 3. Depth distribution profiles of Ba atoms for Si(111) doped with Ba^+ ions before (1, 2) and after (1', 2') contact with air; E_0=0.5 (1, 1') and 5 keV (2, 2').

To elucidate the effect of the ion-implanted layer on the redistribution of atoms at the border of metal-semiconductor, we studied the interphase boundaries of Ni – pure Si and Ni – ion-doped Si (Fig. 4). The thickness of the deposited Ni film was 500 Å in all cases. From Fig.4 shows that a noticeable interdiffusion of atoms occurs at the border Ni – pure Si. The depth of penetration of Si atoms into the Ni film was 200 Å, and that of Ni atoms in Si reached 400-500 Å. The depths of interdiffusion of atoms in the case of amorphous Si decrease. In all cases, in the thickness of the nickel film and in the near-contact region of the matrix, there were carbon and oxygen atoms, the total concentration of which was 8–10 at.%. These atoms were introduced uncontrollably during Ni deposition. In the deeper layers of the matrix (d ≈ 15-20 Å), their concentration did not exceed 2-3 at.%.

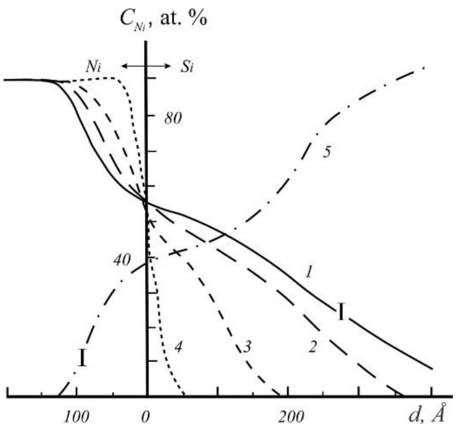

Fig. 4. Depth distribution profiles of Ni atoms of (*1*) pure single-crystal and (*2*) amorphous silicon and silicon doped with Ba^+ ions with an energy of 5 (*3*) and 0.5 keV (*4*); 5-distribution profile of Si in the near-contact region Ni – pure Si (111).

The concentration and penetration depth of Ni atoms in the case of ion-doped samples are much lower (Figure 4, curves 3 and 4) than in the case of pure Si. The smallest diffusion of Ni is observed for Si doped with ions with E_0=0.5 keV. As the energy of the Ba^+ ions increases, its concentration in the near-surface region of Si decreases, and the number of Ni atoms diffused into the depth of the sample increases; there is a certain correlation between changes in the concentration of Ba and Ni atoms in the surface layers of silicon.

An analysis of the obtained results indicates that the observed decrease in the diffusion of atoms of the contacting elements and especially the correlation of their concentration with the concentration of the ion-doping impurity cannot be due only to amorphization of the near-surface layers of the matrix. Apparently, the main reasons for this can be the chemical bonds of Ba with Si, as well as a probable increase in the atomic density (densified matrices) in the region of the maximum distribution of Ba atoms.

On Fig.5 shows the concentration profiles of the distribution of Ni, Ba, and Si atoms in the near-boundary region of the Ni – ion-doped Si system (implantation energy of Ba^+ ions is 0.5 keV). It can be seen that the diffusion ranges of Ba and Si atoms in Ni and atoms ofNi in Si are very small and amount to 25–30 Å. It should be noted that a decrease in the energy of Ba^+ ions (less than 0.5 keV) led to a thinning of the protective layer to 8–10 Å and the formation of a barium film 3–4 monolayers thick on the silicon surface. The latter leads to an increase in the diffusion of Ba atoms in Ni and nickel in the bulk of the matrix. Heating to 800 K for 0.5 h did not change the observed atomic distribution profiles, and only at 800 K was some redistribution of atoms observed.

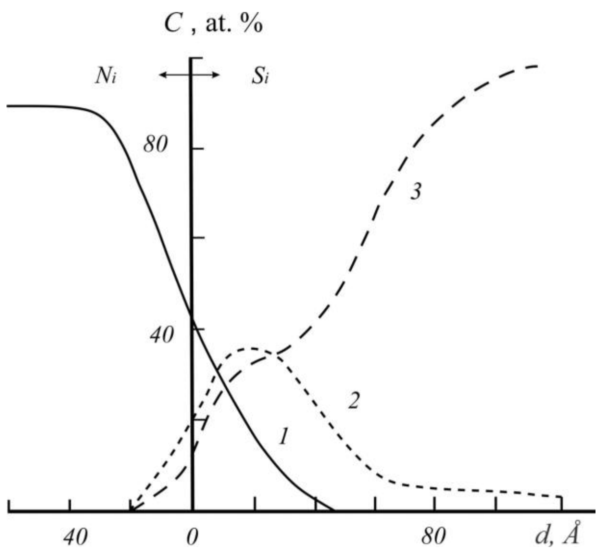

Fig. 5. Distribution profiles of (1) Ni, (2) Ba, and (3) Si atoms in the near-boundary region Ni – ion-doped Si; ion energy Ba^+ E_0=0.5 keV.

4 Conclusion

Thus, upon implantation of low-energy Ba^+ ions (E_0=0.5...1 keV), a diffusion barrier is formed in the near-surface layer of silicon, which prevents intense diffusion of non-indegenous impurities into the depths of silicon samples.

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