ION BEAM MIXING FOR SILICIDE FORMATION

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Abstract

Ion beam mixing has been proposed as a technique for simultaneous doping and metal silicide formation. This work presents a theoretical model for calculating the different parameters required for ion beam mixing through ion implantation. The minimum ion beam energy and dose for complete mixing is calculated. A plot of the obtained energy-dose relation shows that the dose increases linearly with energy. The dose-silicide thickness relation is also plotted. It is found that the thickness of the formed metal silicide increases lineraly with the square root of the applied dose. A good agreement is found between the values and relations of the proposed model and experimental results.

Introduction

Metal silicides are being widely considered for shallow junctions and contacts in VLSI circuits [1]. Recently, attention has been drawn to the formation of silicides by ion implantation. Provided that the primary ions penetrate to the metal/silicon interface and a little beyond, an interfacial zone of mixed metal-silicon will be formed. For many metals this can result in the formation of a metal silicide compound if a suitable phase exists. Simultaneously, the silicon substrate will be doped with the implanted ions. Some heating at moderate temperatures during or after implantation may be necessary to complete the compound-forming process [2]. In this case the temperature is lower than needed to react unimplanted layers.

Ion beam induced mixing can be attributed to one of several mechanisms [3]: (1) Cascade mixing or the repeated displacement of atoms in the solid by successive collision cascades. (2) Recoil mixing which is due to direct collision between incident ions and traget atoms. (3) Enhanced diffusion due to mobile defects such as vacancies and interstitials generated by the incoming ions. (4) Mixing by energy spikes. Under most implantation conditions in semiconductors, mechanisms (1) and (3) are expected to dominate [4].

Theoretical Model

In calculations of silicidation using ion mixing processes, the main parameters we are concerned with are the energy and dose of the incident ions required for silicide formation. If the ion's energy is insufficient to reach the interface no mixing will occur no matter how much the dose is. If the dose is insufficient incomplete mixing will

occur. An important condition that must be fulfilled is that the ions must reach the contact depth in order to avoid outdiffusion of the dopant [5].

Consider a silicon substrate covered by a metal of thickness t_m and density $_m$. The number of disilicide molecules formed by ion mixing per unit area will be equal to the number of metal atoms. Therefore

$$t_{MSi} = \rho_m (M_m + 2M_{Si}) / (\rho_{MSi} M_m) \cdot t_m \qquad (1)$$

where M_m and M_{Si} are the atomic masses of metal and silicon, respectively, t_{MSi} and ρ_{MSi} are the thickness and density of the silicide layer, respectively. The thickness of contact, t_c, is equal to

$$t_c = t_{MSi} - t_m \qquad (2)$$

The relation between the ion range in the silicon substrate, R_c, and the thickness of contact is given by [6].

$$R_c = t_c (1 + M_{Si}/3 M_i) \qquad (3)$$

where M_i is the atomic mass of the implanted ion. Knowing the ion range in silicon, we can obtain E_{Si}, the ion's energy at the

metal/silicon interface. The difference between the initial energy E_o and E_{Si} is lost in electronic and nuclear interactions in the metal film.

The average energy lost by an ion in all nuclear collisions is

$$T_n = T_1 - \frac{R_m}{\lambda}$$ (4)

where T_1 is the average energy lost per collision, R_m is the total distance travelled by the ion in the metal and λ is the mean free path. Using the differential scattering cross section, (E,T), based on the $1/r^2$ potential [7], eq. 4 can be rewritten as

$$= 4M_i \, M_m / (M_i + M_n)^2$$ (5)

and

$$= \frac{4M_i \, M_m}{(M_i + M_m)^2}$$

Where Z_i and Z_m are the atomic numbers of the ions and metal, respectively, a_o is the Bohr radius and e is the electron charge. N is the atomic density, E_d is the threshold energy for displacement.

The energy lost by an ion in electric collisions is equal to

$$T_e = (E_{Si}^{\frac{1}{2}} + \frac{1}{2} KR_m)^2 - E_{Si} \tag{6}$$

where K is a constant [8]. The difference between E_o and E_{Si} is equal to the sum of electronic and nuclear losses. Therefore

$$E_o = (E_{Si} + \frac{1}{2} KR_m)^2 + T_n \tag{7}$$

The dose required for complete mixing must be sufficient for two things: (1) Complete amorphization of the silicon substrate. (2) increase in total diffusion coefficient D of the silicon atoms so that it may reach the metal surface. The dose required for complete amorphization of silicon is given by [7].

$$dose = \frac{(z_{Si}^{2/3} + z_i^{2/3})^{\frac{1}{2}} M_{Si} E_d}{2.48 \times 10^8 z_i z_{Si} e^2 a_o (M_i + M_{Si})} (- E_d/E_{Si})^{-1} \tag{8}$$

As discussed earlier, the ion mixing occurs mainly through cascade mixing and radiation enhanced diffusion. These two mechanisms contribute to the diffusion coefficient in the following manner [9].

$$D = D_c + D_r \exp(- Q/kT) \tag{9}$$

where Q is the activation energy, k is Boltzman constant, and T is the absolute temperature. D_c and D_r are the diffusion coefficients due

to cascade mixing and radiation enhanced diffusion, respectively, and their values are given by [10]

$$D_c = \frac{1}{6} P(x) d^2$$ (10)

and

$$D_r = \sqrt{P(x)D_v/NR_{iv}}$$ (11)

where d is the average displacement of a recoil atom, N is the D_v is the vacancy diffusion coefficient , R_{iv} is the vacancy-interstitial separation at which spontaneous recombination accurs ($\approx$ 10 A^o[9]) and is the fraction of the point defects which escape the cascade to migrate freely through the lattice (0.025 [9,10]). P(x) is the number of displacement per target atom per unit time at depth x and may be calculated using the modified Kinchin Pease relation,

$$P(x) = \frac{0.8}{2NE_d} (dE/dx)_n$$ (12)

where $(dE/dx)_n$ is nuclear stopping power, and is the ion flux. The amount of mixing changes with the diffusion coefficient D according to the relation given by Haff and Switkows ki[11]

$$n(x,t) = \frac{1}{2} erfc (x/\sqrt{4Dt})$$ (13)

where n(x,t) is the fraction of the diffusing element at depth x and
time t from start of implantation. This is illustrated in Fig. 1. It
is clear that n(x,t) is increasing with the diffusion coefficient D.
Since erfc (y > 2) = 0, therefore we assume $(x/\sqrt{4Dt}) \leq 2$ for a
non-zero   value of n(x,t). Taking x = t_m and t = 120 sec, we will
obtain the minimum value of D which will cause the silicon ions to
reach the metal surface.

Results and Discussions

The energy and dose required for ion mixing and silicide formation
was calculated for molybdenum and tungsten films of 100 and 200 A°
thickness, and for arsenic and phosphorus ion beams. The calculated
dose in our model is only enough to ensure that silicon atoms have
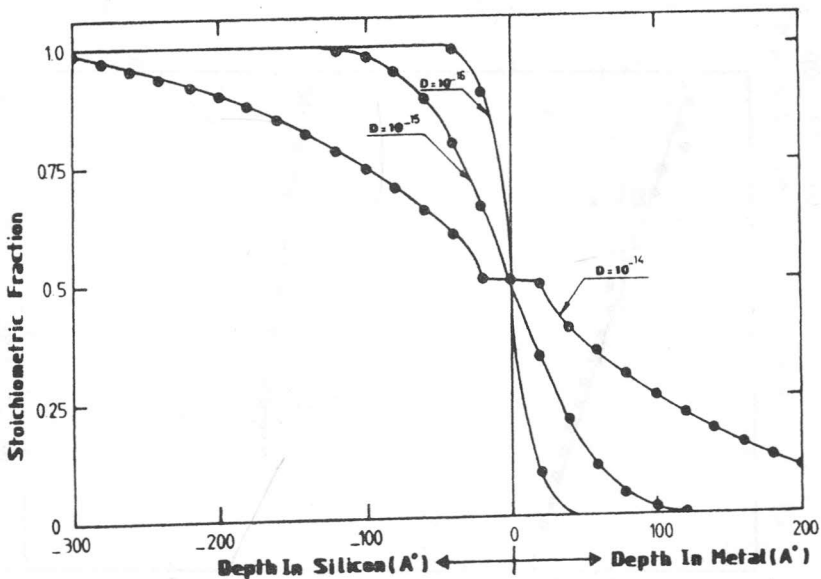reached the metal surface. The same dose was found experimentally to

Fig. 1. Change of Amount of mixing (represented
by n(x,120 sec), the fraction of silicon
in the metal/silicon mixture), as a
function of D, the total diffusion coeff-
icient.

cause complete mixing. This can be explained considering that experimental results were obtained at relatively long time after implantation in which silicon ions had a chance to diffuse further in the metal. For example, for 200 A$^\circ$ Mo/Si system, and arsenic beam, d'Heurle et al. [12] found that 200 KeV ions with 2×10^{16} cm^{-2} dose will cause complete ion mixing. This agrees with our model which gives an ion dose of 1.6×10^{16} cm^{-2} at 200 KeV energy.

Figs. 2 and 3 show the energy-dose relation for arsenic and phosphorus beams on Mo/Si and W/Si systems. The fact that the dose required increases with increasing energy can be easily explained. As the ion energy increases the nuclear energy loss in the metal film will decrease. This causes a decrease in the number of created vacancies. Consequently, a decrease in the diffusion coefficient. Thus, the dose
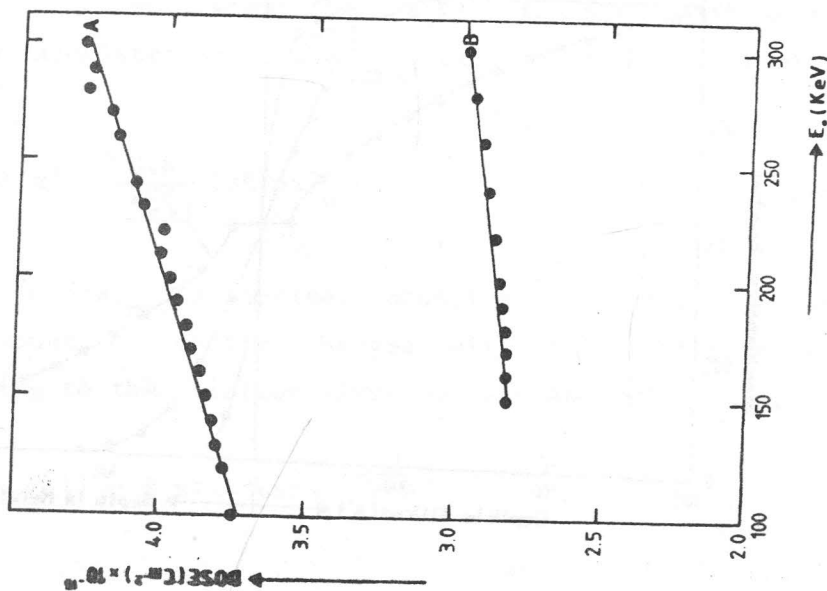

Fig. 2   Energy-Dose relation for As beam on 100 A Mo/Si (A) and 100 AW/Si (B).
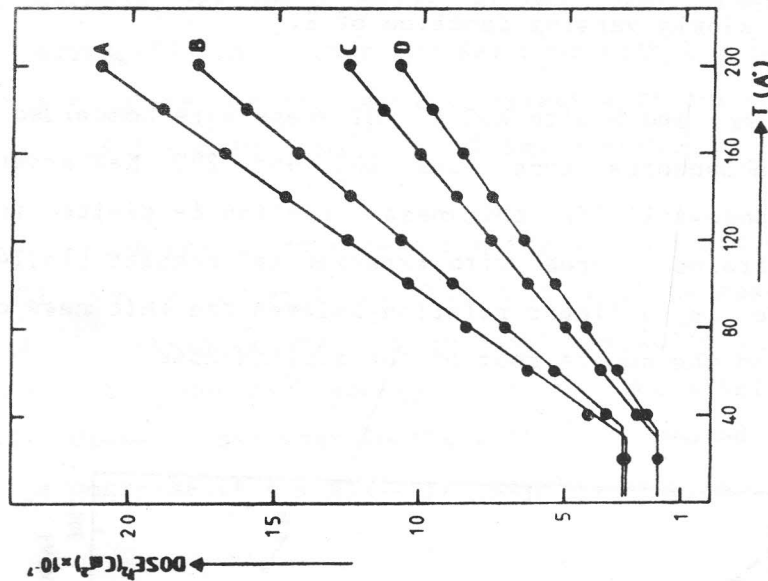
Fig. 4   Dose-Silicide thickness relation for 100 KeV P on Mo/Si(A), 150 KeV P on W/Si (B), 200 KeV As on Mo/Si (C) and 250 KeV As on W/Si (D).

Conclusion

A new method for silicide formation is accomplished by ion beam mixing using ion implantation. A model is presented to calculate the energy and dose required for silicidation, and the results are found to agree with experimental values. It is predicted that the dose required for complete mixing to increase with increasing energy. In agreement with experiments, the thickness of the formed metal silicide was found to increase linearly with the square root of the applied dose.

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