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Grain growth mechanism in heavily arsenic-doped polycrystalline silicon

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The mechanism of grain growth in heavily arsenic-doped polycrystalline silicon has been investigated by developing a kinetic model. A computer simulation technique has been used to determine the grain boundary self-diffusion of the silicon atoms and hence the grain size for different arsenic concentrations, annealing times and temperatures has been estimated. The evaluated numerical values are compared with the available experimental values. Using this model the grain size distribution in arsenic-doped polysilicon for various values of arsenic concentration, annealing time and temperature has been determined. The results are discussed in detail.

1. Introduction

Polycrystalline silicon is commonly used as an interconnect and as a gate material for most metal–oxide–semiconductor (MOS) devices. To reduce the resistivity of polysilicon, it is doped with impurities. Wada and Nishimatsu [1] have investigated dopant-enhanced grain growth in phosphorus-doped polysilicon owing to high-temperature annealing.

When polysilicon is subjected to annealing, its grain boundary will migrate. This process is known as grain growth. Recently many researchers have been attracted by the mechanism of grain growth in various materials. In the case of metals, a driving force exists from the reduction of grain boundary energy during thermal treatment. It is reported that the grain growth mechanism in polysilicon is due to the diffusion of atoms from one grain to another [2]. The determination of energy for the diffusion of atoms from one grain to another is more important because the driving force has an important role in the grain growth mechanism. Many experimental results [1–4] on grain growth in polycrystalline silicon are available. The effect of grain growth conditions on the polycrystalline silicon diameter has been studied [5]. However, concerning the grain growth mechanism only a few results [6–8] have been reported.

Many theoretical reports on grain size distribution are available [9–16], but there are no reports on the grain size distribution in heavily arsenic-doped polysilicon during high-temperature annealing. The investigation of the distribution of grains in the polycrystalline silicon matrix, and hence the knowledge of average grain size, are extremely useful in fabricating high-value resistors and gate electrodes in integrated circuits. In this paper we have evaluated the grain size and size distribution in heavily arsenic-doped polycrystalline silicon as a function of arsenic concentration, annealing time and annealing temperature by proposing a kinetic model. The evaluated numerical values of the grain size have been compared with the available experimental values. The results are discussed.

2. Kinetic model

To determine the grain size and its distribution in arsenic-doped polycrystalline silicon we have used a kinetic model based on the diffusion of silicon atoms from one grain to another. In the absence of any driving force for the grain growth, the net amount of silicon atoms transferred from one grain to another is zero. The driving force for the movement of atoms from one grain to another is related to the grain boundary energy and the radius of the grain. The difference in chemical potential of the silicon atoms on either side of the grain boundary, which is the driving force for grain growth, is given by [8]

$$\Delta\mu = K_1 a^3 \gamma / r \tag{1}$$

where K_1 is a constant related to the geometric shape of the grains (for spherical grains $K_1 = 2$), γ is the grain boundary energy, a is the lattice constant of silicon and r is the grain size.

From basic rate theory, the net rate of atomic transfer across the boundary (from lattice sites of one grain to those of a neighbour) is given by [7]

$$n = \frac{D_g}{\lambda^2}\left[1 - \exp\left(-\frac{\Delta\mu}{kT}\right)\right] \tag{2}$$

where D_g is the self-diffusion constant of the silicon atoms along the grain boundary, k is the Boltzmann constant, T is the annealing temperature and λ is the thickness of the grain boundary. The rate of boundary motion is given by the product of the net rate of atomic transfer across the boundary and the thickness. Therefore, the grain growth rate becomes

$$\frac{dr}{dt} = n\lambda = \frac{D_g}{\lambda}\left[1 - \exp\left(-\frac{\Delta\mu}{kT}\right)\right] \tag{3}$$

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Expanding the exponential, neglecting the cube and higher powers of $\Delta\mu/kT$ and using Equation 1

$$\frac{dr}{dt} = \frac{2D_g}{\lambda}\left(\frac{C}{r}\right)\left[1 - \left(\frac{C}{r}\right)\right] \quad (4)$$

where $C = K_1 a^3\gamma/2kT$.

Integrating Equation 4

$$2D_gCt/\lambda = [(r - C)^2/2 + 2C(r - C) + C^2\log(r - C)]_{r_0}^{r} \quad (5)$$

where t is the time of annealing and r_0 is the initial grain size. Expanding the right-hand side of Equation 5, applying the limits and neglecting the cube and higher powers of C, since C is very small compared with the value of r_0,

$$r = (C^2 + 4D_gCt/\lambda + r_0^2 + 2Cr_0)^{1/2} - C \quad (6)$$

It is noted that the grain size is directly proportional to the square root of the annealing time as reported earlier [5–7].

3. Size distribution of grains

Extending the above kinetic model, the size distributions in polysilicon doped with arsenic have been investigated for various values of arsenic concentrations, times of annealing and annealing temperatures. By introducing a dimensionless variable known as the relative grain size, $U = r/r_{cr}$, in Equation 4 and simplifying

$$\frac{dU^2}{d\tau} = \frac{4D_gC}{\lambda}\left(1 - \frac{C}{Ur_{cr}}\right)\frac{dt}{dr_{cr}^2} - U^2$$

where

$$\frac{1}{d\tau} = \frac{r^2}{dr_{cr}^2}$$

r_{cr} is the average grain size and $d\tau$ represents the time.

$$\frac{dU^2}{d\tau} = S_1\left(1 - \frac{S_2}{U}\right) - U^2$$

where $S_1 = (4D_gC/\lambda)(dt/dr_{cr}^2)$ and $S_2 = C/r_{cr}$.

$$\frac{dU}{d\tau} = \frac{1}{2U}\left[S_1\left(1 - \frac{S_2}{U}\right) - U^2\right] \quad (7)$$

Equation 7 has been solved to determine the steady-state grain size distribution during normal grain growth in polysilicon, using the approach of Hillert [9]. The whole distribution of the individual grain size during the steady state is given by

$$P(U) = -\tfrac{1}{2}\exp(-\beta\psi/2)/(dU/d\tau) \quad (8)$$

where β is a constant ($\beta = 2$ for a two-dimensional system, $\beta = 3$ for a three-dimensional system) and

$$\psi = \int_0^U dU/(-dU/d\tau) \quad (9)$$

From Equations 7 and 9

$$\psi = [\tfrac{2}{3}\log(U^3 - S_1U + S_1S_2)]_0^U + Z \quad (10)$$

where

$$Z = \frac{2S_1}{3}\int_0^U \frac{dU}{U^3 - S_1U - S_1S_2}$$

A numerical integration method has been followed to determine the value of Z. Substituting the values of $dU/d\tau$ and ψ from Equations 7 and 10, respectively, into Equation 8,

$$P(U) = \frac{\beta U^2}{(U^3 - S_1U + S_1S_2)[(U^3 - S_1U + S_1S_2)/S_1S_2]^{\beta/3}\exp(\beta Z/2)} \quad (11)$$

Equation 11 gives the grain size distribution in arsenic-doped polycrystalline silicon.

4. Simulation model

A computer simulation technique has been used to evaluate the numerical values of our theoretical findings. To determine the grain boundary self-diffusion of silicon atoms (D_g), we followed the method used by Mei *et al.* [2]. The grain boundary self-diffusion of silicon atoms along the grain boundary is given by

$$D_g = D^1\phi\frac{\exp(\Delta G_b/kT)}{[1 + AC_1\exp(G_a/kT)]^2} \quad (12)$$

where D^1 is the diffusivity in bulk, ϕ is a constant (its value is 10^{-11} [2]), ΔG_b, the difference in the diffusion activation energy between the grain boundary and bulk, is 3.7 eV, A, the vibrational entropy factor, is 3.02 [17], G_a, the heat segregation, is 39.94 kJ mol^{-1} [17] and C_1 is the atomic fraction of dopants inside the grain, which is a function of grain size as given by [5]

$$C_1 = \frac{N_T}{N_{Si}}\left[\frac{Q_s}{rN_{Si}}\exp\left(\frac{G_a}{kT}\right) + 1\right]^{-1} \quad (13)$$

Here N_T is the total arsenic concentration, N_{Si} is the number of silicon atoms per unit volume, Q_s the effective density of segregation sites at the grain boundary (the value of Q_s is 2.64×10^{19} sites m^{-2} for As [17]) and r is the grain size given by Equation 6. Assuming the initial grain size r_0 to be 0.09 μm, the value of C_1 from Equation 13 and hence the value of grain boundary self-diffusion from Equation 12 have been determined. Using the value of D_g, the grain is allowed to grow for 1 min and the grain size is evaluated at the end of 1 min. Using the new grain size (r) at the end of the first time step of 1 min, the new values of C_1 and D_g have been determined and used for the evaluation of the grain size for the next time step of 1 min. The procedure is repeated until the time of annealing is achieved. Similarly, the simulation procedure has been followed for different times and temperatures of annealing and various dopant concentrations. The grain size distribution in the polysilicon at the end of each time is also evaluated using Equation 11.

5. Results and discussion

Figs 1–6 depict the predicted grain sizes in polysilicon doped with arsenic. Fig. 1 shows grain size as a function of annealing temperature for 1 h annealing for five different dopant concentrations. It is found that the grain size decreases with increase of dopant concentrations. The reported experimental values [2] have also been plotted in the figure. Fig. 2 is drawn between

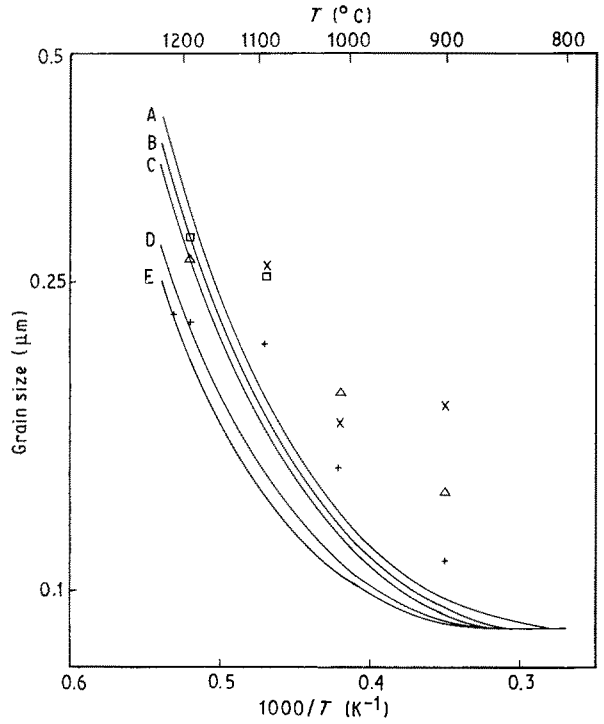

Figure 1 Variation of grain size as a function of temperature for As-doped polysilicon annealing for 1 hour. Δ, +, × and □ are experimental values [2]. (A, □) 1.2×10^{25}, (B, ×) 6.0×10^{25}, (C, △) 1.2×10^{26}, (D) 4.0×10^{26} and (E, +) 6.0×10^{26} atoms m^{-3}.

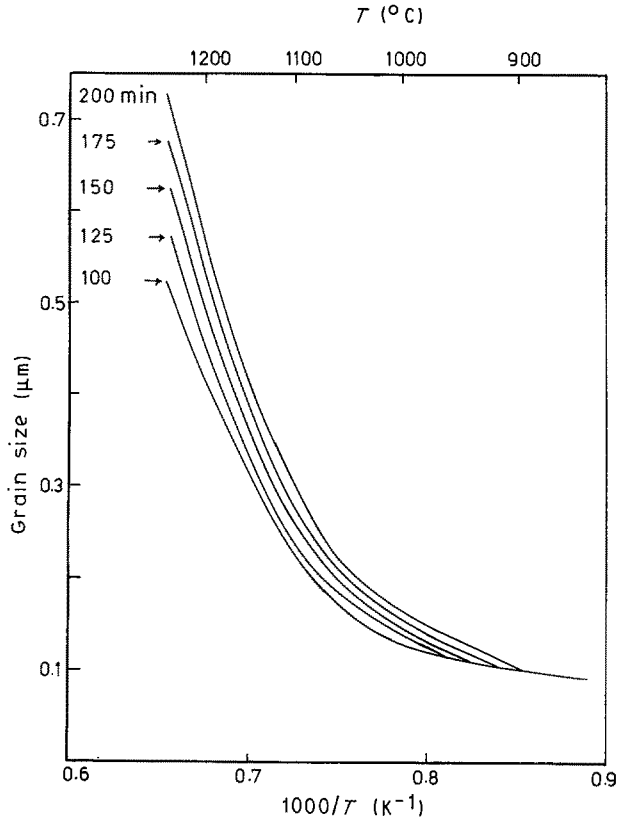

Figure 2 Function of grain size versus annealing temperature for given arsenic concentration 1.2×10^{25} atoms m^{-3} for different annealing times.

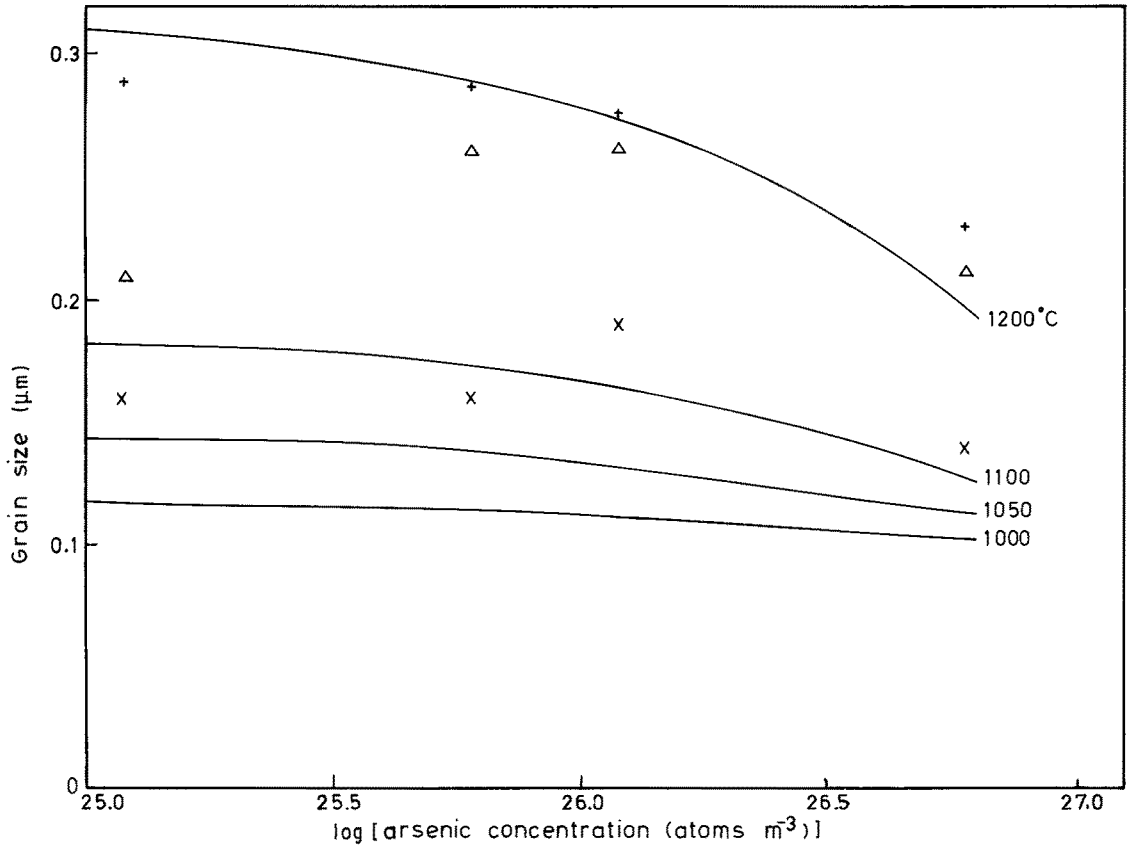

Figure 3 Variation of grain size with the dopant concentrations in As-doped polysilicon after 1 h annealing at four different temperatures. ×, + and △ are experimentally reported values [2]. (+) 1200 °C, (△) 1100 °C and (×) 1000 °C.

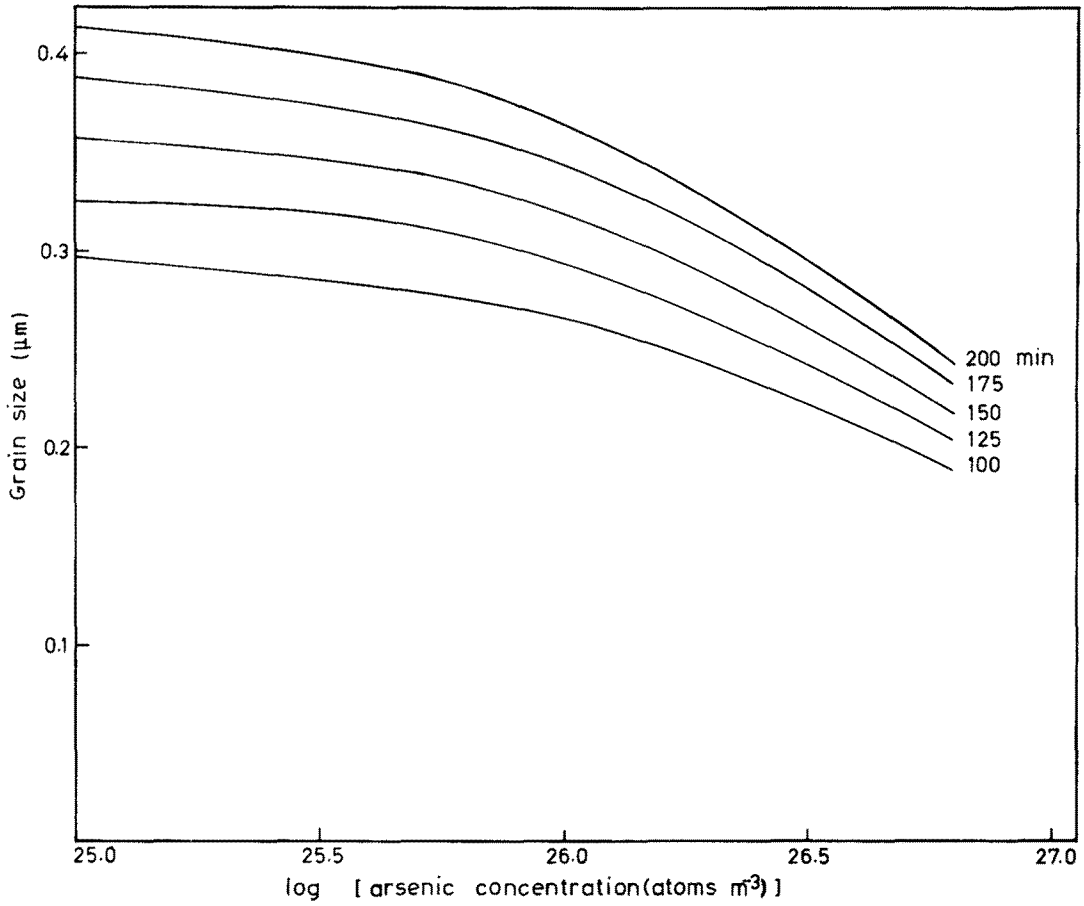

Figure 4 Function of grain size with arsenic concentration for various annealing times and temperature 1423 K.

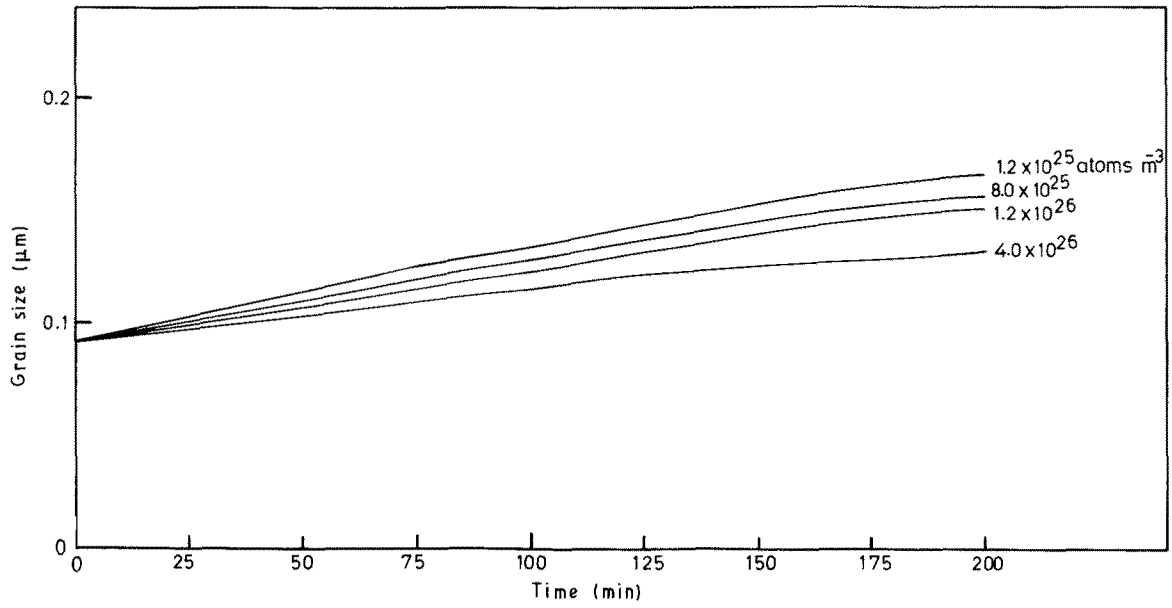

Figure 5 Grain size as a function of annealing time at 1273 K for various As concentrations.

grain size and temperature for the given dopant concentration of 1.2×10^{25} atoms m^{-3} and for five different annealing times. It reveals that grain size increases with time. Fig. 3 shows the grain size as a function of dopant concentrations for 1 h annealing for four different annealing temperatures. It shows that grain size increases with temperature. The reported experimental values [2] have also been shown in the figure. Fig. 4 depict grain size versus arsenic concentration for annealing temperature 1423 K for five different annealing times. From these observations it can be concluded that the grain size increases with time. Fig. 5 depicts grain size versus annealing time for the annealing temperature 1273 K for four various arsenic concentrations. Fig. 6 shows grain size versus annealing time for the dopant concentration 1.2×10^{25} atoms m^{-3} for four different annealing temperatures.

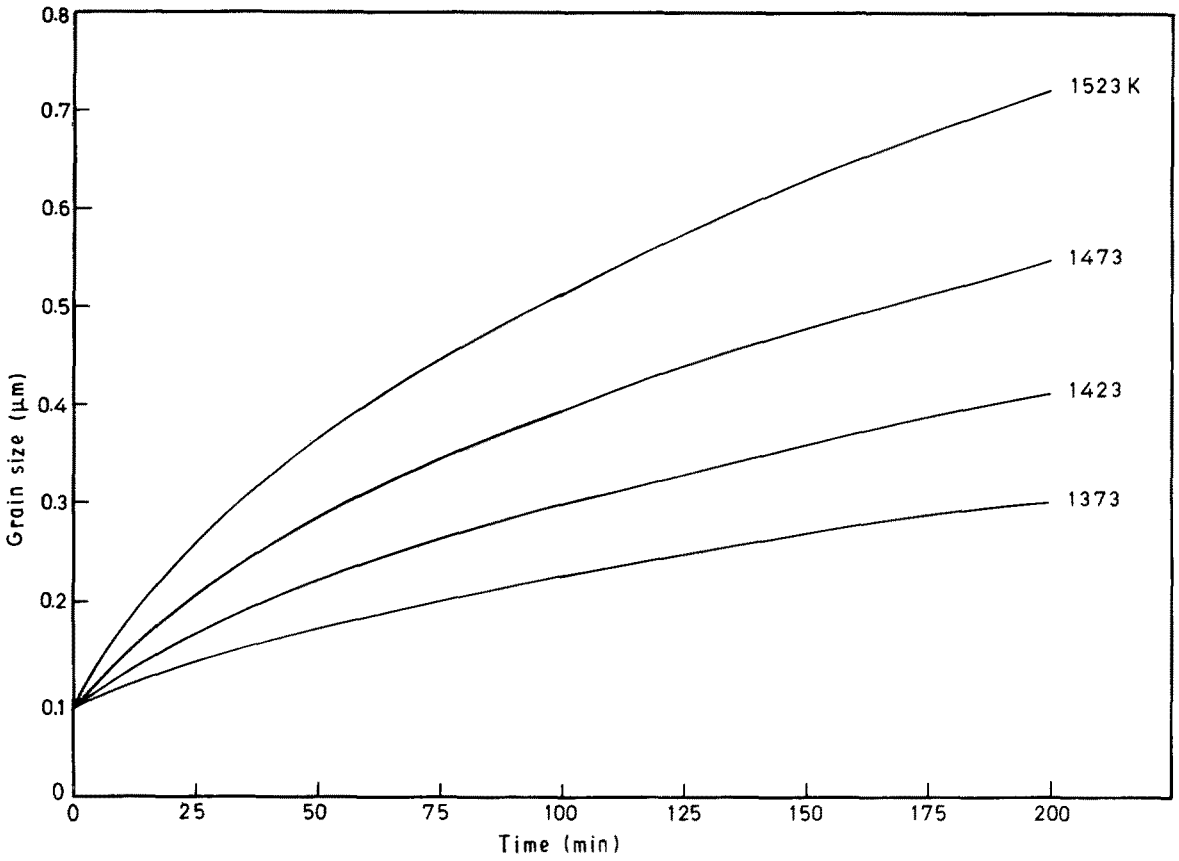

Figure 6 Variation of grain size with annealing time for different annealing temperatures for given As concentration 1.2×10^{25} atoms m^{-3}

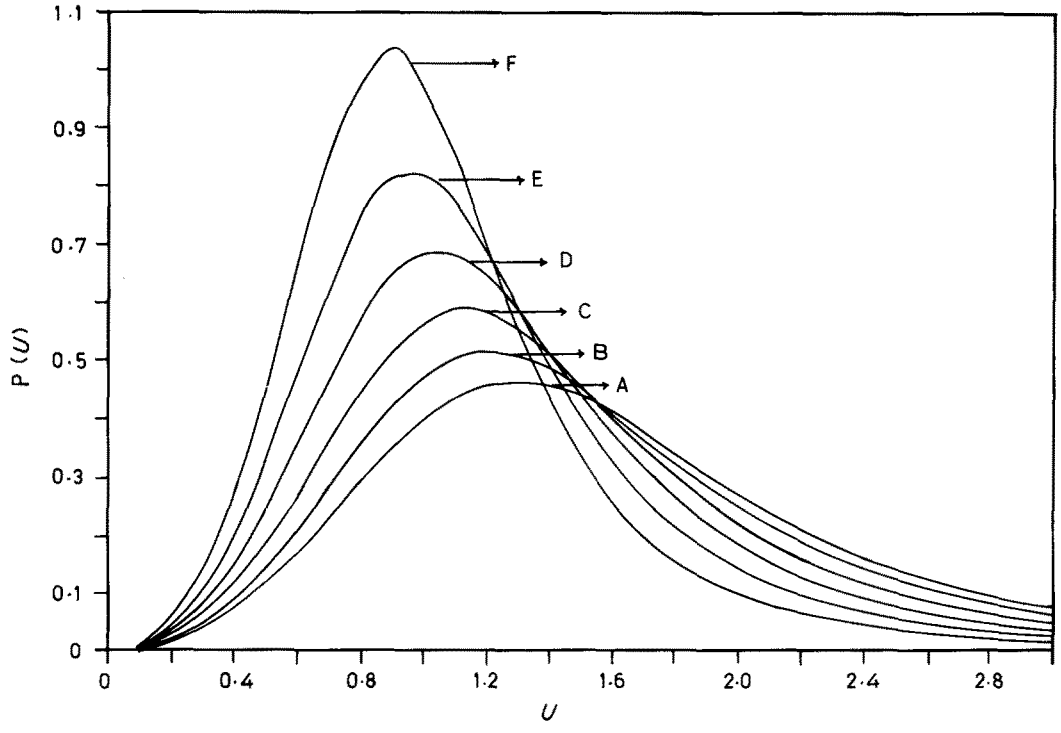

Figure 7 Grain size distribution with relative grain size for six different annealing temperatures for given As concentration 1.2×10^{25} atoms m^{-3} and annealing time 1 h. (A) 1373, (B) 1398, (C) 1423, (D) 1448, (E) 1473 and (F) 1498 K.

Fig. 7 plots the grain size distribution versus relative grain size for the arsenic concentration 1.2×10^{25} atoms m^{-3} for 1 h annealing for six different annealing temperatures. From the graph it is observed that the size distribution attains a maximum value at a single point then decreases and the grain size distribution increases with annealing temperature. Fig. 8 depicts the grain size distribution as a function of relative grain size for the dopant concentration 1.2×10^{25} atoms m^{-3} for the annealing temperature 1473 K for three different annealing times. The broken line in the figure shows Hilleret's [9] size distribution.

Here also the grain size distribution increases to a maximum and decreases for a further increase of relative grain size and the maximum grain size distribution increases with annealing time. Since grain size is a function of annealing time and annealing temperature, the grain size distribution is also a function of annealing time and temperature.

Grain size distribution versus relative grain size is drawn in Fig. 9 for 2 h of annealing, at an annealing temperature of 1448 K and for six various arsenic concentrations. The grain size distribution increases to a maximum at a single point and for a further increase of relative grain size, the distribution decreases. The decrease of grain size distribution is due

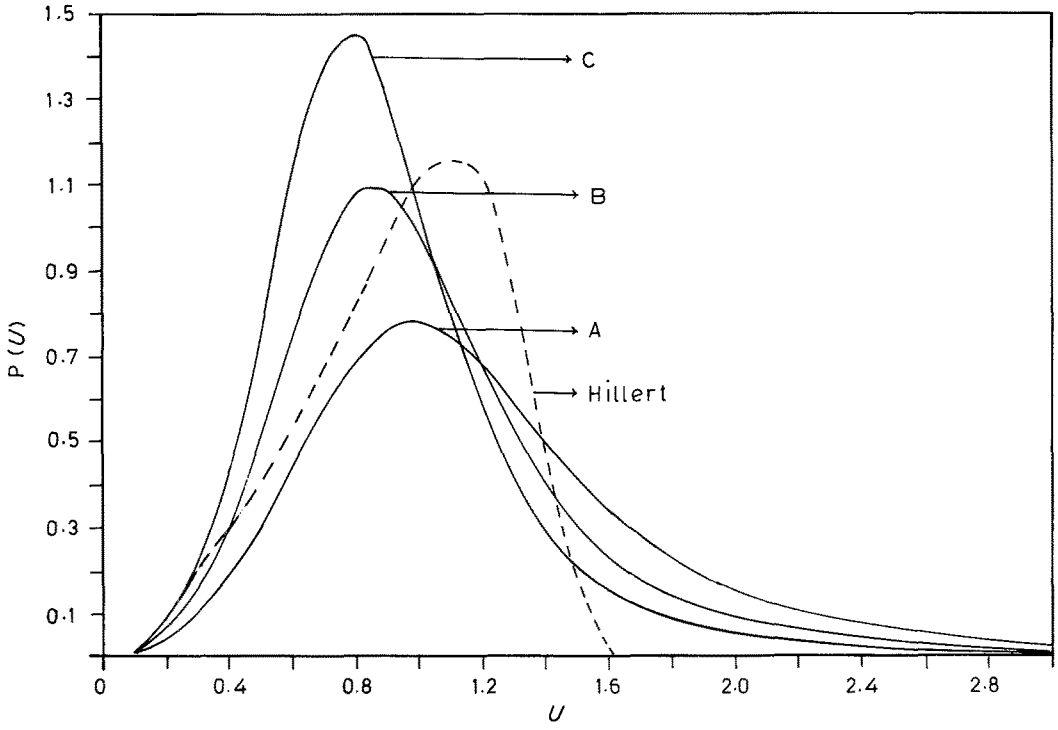

Figure 8 Function of grain size distribution as relative grain size for three different annealing times for annealing temperature 1473 K and As concentration 1.2×10^{25} atoms m^{-3}. The broken line indicates Hillert's grain size distribution [10]. (A) 1 h, (B) 2 h and (C) 3 h.

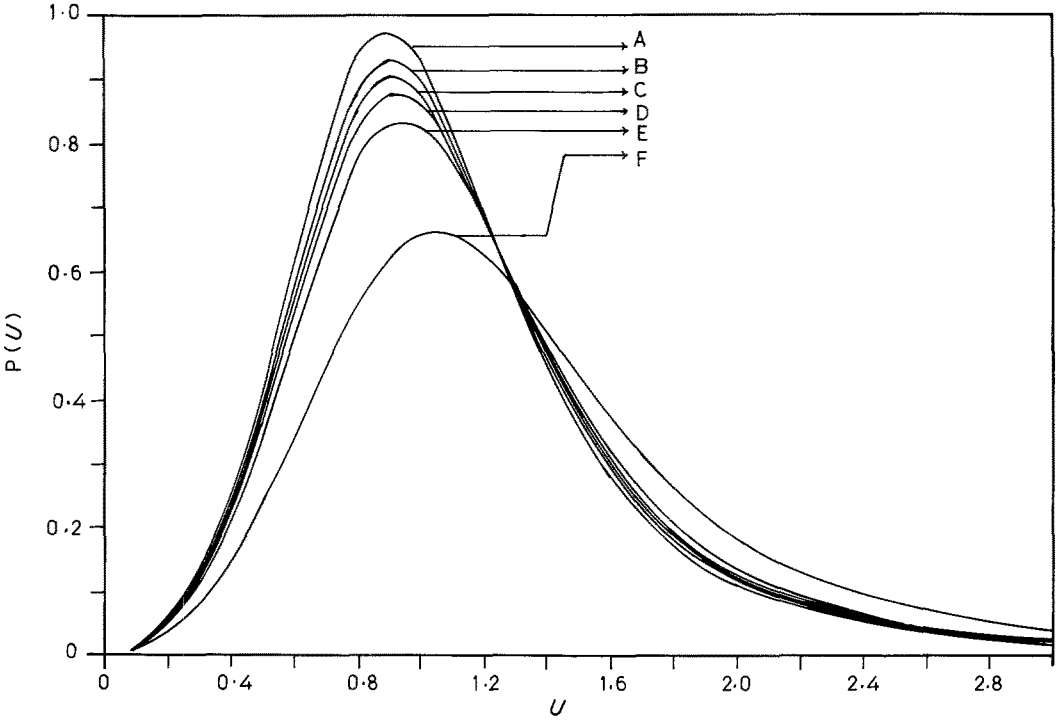

Figure 9 Variation of grain size distribution with relative grain size for six different As concentrations for given annealing time 2 h and temperature 1448 K. (A) 1.2×10^{25}, (B) 4×10^{25}, (C) 6×10^{25}, (D) 8×10^{25}, (E) 1.2×10^{26} and (F) 4×10^{26} atoms m^{-3}.

to the less amount of atoms segregated at the grain boundaries. The nature of Figs 7–9 is in good agreement with reported theoretical results [10–16].

6. Conclusion

From the above results it is concluded that the grain size and size distribution in arsenic-doped polysilicon decrease with arsenic concentration, but they increase with annealing temperature and annealing time. The reason for the decrease of grain size and size distribution with concentration is the less amount of atoms segregated at the grain boundaries.

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