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## Mechanism of Gold Diffusion into Silicon

10 APRIL 1963

*Prepared by*  
W. R. WILCOX  
*Materials Sciences Laboratory*  
*Aerospace Corporation*

and

T. J. LA CHAPELLE  
*Pacific Semiconductors, Incorporated*  
*Lawndale, California*

*Prepared for* COMMANDER SPACE SYSTEMS DIVISION  
UNITED STATES AIR FORCE  
*Inglewood, California*

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**MECHANISM OF GOLD DIFFUSION INTO SILICON\***

**Prepared by**

**W. R. Wilcox  
Materials Sciences Laboratory  
Aerospace Corporation**

**and**

**T. J. LaChapelle  
Pacific Semiconductors, Incorporated  
Lawndale, California**

**AEROSPACE CORPORATION  
El Segundo, California**

**Contract No. AF 04(695)-169**

**10 April 1963**

**Prepared for  
COMMANDER SPACE SYSTEMS DIVISION  
UNITED STATES AIR FORCE  
Inglewood, California**

**\* The laboratory investigations reported herein were performed while both authors were affiliated with Pacific Semiconductors, Inc. Final analyses and reporting were conducted at Aerospace Corporation, under Contract No. AF 04(695)-169.**

## ABSTRACT

Gold was found to diffuse into silicon by a complex mechanism involving a vacancy-controlled interstitial-substitutional equilibrium. This led to very complex diffusion concentration profiles. In analysing the problem, a new experimental value was found for the self-diffusion coefficient of silicon,  $1.81 \times 10^4 \exp(-112 \pm 20 \text{ kcal/RT}) \text{ cm}^2/\text{sec}$ , which compared very favorably with previous data on diffusion of bismuth, germanium, and tin in silicon. The interstitial gold-diffusion coefficient was found to be  $2.4 \times 10^{-4} \exp(-8.9 \pm 2 \text{ kcal/RT})$ , the substitutional gold-diffusion coefficient to be  $2.75 \times 10^{-3} \exp(-47 \pm 10 \text{ kcal/RT})$ , the equilibrium-interstitial gold solubility to be  $5.95 \times 10^{24} \exp(-58 \pm 10 \text{ kcal/RT})$ , and the equilibrium-substitutional gold solubility (Collin's data) below  $1200^\circ\text{C}$  to be  $8.15 \times 10^{22} \exp(-40.6 \text{ kcal/RT})$ .

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## I. INTRODUCTION

Gold conveniently furnishes recombination centers in silicon.<sup>1-5</sup> Because of this, gold has been deliberately diffused into silicon to make high-speed semiconductor devices. The diffusion of gold into silicon was first studied in detail by Struthers using radiotracers.<sup>6</sup> The diffusion coefficients measured gave a good Arrhenius plot from 800°C to 1200°C to yield  $D = 0.011 \exp(-25,800/RT)$ . More recent work, however, has indicated that gold diffuses into silicon at a much slower rate.<sup>7,8</sup> Limited evidence that the diffusion may be structure-sensitive was also reported.<sup>7</sup> It was observed by Dash that gold diffusion at 1150°C resulted in the climb of dislocations.<sup>9</sup> Dash suggested that this phenomenon could be explained by the substitutional-interstitial diffusion mechanism hypothesized for diffusion of copper into germanium.<sup>10-12</sup> In this mechanism, the diffusing atoms move in two manners: interstitially and substitutionally. A high interstitial diffusion rate is combined with low interstitial solubility. Conversely, a low substitutional diffusion rate is combined with high substitutional solubility. The net result is that the diffusive flux is carried almost entirely by interstitial atoms. The interstitials then combine with vacancies to form substitutional atoms. The consuming of vacancies leads to dislocation climb.



The purpose of the work described in this paper was to determine, quantitatively, the mechanism of gold diffusion into silicon. Measurements of the diffusion were carried out from 700°C to 1300°C using radiotracer Au<sup>198</sup> and also Au<sup>199</sup>. Almost 100 wafers were diffused, including dislocation-free Czochralski silicon and floating-zone material (having about  $10^4$  dislocations/cm<sup>2</sup>), high and low resistivity n- and p-type silicon, and previously-diffusion-doped samples.<sup>13</sup> The substitutional-interstitial mechanism was verified, and the parameters involved were determined. Values were determined for interstitial gold solubility, interstitial gold diffusion coefficient, substitutional gold diffusion coefficient, and the self-diffusion rate of silicon.

## II. EXPERIMENTAL PROCEDURE

The experimental techniques used in this work are reported elsewhere in much greater detail than is attempted here.<sup>14</sup> Both (111) floating-zone grown silicon of about  $10^4$  dislocations/cm<sup>2</sup> and dislocation-free (100) Czochralski-grown silicon were used. Comparison with dislocation-free (111) Czochralski-grown material showed that crystal orientation did not affect the gold diffusion. Therefore, in the figures to follow, (100) is taken to mean Czochralski material and (111) to mean floating-zone material. The specimens were in the form of thick cylindrical wafers of about 1 to 2 cm in diameter and 0.5 cm in thickness. The wafers were parallel-lapped with 13-micron garnet. Extreme

care was taken to attain a very clean, oxide-free surface before plating of the gold which was tagged with radiotracers. Both  $\text{Au}^{198}$  and  $\text{Au}^{199}$  were used at different times in tagging stable gold-chloride solutions with radiotracer. Nearly carrier-free  $\text{Au}^{199}$  was also used, undiluted (as supplied by Oak Ridge National Laboratory), in some experiments to produce very low surface concentrations of gold. The gold was chemi-plated onto the wafers by injecting a dilute gold chloride solution into hydrofluoric acid on the surface of the wafer. Autoradiographs before and after diffusion showed that a very uniform layer was obtained (Ref. 14). The wafers were then encapsulated in quartz in an argon atmosphere and placed in the diffusion furnace controlled to  $\pm 2^\circ\text{C}$  for a period of time ranging from 15 minutes to several days. After diffusion, the capsules were quenched by placing them on a massive brass block. Excess surface activity was removed by dissolving the gold with aqua regia. Counting was then begun using a Geiger-Muller tube. Counting accuracy was usually on the order of a few percent. A collimator on the wafer was used to eliminate edge effects and non-parallelism. Thin layers were removed using a high precision machine with fine silicon-carbide paper. Thicknesses were measured by a Mikrokator and by a Mettler microbalance to about  $5 \times 10^{-5}$  cm. Best results were obtained by counting the wafers rather than the paper. The counting rate versus distance was converted to a concentration profile, using the techniques described in Ref. 14.

### III. EXPERIMENTAL RESULTS

The net results of the experiments were plots of gold concentration versus distance into the silicon. The initial experiments were performed between 800°C and 1100°C on dislocation-free silicon. The diffusion was much slower than reported by Struthers,<sup>6</sup> as shown in Fig. 1. In addition, the concentration profiles did not remotely resemble a complementary-error function distribution, which would be expected for a saturated surface condition with a constant diffusion coefficient. It was found, however, that when plotted on log-log paper the profiles were all nearly identical. An empirical curve of the results is shown in Fig. 2. An interesting observation is that the portion of this curve from a concentration of about 10 to 98 percent of the solubility gives a very good straight-line plot of log concentration versus  $\sqrt{x/Kt}$ . The values of K for various materials and diffusion conditions are given in greater detail in Ref. 14. The effect of high prior doping with n- and p-type impurities is also discussed in Ref. 14. Phosphorous-diffused layers with high surface concentrations were found to both hinder the gold diffusion rates and to increase the gold solubilities.

Further experiments revealed that the diffusion rates were higher when floating-zone silicon was used than when dislocation-free silicon was used. It was also found that the ideal error-function complement profile was obtained for high temperatures (1300°C), Fig. 3, and for very long diffusion times at lower temperatures (700°C), Fig. 4. In Fig. 3, note the evidence of out-diffusion within  $10^{-3}$  cm of the specimen surface. This out-diffusion is caused by reduced solubility during cooling from the

diffusion temperature at the end of the run. As would be expected, the out-diffusion was more severe in the high-dislocation-density silicon. Figure 3 also shows Gaussian distributions obtained under conditions of very low surface concentration, designated C. F. in the figures (for nearly carrier-free radiotracer). It was possible to obtain Gaussian distributions at 1200°C, Fig. 5, and even at 1000°C under conditions of very low surface concentrations and high dislocation density. Figure 5 also shows that the diffusion profiles for dislocation-free silicon had already deviated from ideal and were approaching those of Fig. 2. Figure 6 shows typical concentration profiles obtained for diffusion at 1100°C. Note that even the profiles for the (111) floating-zone silicon deviated from the ideal error-function complement at 1100°C.

From the foregoing results, diffusion coefficients were calculated and are shown in Fig. 7 as  $\log D$  versus  $1/T$  (an Arrhenius plot). Calculation of diffusion coefficients for the error-function complement (erfc) and Gaussian-shaped profiles were easily obtained by superimposing log-log plots of these curves on the data. The more complex experimental profiles were analyzed by similarly superimposing on a log-log erfc plot those data points which seemed to fit. Many of the profiles, for example, had erfc tails, as illustrated in Fig. 6. The erfc tails at 800°C and 900°C were much more pronounced than in Fig. 6. Extrapolation of the erfc fit to the tails back to the surface of the sample also gave values for a solubility. As will be seen later, these tails are believed to be caused by interstitial diffusion alone. Hence, the extrapolated surface concentration is believed to be the interstitial gold solubility. The ratio of total gold solubility to

the interstitial gold solubility is given in Fig. 8, where it is compared with values obtained from calculations using data in Fig. 7. Because the interstitial solubility is so much lower than the substitutional solubility, the substitutional solubility is very nearly equal to the total gold solubility. Fitting the erfc curve to the rest of the data of complex profiles likewise gave diffusion coefficients, shown in Fig. 7. The diffusion coefficients given by Boltaks<sup>7</sup> and Struthers<sup>6</sup> are also shown in Fig. 7.

#### IV. DISCUSSION

In attempting to determine the best mechanism for gold diffusion in silicon based on the experimental data, we will assume a substitutional-interstitial process and analyze the data on this basis. If the results are reasonable, this can be taken as strong evidence supporting the assumed mechanism.

The various types of diffusion coefficients which can arise with the assumed mechanism are summarized in Table 1. The method of derivation is illustrated in the Appendix.

Table 1. Diffusion Coefficients Arising in Substitutional-Interstitial Diffusion Mechanism

Type of Curve	Case	Assumptions <sup>a</sup>	Diffusion Coefficient <sup>a</sup>
Erfc Overall	(1)	$C_v = (C_v)_s$ , high $N_{dis}$ and/or high T	$\frac{(C_i)_s}{(C_i)_s + (C_{sub})_s} D_i$
	(2)	Long time, low T	$D_{sub}$
	(3)	$C_i = (C_i)_s$ , low $N_{dis}$	$\frac{(C_v)_s}{(C_v)_s + (C_{sub})_s} D_v$
Gaussian	(4)	Low surface concentration, $C_i \ll C_v$	$\frac{(C_i)_s}{(C_i)_s + (C_{sub})_s} D_i$
	(5)	low surface concentration, $C_i \gg C_v$	$D_i$
Tail Region	(6)	$C_i \ll C_v$	$\frac{(C_i)_s}{(C_i)_s + (C_{sub})_s} D_i$
	(7)	$C_i \gg C_v$	$D_i$
Surface Region	(8)	Long time, low T	$D_{sub}$
	(9)	$C_i = (C_i)_s$ , low $N_{dis}$	$\frac{(C_v)_s}{(C_v)_s + (C_{sub})_s} D_v$
<sup>a</sup> $N_{dis}$ denotes dislocation density, T denotes temperature, C denotes concentration, D denotes diffusion coefficient. Subscripts as follows: i = interstitial gold, sub = substitutional gold, v = vacancy, s = saturation or solubility value.			

If the diffusion coefficients and concentrations of vacancies, interstitial gold, and substitutional gold can all be assumed to vary according to the Arrhenius law,<sup>15</sup> then a plot of  $\log D$  versus  $1/T$  should show a straight line. Figure 7 shows, in fact, three apparent straight lines, which are designated as Curves I, II, and III. The equations of these lines in  $\text{cm}^2/\text{sec}$  are

$$\text{Curve I: } D = 2.75 \times 10^{-3} \exp (-47,400/RT) , \quad (1)$$

$$\text{Curve II: } D = 1.15 \times 10^{-3} \exp (-71,800/RT) , \quad (2)$$

$$\text{Curve III: } D = 1.78 \times 10^{-2} \exp (-26,000/RT) . \quad (3)$$

The problem is to determine the meaning of these curves. From Table 1, it is observed that four different diffusion coefficients might arise. We must determine which of the coefficients is applicable to each measured curve.

If we consider the vacancy-diffusion-controlled situation (Case 3, Table 1), then the effective diffusion coefficient  $D_{\text{Au}}$  is given by

$$D_{\text{Au}} = \frac{(C_v)_s}{(C_{\text{sub}})_s} D_v . \quad (4)$$

Here, it is assumed that  $(C_v)_s \ll (C_{sub})_s$ , which is reasonable. Note, however, that

$$\left. \begin{aligned} (C_v)_s D_v &= (X_v)_s \left(\frac{N\rho}{W}\right) D_v \\ &= D_{sd} \left(\frac{N\rho}{W}\right) \end{aligned} \right\} \quad (5)$$

where  $(X_v)_s$  is the equilibrium atom fraction of vacancies in silicon,  $N$  is Avogadro's number,  $\rho$  is the density of silicon, and  $W$  is the atomic weight of silicon. The term  $(N\rho/W)$  is actually the number of silicon atoms per unit volume.

Substituting Eq. (5) into Eq. (4) and solving for  $D_{sd}$  we obtain

$$D_{sd} = (C_{sub})_s D_{Au} \left(\frac{W}{N\rho}\right) \quad (6)$$

If it is assumed that  $(C_{sub})_s \gg (C_i)_s$ , which is in fact shown in Fig. 8, then the equilibrium substitutional gold solubility  $(C_{sub})_s$  is very nearly equal to the total gold solubility, as measured by Collins et al.<sup>3</sup> and by Struthers.<sup>6</sup> With this,  $D_{sd}$  can be calculated using Eq. (6) and the curves I, II, and III, in turn. The true result should be approximately equal to the diffusion coefficients known for substitutional elements in silicon, and, in particular, for the Group IV elements, germanium and tin.



Collins' data<sup>3</sup> for gold solubility can be given by

$$(C_{\text{sub}})_s = 8.15 \times 10^{22} \exp(-40,600/RT) \text{ (gold atoms/cm}^3 \text{ Si)} \quad (7)$$

This is particularly accurate below 1200°C.

Substituting Eq. (7) and Eq. (1), (2), and (3), in turn, into Eq. (6), we obtain, respectively:

$$\text{Curve I: } D_{sd} = 4.32 \times 10^{-3} \exp(-88,000/RT) \quad , \quad (8)$$

$$\text{Curve II: } D_{sd} = 1.81 \times 10^4 \exp(-112,400/RT) \quad , \quad (9)$$

$$\text{Curve III: } D_{sd} = 2.8 \times 10^{-2} \exp(-67,200/RT) \quad . \quad (10)$$

As shown in Fig. 9, the silicon self-diffusion coefficient determined from Curve II, Eq. (9), is very close to the diffusion coefficients of bismuth,<sup>16-18</sup> tin,<sup>19</sup> germanium,<sup>17,18</sup> and fairly near that for indium<sup>16</sup> in silicon.

The gold solubility given by Struthers<sup>6</sup> differs from the data of Collins, used above. Struthers found, approximately,

$$(C_{\text{sub}})_s = 3 \times 10^{21} \exp(-15,300/RT) \quad . \quad (11)$$

This gives, for Curve II:

$$D_{sd} = 6.63 \times 10 \exp (-87,100/RT) \quad . \quad (12)$$

This is also shown in Fig. 9. It appears not to give as good an agreement as that found using the solubility data of Collins. Although this is not entirely certain, we shall tentatively conclude from this that Collins' data for gold solubility is better than that of Struthers.

On the basis of the above calculations and comparisons, we conclude that Curve II of Fig. 7 represents the vacancy-controlled diffusion

$$\frac{(C_v)_s}{(C_{sub})_s} D_v \quad .$$

The only other possible explanation is that this curve is, instead,

$$\frac{(C_i)_s}{(C_{sub})_s} D_i \quad .$$

In such an event, Curve III would have to represent  $D_i$ . The ratio of values on Curve III to those on Curve II must then yield values for  $(C_{sub})_s/(C_i)_s$  if this is true. These values are to be compared with the experimental ratios given in Fig. 8. Because there is virtually no agreement, we have shown that Curve II cannot represent the interstitial-controlled diffusion. Therefore Curve II must represent

$$\frac{(C_v)_s}{(C_{sub})_s} D_v$$

as originally concluded. Curve III must be

$$\frac{(C_i)_s}{(C_{sub})_s} D_i$$

It cannot be  $D_i$  because, as we have just shown, this would necessitate a lower curve for

$$\frac{(C_i)}{(C_{sub})_s} D_i$$

which is not present. It cannot be  $D_{sub}$  because the values are far too large for substitutional diffusion in silicon. Using the experimental results in Fig. 8 for  $(C_{sub})_s/(C_i)_s$  (as determined from the tails on the concentration profiles) together with Eq. (3) for Curve III, we find that

$$D_i = 2.44 \times 10^{-4} \exp(-8,900/RT) \quad (13)$$

From this equation we calculate that, at  $1200^\circ\text{C}$ ,  $D_i = 1.3 \times 10^{-5}$  and, at  $1000^\circ\text{C}$ ,  $D_i = 7.5 \times 10^{-6}$ .

This compares very well with the interstitial diffusants: lithium,<sup>20</sup> nickel,<sup>20</sup> copper,<sup>6, 21-23</sup> helium,<sup>24</sup> and hydrogen<sup>24</sup> in silicon.

Now only Curve I remains. By the foregoing process of elimination and by virtue of the low values, Curve I must represent  $D_{\text{sub}}$ , the pure substitutional diffusion.

As a final point, it is worthwhile to re-examine the older data for gold diffusion in silicon. Struthers' data<sup>6</sup> are shown in Fig. 7 as the S-points and Boltaks'<sup>7</sup> by B-points. Struthers' data fall very nearly on Curve III for interstitial-controlled diffusion. From this, it is surmised that the original experimental conditions were probably as follows: very low perfection silicon with more than  $10^3$  dislocations/cm<sup>2</sup> and/or a surface concentration below saturation. Struthers has, in fact, verified that both of these were his experimental conditions.<sup>25</sup> Boltaks' data, on the other hand, fall very nearly on the vacancy-controlled-diffusion Curve II, indicating that he used saturated surface conditions.

## V. CONCLUSIONS

It has been determined that gold diffuses into silicon by a mechanism analogous to that of copper diffusing into germanium. Movement of gold atoms primarily involves an interstitial diffusion, controlled by the concentration of vacancies (which are necessary to attain the higher substitutional concentrations). Such a complex mechanism often

leads to unusual diffusion-concentration profiles, as exemplified by the most common one, shown in Fig. 2. Prediction of the exact concentration profile, a priori, would necessitate a numerical-computer solution of the differential equations describing simultaneous diffusion of interstitials, substitutionals, and vacancies. Since this mechanism usually causes a strong dependence of the diffusion rate on crystalline perfection and on quantity of diffusant the aforementioned computer solution for a diffusion-concentration profile would necessitate knowledge of the rate of vacancy generation by dislocations in silicon. Values for the latter have not yet been determined.

In the course of these analyses, the parameters of fundamental importance in the diffusion of gold into silicon have been determined as follows.

Self-diffusion coefficient of silicon ( $\text{cm}^2/\text{sec}$ ), Fig. 4:

$$D_{sd} = 1.81 \times 10^4 \exp (-112 \pm 20 \text{ kcal/RT}) \quad (9)$$

Interstitial gold-diffusion rate in silicon ( $\text{cm}^2/\text{sec}$ ):

$$D_i = 2.44 \times 10^{-4} \exp (-8.9 \pm 2 \text{ kcal/RT}) \quad (13)$$

Substitutional gold-diffusion rate in silicon ( $\text{cm}^2/\text{sec}$ ):

$$D_{sub} = 2.75 \times 10^{-3} \exp (-47 \pm 10 \text{ kcal/RT}) \quad (1)$$

Equilibrium-substitutional gold solubility<sup>1</sup> (atoms/cm<sup>3</sup>) below  
1200°C:

$$(C_{\text{sub}})_s = 8.15 \times 10^{22} \exp (-40.6 \text{ kcal/RT}) \quad (7)$$

Equilibrium-interstitial gold solubility (atoms/cm<sup>3</sup>):

$$(C_i)_s = 5.95 \times 10^{24} \exp (-58 \pm 10 \text{ kcal/RT}) \quad (14)$$

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## APPENDIX: TYPICAL DIFFUSION SOLUTIONS

Following are two typical solutions for limiting cases of a vacancy-controlled interstitial-substitutional diffusion. The reaction of an interstitial gold atom going into a substitutional position is represented by



where  $V$  is a vacancy.

It is assumed that the concentration of these three is at equilibrium at all times. This is expressed by

$$\frac{C_{\text{sub}}}{C_i C_v} = K \quad , \quad (16)$$

where  $K$  is an equilibrium constant which is a function of temperature alone.

### Case A

Assume  $C_v = (C_v)_s$ , the maximum solubility of vacancies:

$$D_{\text{sub}} \ll D_v; \text{ and } D_{\text{sub}} \ll D_i \quad .$$



The first condition holds for a very high dislocation density (since vacancies are produced at dislocations) or where the gold concentration is so low that few vacancies are consumed. The gold concentration is also very low for the first gold atoms that penetrate deeply into the crystal. The first condition may also be true even in dislocation-free crystals at high temperatures where the number and rate of generation of vacancies is greater. The second and third conditions, which state that the substitutional atoms are relatively stationary, are known to be at least approximately true.

The expression for interstitial diffusion is

$$D_i \frac{\partial^2 C_i}{\partial x^2} = \frac{\partial C_i}{\partial t} + \frac{\partial C_{\text{sub}}}{\partial t} \quad (17)$$

But, from Eq. (16), we know that

$$C_{\text{sub}} = K C_i (C_v)_s \quad (18)$$

Therefore, Eq. (17) becomes

$$D_i \frac{\partial^2 C_i}{\partial x^2} = \left[ 1 + K(C_v)_s \right] \frac{\partial C_i}{\partial t} \quad (19)$$

For constant interstitial surface concentration, the solution to this is

$$C_i = (C_i)_s \operatorname{erfc} \left\{ \frac{x}{2[(D_i)_{\text{eff}} t]^{1/2}} \right\} \quad (20)$$

where

$$\left. \begin{aligned} (D_i)_{\text{eff}} &= \frac{D_i}{1 + K(C_v)_s} \\ &= \frac{(C_i)_s}{(C_i)_s + (C_{\text{sub}})_s} D_i \end{aligned} \right\} \quad (21)$$

Using the equilibrium expression, Eq. (18), we find that

$$C_{\text{sub}} = (C_{\text{sub}})_s \operatorname{erfc} \left( \frac{x}{2[(D_i)_{\text{eff}} t]^{1/2}} \right) \quad (22)$$

Hence, the effective diffusion coefficient for gold is

$$\frac{(C_i)_s}{(C_i)_s + (C_{\text{sub}})_s} D_i \approx \frac{(C_i)_s}{(C_{\text{sub}})_s} D_i \quad (23)$$

assuming

$$(C_i)_s \ll (C_{\text{sub}})_s$$

Case B

Assume  $D_i \gg D_{\text{sub}}$ ; then

$$D_i \frac{\partial C_i}{\partial x} \gg D_v \frac{\partial C_v}{\partial x} \quad (24)$$

and that the silicon is dislocation free.

In essence, it is assumed that only the interstitial gold atoms move, so that the vacancy concentration is the saturated value reduced by the number of substitutional gold atoms, i. e. ,

$$C_v = (C_v)_s - C_{sub} \quad (25)$$

Substituting this into Eq. (6) we find that

$$\frac{C_{sub}}{C_i [(C_v)_s - C_{sub}]} = K \quad (26)$$

Differentiating with respect to time, there results

$$\frac{\partial C_{sub}}{\partial t} = \left[ \frac{K(C_v)_s}{1 + K C_i} - \frac{K^2 C_i (C_v)_s}{(1 + K C_i)^2} \right] \frac{\partial C_i}{\partial t} \quad (27)$$

Substituting this into Eq. (17), we obtain

$$D_i \frac{\partial^2 C_i}{\partial x^2} = \frac{1}{f(C_i)} \frac{\partial C_i}{\partial t} \quad (28)$$

where

$$f(C_i) = \frac{(1 + K C_i)^2}{(1 + K C_i)^2 + K (C_v)_s} \quad (29)$$

For constant interstitial surface concentration, the solution to this is<sup>26</sup>

$$C_i = (C_i)_s \operatorname{erfc} \left\{ \frac{x}{[(D_i)_{\text{eff}} t]^{1/2}} \right\} \quad , \quad (30)$$

where

$$(D_i)_{\text{eff}} = f(C_i) D_i \quad .$$

This, in turn, gives an effective diffusion coefficient for the total gold content which is a function only of concentration. This is not much help quantitatively but indicates that  $C/C_s$  can be a single function of  $x/\sqrt{t}$  at a given temperature (as was found experimentally in Fig. 2) and still conform to the present mechanism.

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## FIGURES

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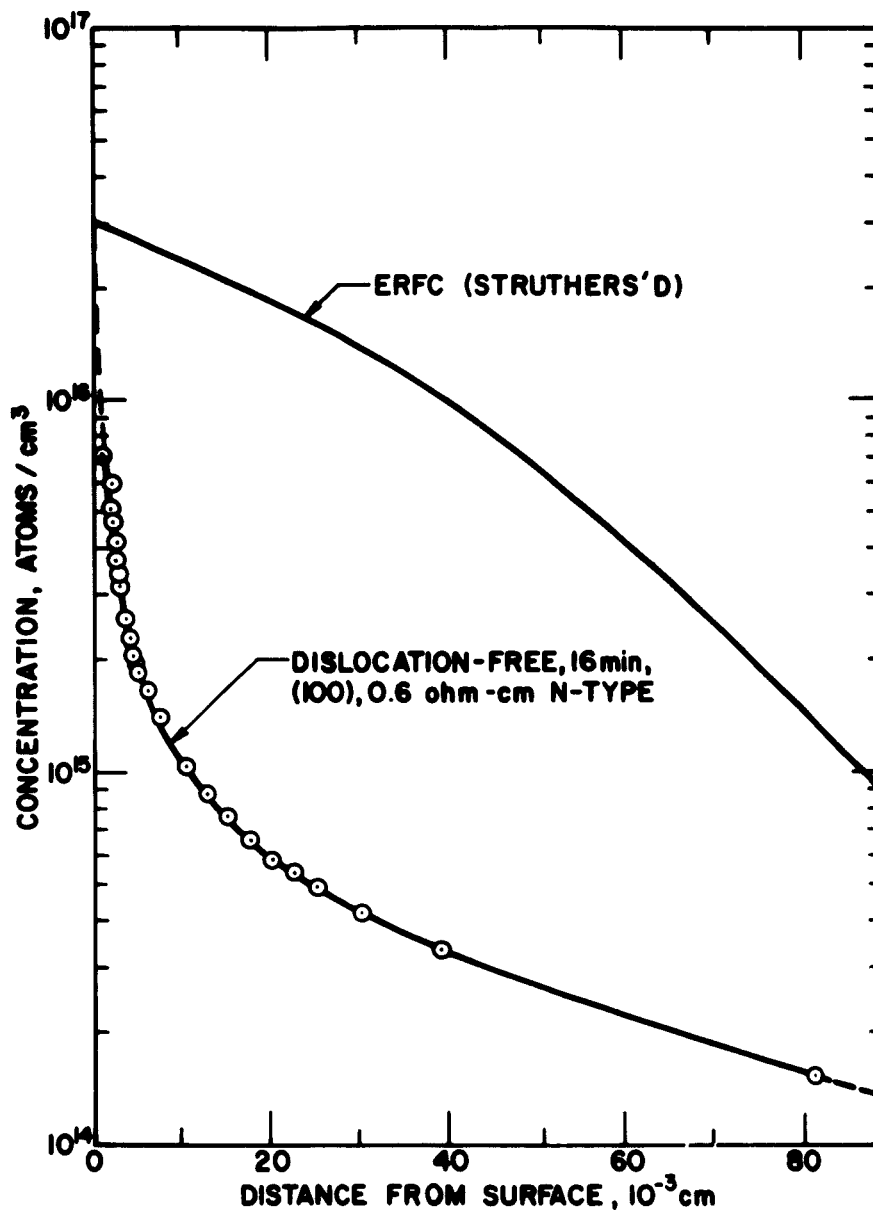
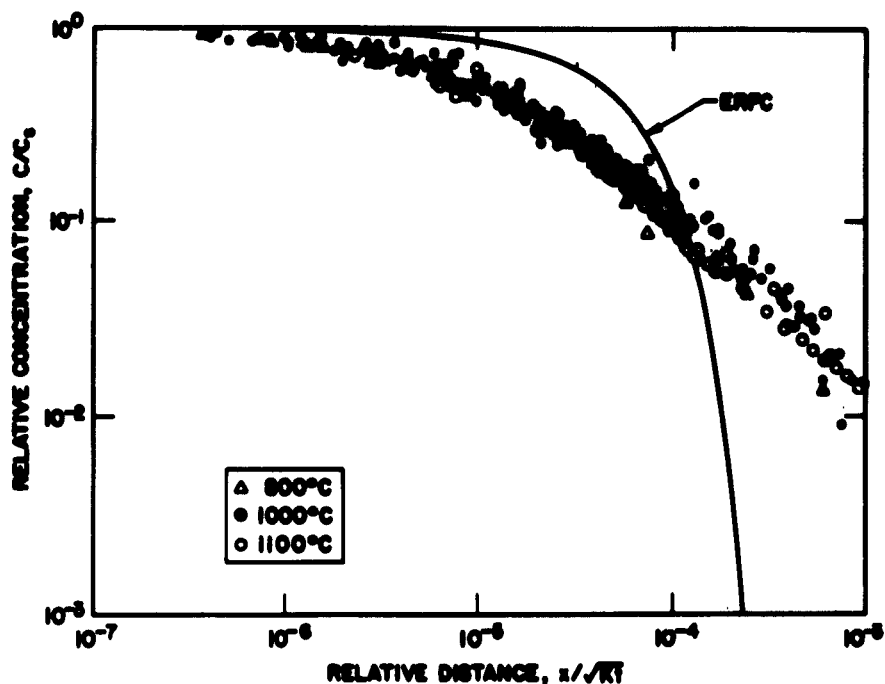


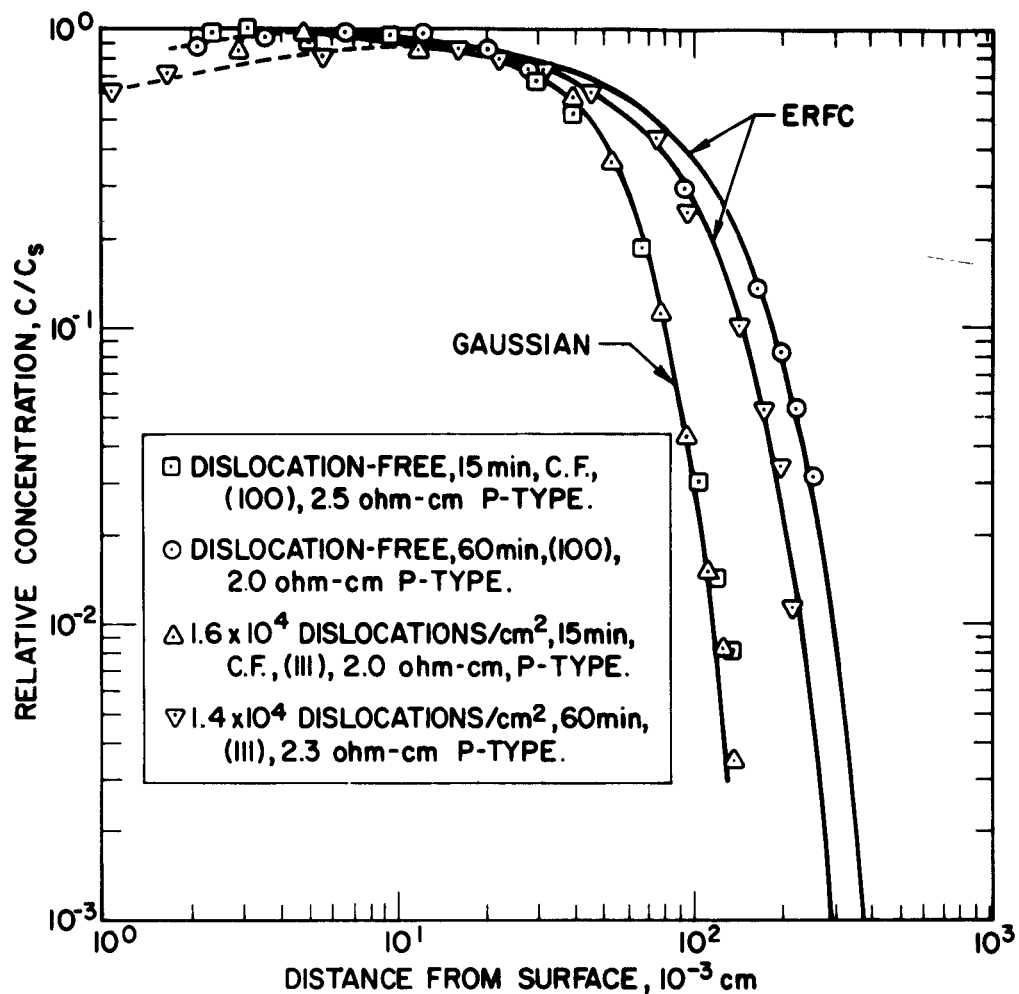
Fig. 1. Concentration Profile for Gold Diffusion into Dislocation-Free Silicon at 1097°C; Compared to Struthers' Results





Error-function complement curve is shown for comparison of shape only, relative position being unimportant. Here  $C$  represents the gold concentration at distance  $x$  from the surface (where the concentration is equal to the solubility value  $C_s$ ),  $t$  is the time of diffusion and  $K$  is a constant necessary to superimpose the data, and may be considered to be an effective diffusion coefficient.

Fig. 2. Empirical Correlation of Concentration for Gold Diffusion into Dislocation-Free Silicon from 800°C to 1100°C



C. F. denotes that undiluted radiotracer ( $\text{Au}^{199}$  as supplied) was used in plating surface before diffusion.

Fig. 3. Concentration Profiles for Gold Diffused into Silicon at  $1300^\circ\text{C}$

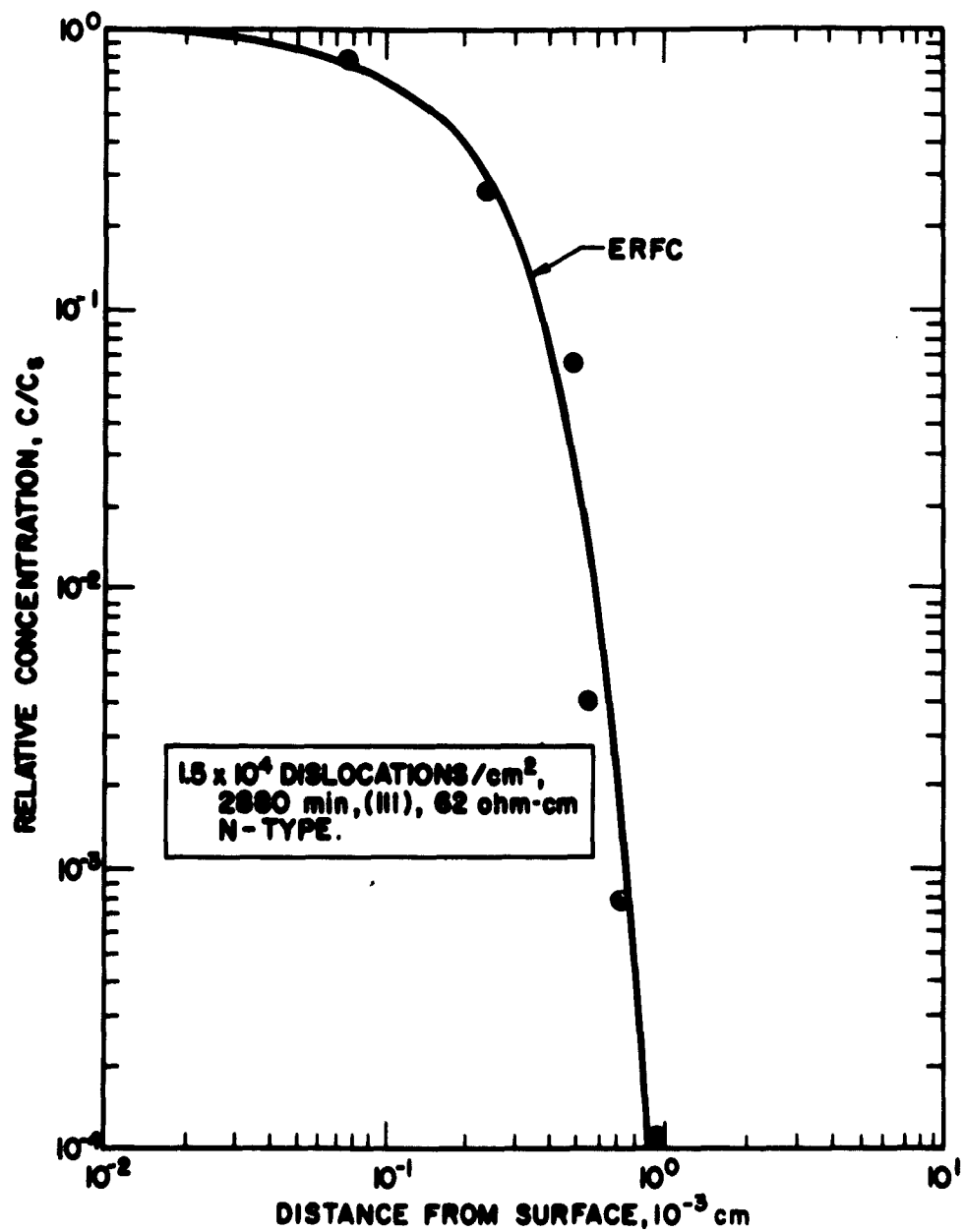


Fig. 4. Distribution of Gold Diffused into Silicon at  $700^{\circ}\text{C}$

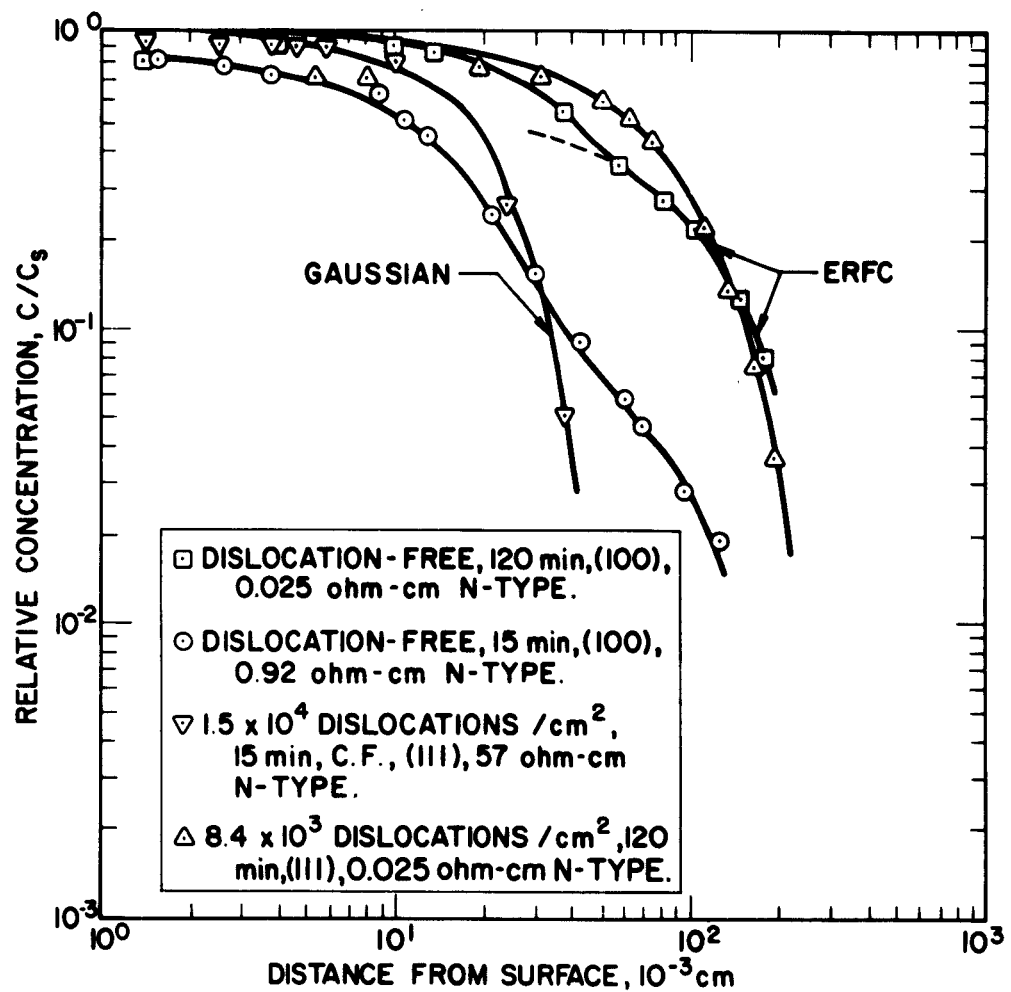


Fig. 5. Distribution of Gold Diffused into Silicon at 1200°C

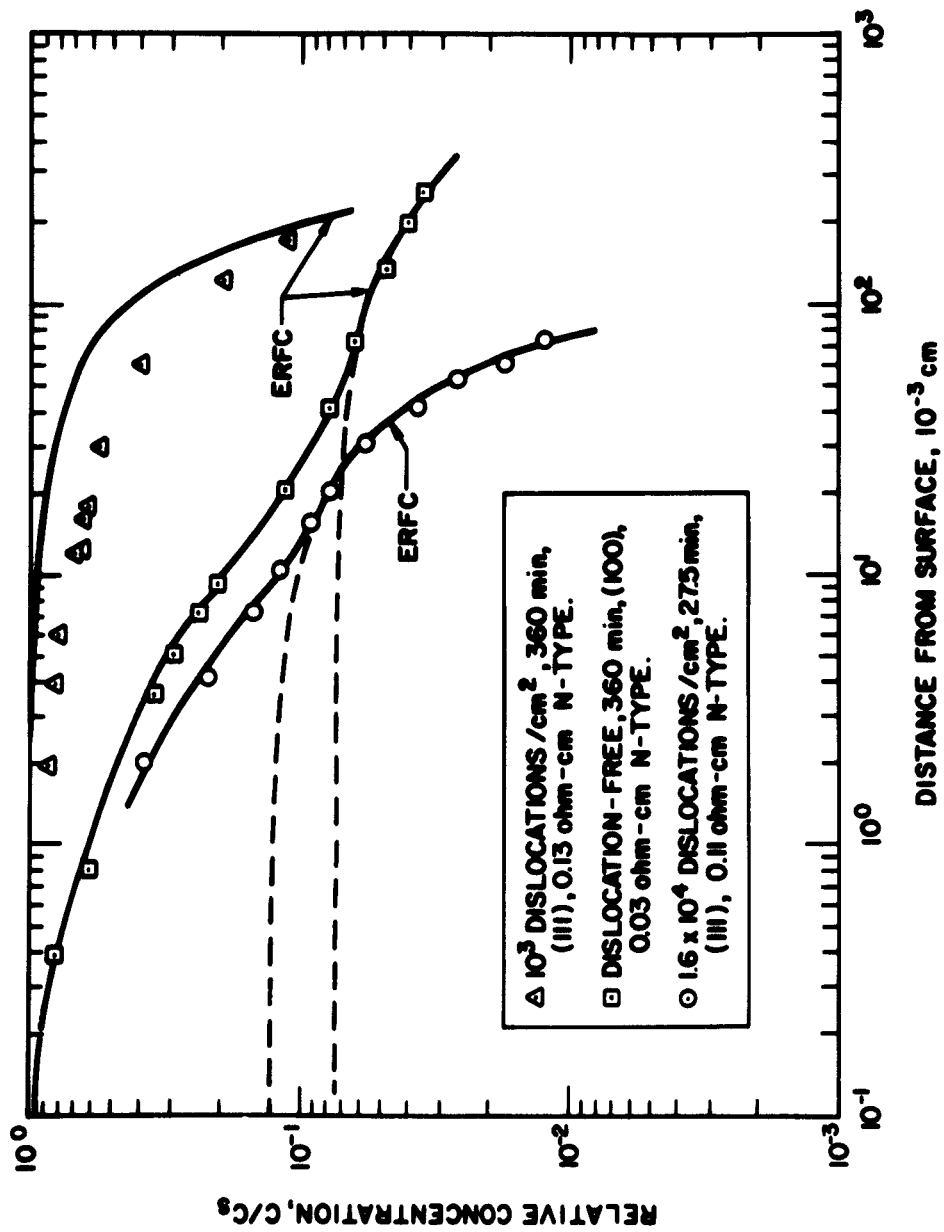


Fig. 6. Distribution of Gold Diffused into Silicon at  $1000^\circ\text{C}$

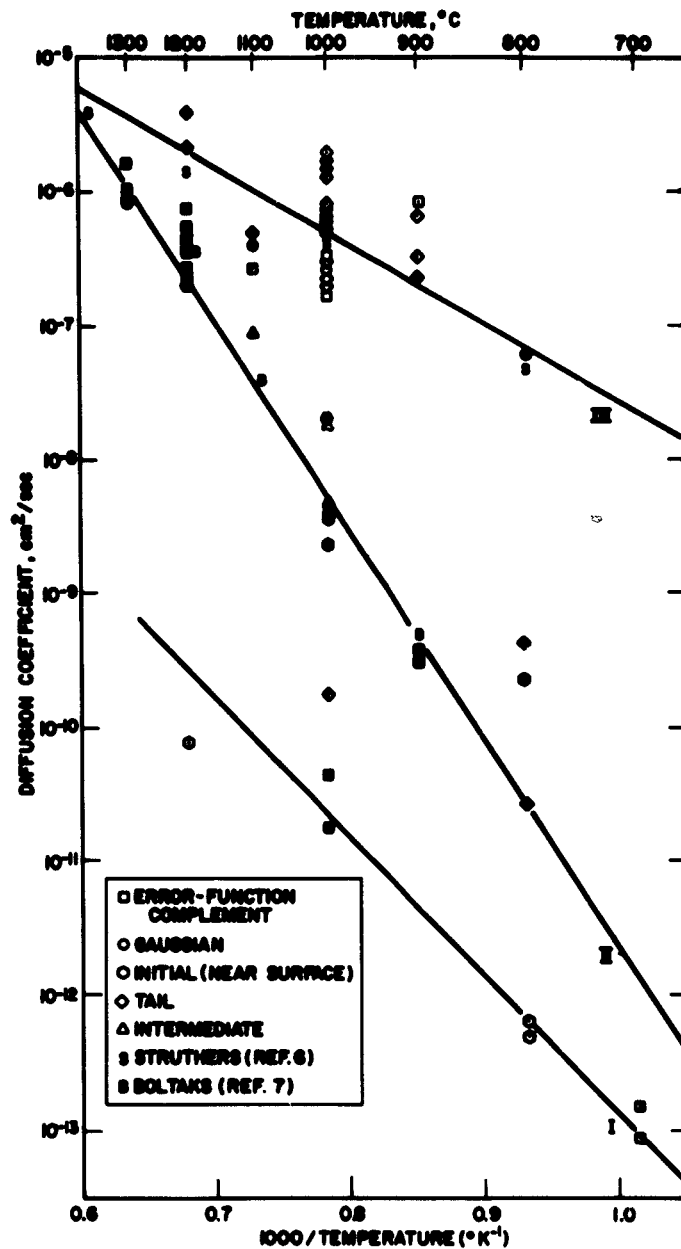


Fig. 7. Diffusion Coefficients Calculated from Experimental Diffusion Concentration Profiles as a Function of Inverse Temperature (Arrhenius Plot)

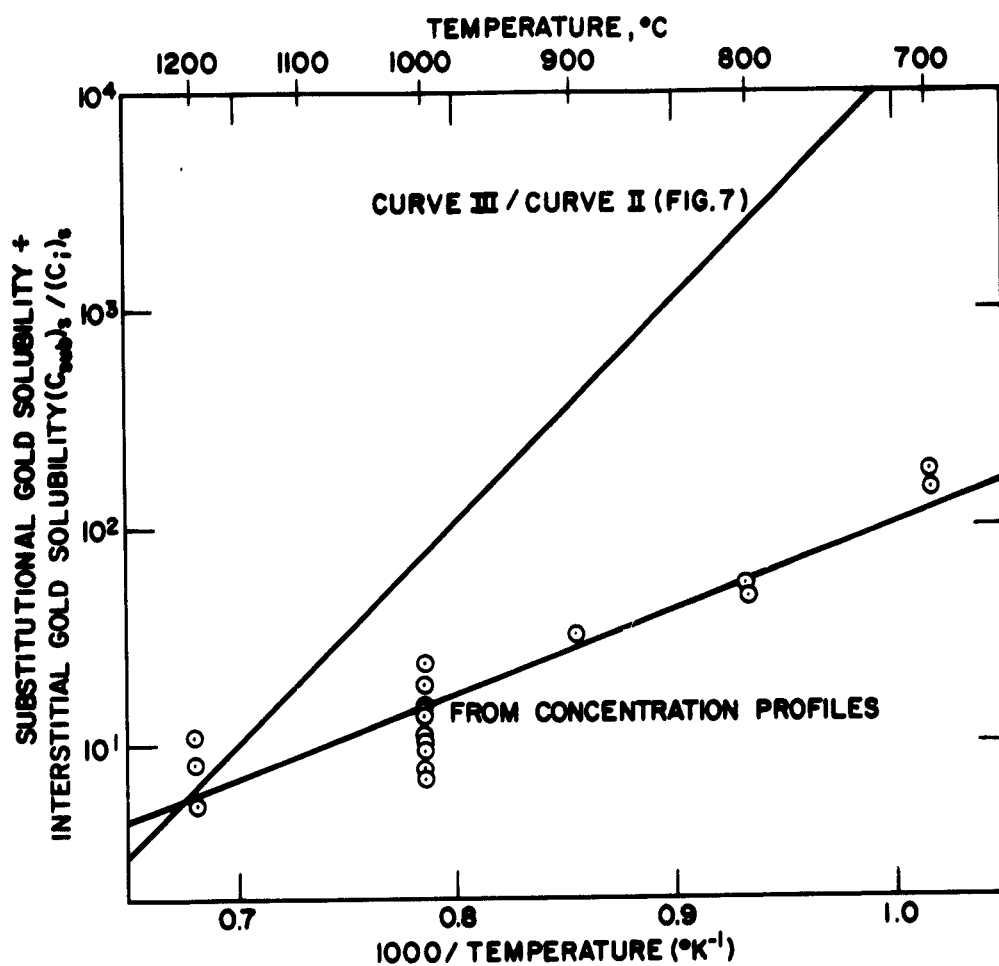


Fig. 8. Ratio of Substitutional to Interstitial Gold Concentrations, as Calculated from Experimental Diffusion Concentration Profiles and from Curves II and III in Fig. 7

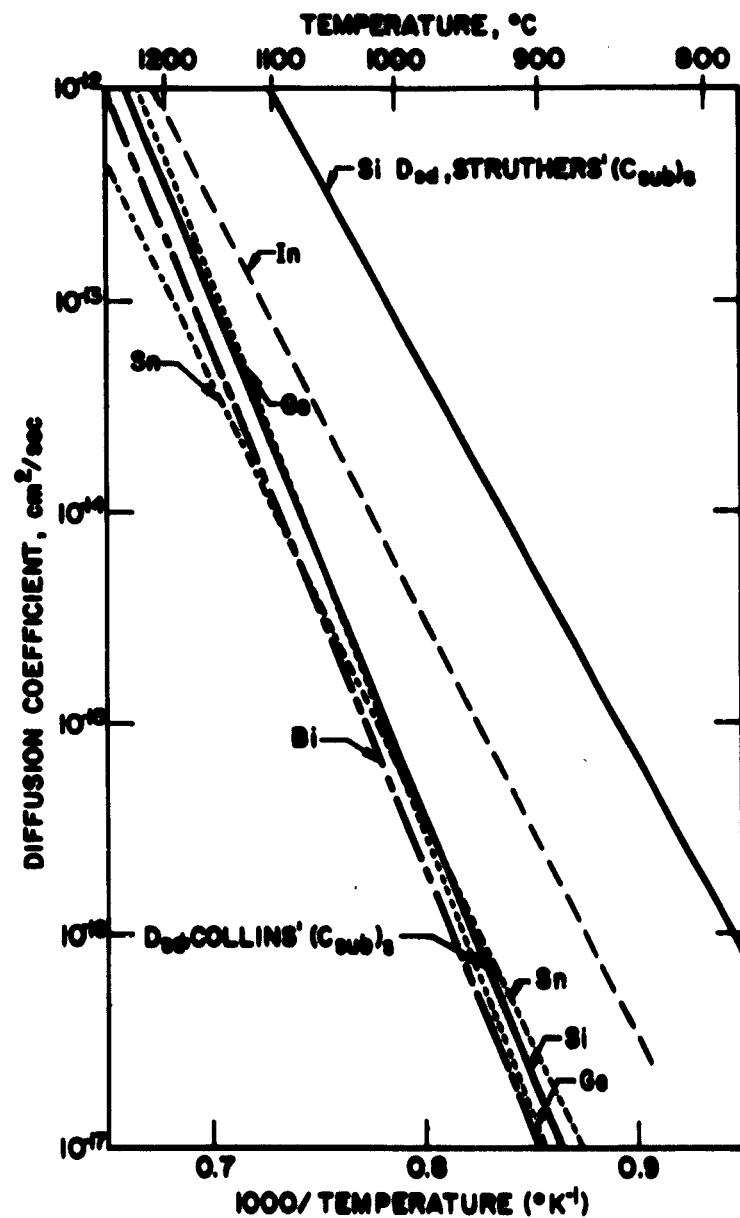


Fig. 9. Comparison of Calculated Self-Diffusion Coefficient of Silicon with Previous Data for Impurity Diffusion into Silicon



<p>● UNCLASSIFIED</p>	<p>Aerospace Corporation, El Segundo, California. MECHANISM OF GOLD DIFFUSION INTO SILICON. Prepared by W. R. Wilcox (Materials Sciences Laboratory, Aerospace Corporation) and T. J. LaChapelle (Pacific Semiconductors, Incorporated). 10 April 1963. [48] p. incl. illus. (Report TDR-169(3240-01)TN-1; SSD-TDR-63-70) (Contract AF 04(695)-169) Unclassified report</p> <p>Gold was found to diffuse into silicon by a complex mechanism involving a vacancy-controlled interstitial-substitutional equilibrium. This led to very complex diffusion concentration profiles. In analyzing the problem, a new experimental value was found for the self-diffusion coefficient of silicon, <math>1.81 \times 10^4 \exp(-112 \pm 20 \text{ kcal/RT}) \text{ cm}^2/\text{sec}</math>, which compared very favorably with previous data on diffusion of bismuth, germanium, and tin in silicon. The interstitial gold-diffusion coefficient was found to be <math>2.4 \times 10^{-4} \exp(-8.9 \pm 2 \text{ kcal/RT})</math>, (over)</p>
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