CALCULATIONS OF DISLOCATION PIPE DIFFUSION

J. Mimkes

Fachbereich Physik, Gesamthochschule Paderborn, F.R.G.

Résumé.- Les mesures de profils de diffusion ont été interprétées à partir de la solution complète de l'équation de la diffusion dans le canal des dislocations. Deux paramètres ont été ajustés : la diffusivité dans le canal des dislocations D', et le rayon du canal des dislocations a. Les valeurs obtenues pour D' se trouvent en bon accord avec celles déjà données par d'autres auteurs. Par contre les valeurs obtenues pour a sont souvent plus élevées, à cause des erreurs expérimentales dans la détermination de la densité de dislocations.
Cependant, la zone de concentration élevée n'est pas limitée au coeur des dislocations; elle dépend de la diffusivité en volume D, et peut être caractérisée par le rayon effectif de la diffusion le long des dislocations, $R = 2\sqrt{Dt}$.

Abstract.- Experimental diffusion profiles have been analyzed by a complete solution of the pipe diffusion equations, using two fitting parameters, pipe diffusivity D' and dislocation pipe radius a. The pipe diffusivity D' agrees well with values obtained by other authors. The pipe radius often turns out very large due to the inaccuracy of the experimental dislocation density.
However, the area of high concentration along the dislocation is not confined to the dislocation core, but depends on the diffusivity D of the bulk and may be characterized by an effective diffusion pipe radius $R = 2\sqrt{Dt}$.

1. Introduction.- In diffusion experiments dislocations have often been observed /1/ to form a short cut for the diffusion process. As the diffusivity in the dislocation pipe may be up to 1000 times higher than in the bulk, pipe diffusion is of considerable interest to materials research.

2. Pipe diffusion model.- In order to calculate pipe diffusion data the differential equations of pipe diffusion have to be solved.

In a simple model isolated dislocations may be approximated by infinite pipes of radius a and diffusivity D' penetrating the crystal perpendicular to the surface. The concentration c' of diffusing material is assumed to be of radial symmetry in the pipe :

$$D'\left(\frac{\partial^2 c'}{\partial r^2} + \frac{1}{r}\frac{\partial c'}{\partial r} + \frac{\partial^2 c'}{\partial z^2}\right) = \frac{\partial c'}{\partial t} - \gamma\,\delta(z)\cdot\delta(t) \quad r<a \quad (1)$$

γ is the initial concentration of an instantaneous source at the surface z = o.

In the bulk diffusion is determined by the diffusivity D :

$$D\left(\frac{\partial^2 c}{\partial r^2} + \frac{1}{r}\frac{\partial c}{\partial r} + \frac{\partial^2 c}{\partial z^2}\right) = \frac{\partial c}{\partial t} - \gamma\,\delta(z)\delta(t) \qquad r>a \quad (2)$$

At the boundary of the dislocation pipe we have

$$c = c \quad D\frac{\partial c}{\partial r} = D'\frac{\partial c'}{\partial r} \qquad r=a \quad (3)$$

These equations may be solved by Fourier-Laplace transformations similar to the approach to grainboundary diffusion by Whipple /2/ and Suzuoka /3/ and will yield a similar result for c(r,z,t) /4/.

For the evaluation of sectioning experiments the solution has to be integrated with respect to the radius r :

$$Q(z,t) = \int_0^\infty c(r,z,t,)\cdot 2\pi r dr = \frac{\gamma}{\sqrt{\pi D t}}\left(Q_o(z,t) + N_d \pi a^2 \cdot Q_1(z,t)\right) \quad (4)$$

$$Q_o(z,t) = \exp(-z^2/4Dt) \quad (5)$$

$$Q_1(z,t) = \int_1^\Delta \int_0^\infty (1+r)^{1/2}\,\mathrm{erfc}\left\{\frac{1}{2}\sqrt{\frac{\Delta-1}{\Delta-\sigma}}\left(\frac{ar}{\sqrt{Dt}} + \frac{2}{a}\,\frac{\sigma-1}{\Delta-1}\sqrt{Dt}\right)\right\}\,dr\cdot\left(\frac{z^2}{2\sigma Dt} - 1\right)\exp\left(-\frac{z^2}{4\sigma Dt} - \frac{\sigma-1}{\Delta-1}\,\frac{Dt}{a^2}\right)\frac{d\sigma}{\sigma^{3/2}} \quad (6)$$

Q_o is the total[(1)] amount of material that has diffused the distance z from the surface F : Q_1 is the amount of material that has diffused into the bulk through the dislocation. $\Delta = D'/D$ is the ratio of diffusivities in pipe and bulk, respectively, a is the radius of the pipe. Sectioning experiments may be evaluated by fitting the two parameters D' and a to the experimental data, which must contain the diffused amount Q, the sectioning depth z, diffusion time t, and the dislocation density N_d.

Experimental results have been analyzed /5/ according to equations (4) - (6) for various materials.

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(1) In order to evaluate non homogeneous dislocation distributions equation (6) differs slightly from ref. /4/.

The diffusivities agree well with the expected values and lead to satisfying results for the first fitting parameter $\Delta = D'/D$.

The second fitting parameter, the radius a of the dislocation pipe has given less satisfying results, the pipe radius for self-diffusion in gold /6/ is calculated at the order of 50 Å.

This is, however, due to the fact, that in contrast to the high accuracy of the diffusion data the accuracy of the dislocation density often has been neglected. As the dislocation density N_d enters directly into the calculations of the pipe radius,

$N_d^2 \cdot a \sim \text{const}$

the pipe radius a will be the smaller the higher the dislocation density is assumed /8/.

Only great care in determining the true dislocation density will yield a correct pipe radius a.

However, it may be noted, that the diffusion profile around a single dislocation is almost independent of the pipe radius a, and will extend over large distances into the bulk of the crystal. This will lead to a very large effective radius for pipe diffusion data of Nb into Ta by Pawel and Lundy /7/ in figure 1.

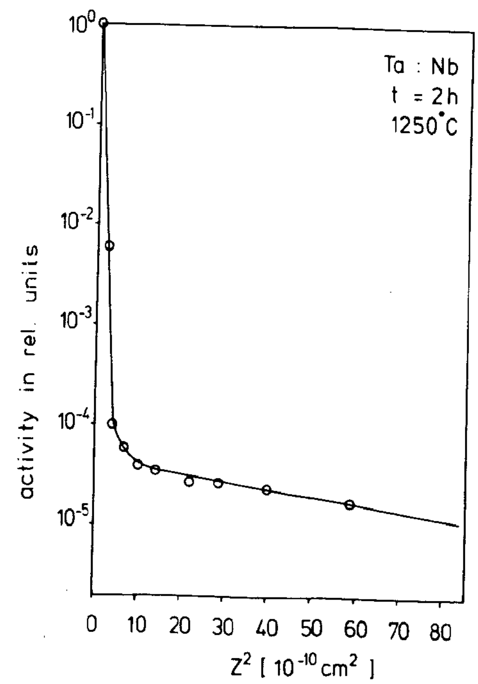

Fig. 1 : Profile of Nb diffusion into Ta. Open circles give experimental data of activity as function of the square of penetration depth z^2 according to ref. /7/. The solid line corresponds to the fit $N_d = 10^7\ cm^{-2}$, a = 170 Å, Δ = 1700, D = $1{,}5\times10^{-15}$ $cm^2\ s^{-1}$ in equation (4).

The data may be fitted by $N_d = 10^7\ cm^2$ (a factor of 100 larger than given by the authors), Δ=1700 and a = 170 Å. This pipe radius still is too large and a higher dislocation density may have to be assumed.

However, the diffusion profile around a dislocation turned out to be almost independent of the pipe radius (or the dislocation density assumed). Figure 2 shows the concentration c(r,z,t) as a function of r to extend over more than six times the assumed pipe radius of 170 Å.

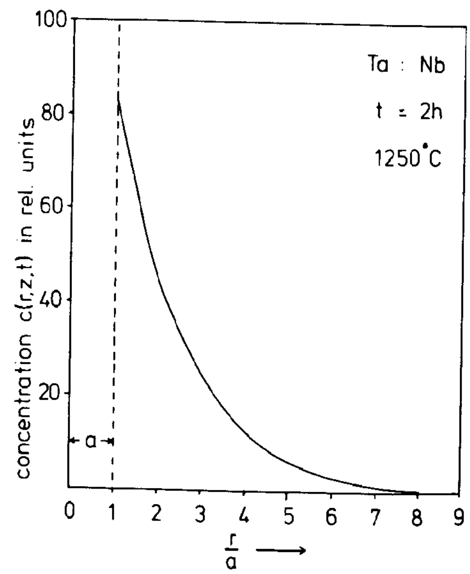

Fig. 2 : Profile of Nb diffusion into Ta. The concentration c(r,z,t) has been calculated as a function of distance r from the dislocation at a penetration depth z = 7000 Å for the same fitting parameters as in figure 1.

As we have to integrate $c(r)\cdot 2\pi r$ over r in order to obtain the total concentration per section the function $f(r) = c(r)\cdot 2\pi r$ has been plotted in figure 3.

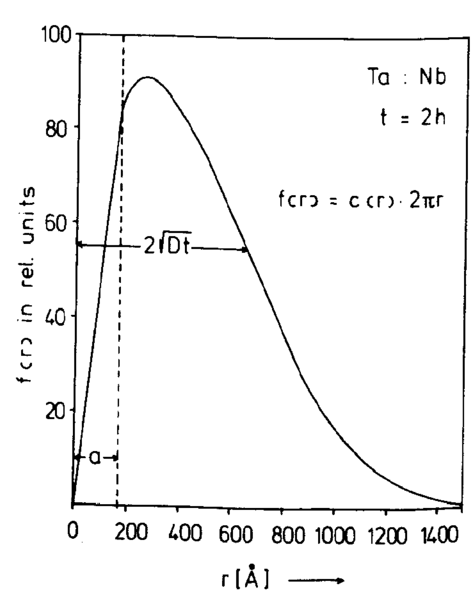

Fig. 3 : Profile of Nb diffusion into Ta. $f(r,z,t) = 2\pi r\cdot c(r,z,t)$ has been calculated for the penetration depth z = 7000 Å and the same fitting parameters as in figure 1.

This figure reveals two results :

1. the material inside the dislocation pipe does not contribute much to the total amount of a section,
2. the material diffused through the pipes extends over a large distance into the bulk of the crystal. This distance will be controlled by the diffusivity of the bulk, and will be of the order $R = 2\sqrt{Dt}$, or in figure 3, R = 650 Å.

Independently of the radius a of the dislocation core the diffusion effective pipe radius $R = 2\sqrt{Dt}$ will govern pipe diffusion and will cause a large amount of material to travel along dislocations as diffusion short cuts.

An application of the solutions of pipe diffusions to tetrahedrally coordinated semiconductors will be given in the following paper.

References

/1/ Hofmann, R.E., and Turnbull, D., J. Appl. Phys., 22 (1951) 634.

/2/ Whipple, R.T.P., Philos. Mag., 45 (1954) 1225.

/3/ Suzuoka, T., J. Phys. Soc. Japan, 19 (1964) 839.

/4/ Mimkes, J. and Wuttig, M., Phys. Rev., B 2 (1970) 1619.

/5/ Mimkes, J., Thin Solid Films, 25 (1975) 221.

/6/ Gupta, D., Phys. Rev., B 7 (1973) 586.

/7/ Pawel, R.E. and Lundy, T.S., Acta Metall., 13 (1965) 345.

/8/ Ahlborn, K. and Schröter, W., this conference.