NUMERICAL SOLUTION OF DOPANT DIFFUSION EQUATIONS

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SUMMARY

A description is given of the application of the Moving
Finite Element (MFE) method to the solution of a non-linear
diffusion equation modelling the behaviour of dopant in
crystalline silicon. The method approximates the dopant
concentration by a piecewise linear representation, as with
conventional finite elements, but on a moving mesh whose
position is computed at the same time as the solution.
Although the number of unknowns is doubled in this way, the
method is able to model moving features, such as steep fronts,
with far fewer nodes. A number of special features of the
method as applied here will be explained. Unlike in its
original form no penalty functions are used, and this enables
inversion of the full mass matrix and simple explicit Euler
time stepping.

The dopant concentrations encountered in the diffusion
problem range over many orders of magnitude. In order to
obtain uniform resolution of the concentration some data
compression is required which must be devised in such a
way that the physics of the problem, contained in the variable
diffusion coefficient, is adequately represented. It has
been found that an appropriate dependent variable to use is
a velocity potential associated with the diffusion velocity.

To illustrate the behaviour of the method the solution
to a one-dimensional test problem will be presented.

1. INTRODUCTION

In order to predict the expected electrical behaviour of a semiconductor device it is necessary to know the distribution of dopant atoms within the device. When using crystalline silicon these dopant atoms are typically introduced into the crystal by ion implantation, which results in a high concentration in a shallow region near the crystal surface. The dopant then diffuses through the crystal during subsequent heat treatments. It is a model of this diffusion process that is considered here.

A discussion of diffusion mechanisms involved in dopant diffusion in crystalline silicon can be found in Fair [1]. The dopant in a crystal can exist in two forms, mobile single atoms or stationary clusters of atoms. We shall denote the concentration of the first type of dopant by c_A and the second by c_c, the total concentration being given by $c_A + c_c$. Although the diffusion of dopant is due only to the movement of the mobile atoms the rate of diffusion is determined by the electrical charge nearby. Both types of atoms can be electrically charged and so clustering alters the diffusion rate.

The diffusion process can be modelled by the differential equation

$$\frac{\partial}{\partial t}(c_A + c_c) = \underline{\nabla} \cdot \left\{ D_i \frac{1 + \beta(n_e/n_i)}{1+\beta} \left(\underline{\nabla} c_A + \alpha c_A \frac{\underline{\nabla} n_e}{n_e} \right) \right\} \qquad (1.1)$$

where β, n_i, D_i, α are constants and n_e is the local electrical charge which is taken as

$$n_e = \frac{1}{2}\left[\frac{\alpha}{\alpha+1}\,c_A + \frac{1}{\alpha+1}\,c_c\right] + \frac{1}{2}\sqrt{\left\{\left(\frac{\alpha}{\alpha+1}c_A + \frac{1}{\alpha+1}c_c\right)^2 + 4n_i^2\right\}} \quad (1.2)$$

where α represents the ratio of the electric charge of a mobile atom to that of a clustered atom.

It is possible for clustered atoms to become mobile and vice versa and this is modelled by a simple first order chemical reaction assumed to be in equilibrium so that some function of c_c and c_A is known. The model for arsenic is usually taken as

$$kc_A^3 n_e = c_c. \quad (1.3)$$

From the above equations it is possible (because only one dopant is being considered) to write an equation

$$\frac{\partial c}{\partial t} = \underline{\nabla}. \ D(c)\ \underline{\nabla}\ c \quad (1.4)$$

for the total concentration $c(=c_A+c_c)$, where the form of the diffusion coefficient $(D(c)$ is shown in fig.1 for typical concentrations encountered. The most significant property of $D(c)$ is its variation over about two orders of magnitude.

Figure 1. ARSENIC DIFFUSION COEFFICIENT $D(c)$
AT A TEMPERATURE OF 1223.0 K
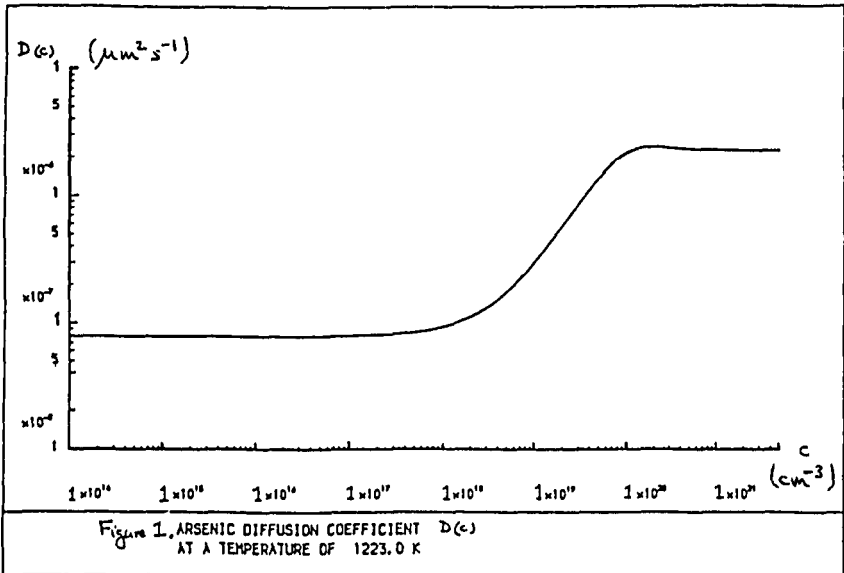
When the dopant is initially implanted in the crystal it occupies a thin region just below the surface. Typically the distribution is taken to be Gaussian with distance below the surface. After heat treatment the distribution of dopant is required because it is the dominant factor in determining the behaviour of the resulting device. In particular, the position of the 'junction' and the dopant distribution about the junction is crucial. This distribution is difficult to calculate numerically because it occurs at concentrations of about 10^{14} cm^{-3}, which are typically 5 or 6 orders of magnitude smaller than the maximum concentration. The profile of the dopant is also difficult to calculate because it involves a steep front and the full history of the dopant profile is crucial to the distribution calculated about the junction.

There are two ways in which we have contributed to overcoming these problems. The first is to introduce an important change of variable which has the effect of data compression and of making it easier to capture the steep front numerically. If the concentration c is used as the variable then, as a consequence of the range of values taken by c, good resolution is obtained only in the region of high concentration and large errors are introduced near the junction. Possible transformations to different variables (including ln c) have been considered by Please and Sweby (2), who have found that a velocity potential associated with D(c) is able to give a good representation of the concentration over the entire solution range. This transformation, which is adopted here, involves solving for ϕ where

$$\phi = \frac{c}{n_i} + \ln \frac{c}{n_i} \tag{1.5}$$

For large c, ϕ behaves like c itself while for small c, ϕ behaves like ln c. Equation (4) is now being transformed into a slightly different non-linear diffusion equation for the variable ϕ.

The second idea which has been contributed to this work is to employ the Moving Finite Element (MFE) method as the numerical solution procedure. The problem of tracking steep moving fronts has been considered by many workers, using both finite differences and finite elements. Finite elements are attractive in general through their capacity to work with irregular meshes while the MFE method gives the added capability of following steep fronts by moving the mesh with the front. In the second section of this paper we review the essential details of the method.

2. THE MFE METHOD

We now give a short account of the Moving Finite Element method, as introduced by Miller (3) and considered further by Wathen and Baines (4), Johnson (5).

We consider approximate solutions to the general evolution equation

$$u_t - L(u) = 0 \qquad\qquad (2.1)$$

where L is the spatial differential operator under consideration.

In the present case the function u will be the velocity potential ϕ. In the present paper we confine the theory and the numerical results to one-dimensional problems.

We take a semi-discrete approximation

$$U(x,t) \approx \sum_{j=1}^{N} U_j(t)\, \alpha_j\{x,\underline{s}(t)\} \qquad\qquad (2.2)$$

where α_j is a standard piecewise linear finite element basis function on the grid defined by the N-dimensional vector $\underline{s}$ of time dependent nodal positions (see Figs. 2.1 and 2.2).
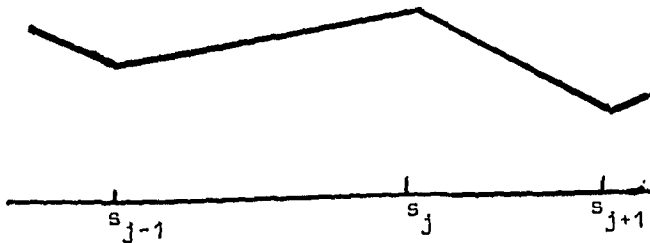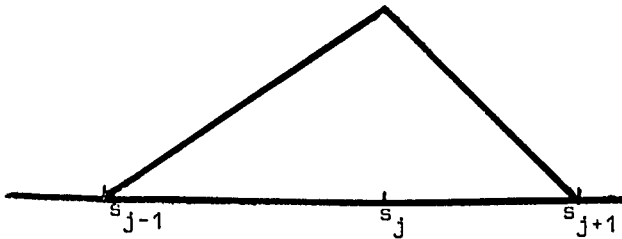

Figure 2.1

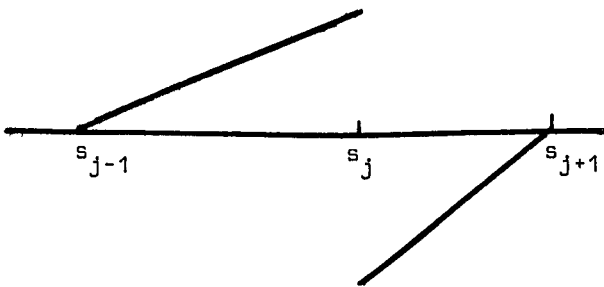Piece-wise linear approximation $U(x,t)$

Figure 2.2

Basis function α_j

Figure 2.3

Basis function β_j

Partial differentiation of (2.2) with respect to time yields

$$U_t(x,t) = \sum_{j=1}^{N} \dot{U}_j \alpha_j(x,\underline{s}(t)) + \dot{s}_j \beta_j(x,\underline{U}(t),\underline{s}(t)) \quad (2.3)$$

where the dot denotes time differentiation and where

$$\beta_j = - \frac{\partial U}{\partial x} \alpha_j$$

may be regarded as a second type of basis function (see

Fig. 2.3). The basis function α_j is given by

$$
\alpha_j = \begin{cases}
\dfrac{x - s_{j-1}}{\Delta s_j} & \text{for } s_{j-1} \le x \le s_j \\[2em]
\dfrac{s_{j+1} - x}{\Delta s_{j+1}} & \text{for } s_j \le x \le s_{j+1} \\[2em]
0 & \text{otherwise}
\end{cases}
$$

where $\Delta s_j = s_j - s_{j-1}$.

The basis function β_j is given by

$$
\beta_j = \begin{cases}
- m_j \alpha_j & \text{for } s_{j-1} \le x < s_j \\[1em]
- m_{j+1} \alpha_j & \text{for } s_j < x \le s_{j+1}
\end{cases}
$$

where $m_j = \dfrac{\Delta U_j}{\Delta s_j}$ is the gradient of the approximation U on the jth element.

Minimising the square of the L_2 norm of the residual of the left hand side of (2.1)

$$
|| U_t - L(U) ||_{L_2}^2
$$

with respect to the 2N parameters $\dot{U}_j, \dot{s}_j$ yields the set of 2N equations.

$$
\langle U_t - L(U), \alpha_j \rangle = 0 \tag{2.4}
$$

$$
\langle U_t - L(U), \beta_j \rangle = 0
$$

$$
(j = 1, \ldots, N)
$$

where $\langle U, V \rangle$ denotes the integral $\int UV dx$. Substituting U_t given by (2.4) then gives the non-linear system

of ordinary differential equations

$$A(\underline{y})\dot{\underline{y}} = \underline{g}(\underline{y})$$ (2.5)

which are known as the MFE equations. In (2.5)

$$\underline{y} = (U_1, s_1, \ldots, U_N, s_N)^T,$$

$A(\underline{y})$ is the MFE matrix which is square, symmetric and 2 x 2 block tridiagonal with blocks given by

$$A_{ij} = \begin{bmatrix} <\alpha_i, \alpha_j> & <\alpha_i, \beta_j> \\ \\ <\beta_i, \alpha_j> & <\beta_i, \beta_j> \end{bmatrix}$$ (2.6)

and the elements of the vector $\underline{g}(y)$ are defined by

$$g_{2i-1} = <L(U), \alpha_i>$$ (2.7)

$$g_{2i} = <L(U), \beta_i>$$

$$(i = 1, \ldots, N)$$

The matrix $A(y)$ of the system (2.5) of ordinary differential equations may be inverted using the pre-conditioned conjugate gradient method. It has been shown by Wathen (6) that the preconditioning of $A(y)$ by the inverse of its diagonal blocks results in a very well-conditioned matrix and as a result the conjugate gradient method converges in a few steps. We therefore easily obtain

$$\dot{\underline{y}} = (A(\underline{y}))^{-1} \underline{g}(\underline{y})$$ (2.8)

In order to obtain the evolution of U_i and s_i from (2.8) we must use a time stepping algorithm. It has been found that, provided no penalty functions are used in the minimisation, explicit Euler time stepping is sufficient.

If $L(u)$ contains second derivatives (as it does in the present application) the MFE method requires the evaluation of the inner products

$$<L(U), \beta_i>$$

where U_{xx} exists only as a sum of delta functions at the

nodes and β_i is discontinuous at the nodes. One way round the problem is to seek an approximate solution which has a finite L_2 norm, but this of course leads to an entirely different structure for the resulting MFE matrix. As an alternative, and in order to take advantage of the structure of the MFE matrix in (2.6), as analysed by Wathen & Baines (4), we persevere with the approximation defined by (2.2), but introduce a special interpretation of the inner products (2.7) appearing on the right hand side of the MFE equations (2.5).

Following Morton (7) we replace the inner products $<U_{xx},\alpha_i>$, $<U_{xx},\beta_i>$ appearing on the right hand side of (2.5)

by $<w_{xx},\alpha_i>$, $<w_{xx},\beta_i>$, respectively, where $w_x(x)$ is

some "recovered" function lying in a smoother space than

$U_x(x)$, such that w_{xx} has a finite L_2 norm.

In the numerical results obtained by the method we have chosen w_x on element i as the quadratic defined by interpolating the values

$$
w_x(x) = \begin{cases} \frac{1}{2}(m_{i-1} + m_i) & \text{at } x = s_{i-1} \qquad (2.9) \\[2mm] m_i & \text{at } x = \frac{1}{2}(s_{i-1} + s_i) \\[2mm] \frac{1}{2}(m_i + m_{i+1}) & \text{at } x = s_i \end{cases}
$$

Note that $w_x(x)$ is in general discontinuous at the nodes. We then obtain

$$
<w_{xx},\alpha_i> = \frac{1}{12}\{(m_i + 10m_{i+1} + m_{i+2}) - (m_{i-1} + 10m_i + m_{i+1})\}
$$

Also
$$
(2.10)
$$

$$
<w_{xx},\beta_i> = \frac{-1}{12}\cdot\{m_{i+1}(m_{i+1} + 10m_{i+1} + m_{i+2}) - m_i(m_{i-1} + 10m_i + m_{i+1})\}
$$

$$
(2.11)
$$

The values may also be approximated by a weighted recovery method.

One other difficulty with the MFE method is that the inverse of A may be ill-conditoned when nodes are almost collinear or elements become very small. In the results given here an averaging device has been used to overcome these problems.

3. NUMERICAL RESULTS

In figures 3, 4 and 5 we show how the transformation
assists the numerical solution of a dopant diffusion problem.
We consider arsenic diffusion in silicon, which is governed
by the diffusion equation (1.1) with $\beta = 100$,
$n_i = 5 \times 10^{-18}$ cm^{-3}. The transformation (1.5) is applied to
obtain a new diffusion equation satisfied by ϕ which is
approximated by an MFE description. The problem is solved
on the interval $0 \leq x \leq 1$ with Neumann boundary conditions
at both ends. As the initial distribution we take a Gaussian
profile centred at $x = 0.25$ with a standard deviation of
0.05. The height of the Gaussian is approximately 10^{21},
although the problem is solved in non-dimensional form.

The solution of this problem includes steep moving fronts
which propagate outwards from the centre of the Gaussian
while the magnitude of the peak is attenuated. The left-
moving front impinges on the $x = 0$ fixed boundary while the
right-moving front propagates freely.

Figure 3 shows the solution for the transformed variable
ϕ at times 0, 2500 and 5000 seconds. Figure 4 gives the
corresponding graphs for the concentration c while figure 5
shows the more commonly used $\ln c$ (omitting the part of the
curve below the axis.). In figures 4 and 5 the dotted line
denotes the active concentration while the full line gives
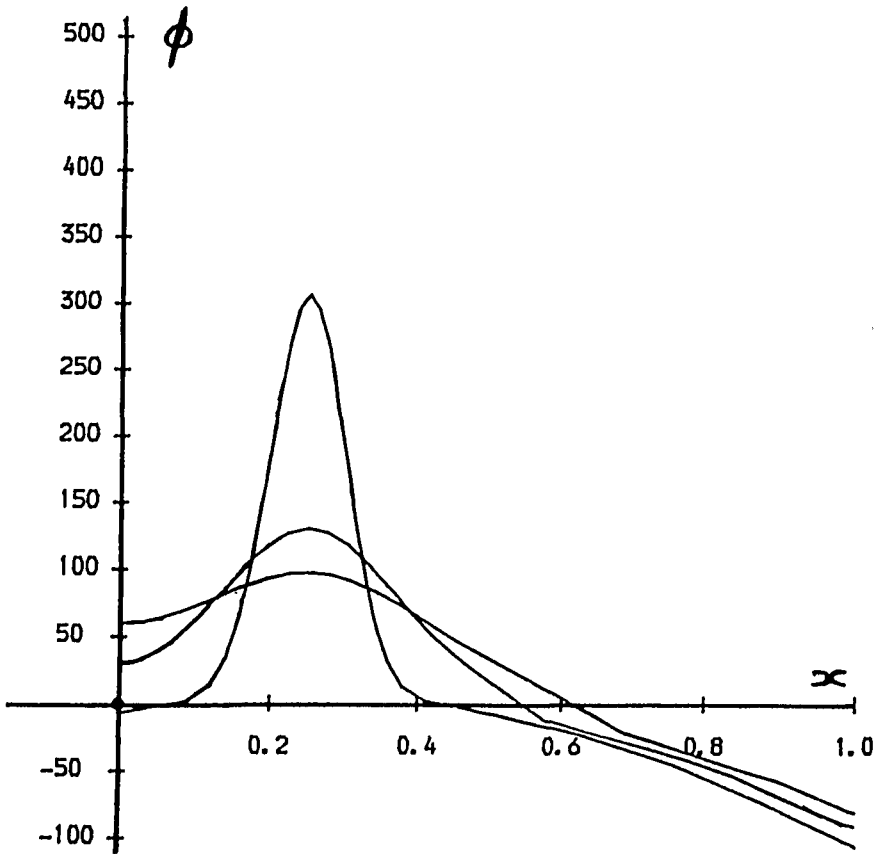the total concentration.

Figure 3 $\phi = \dfrac{c}{n_i} + \ln \dfrac{c}{n_i}$ for the dopant diffusion problem.
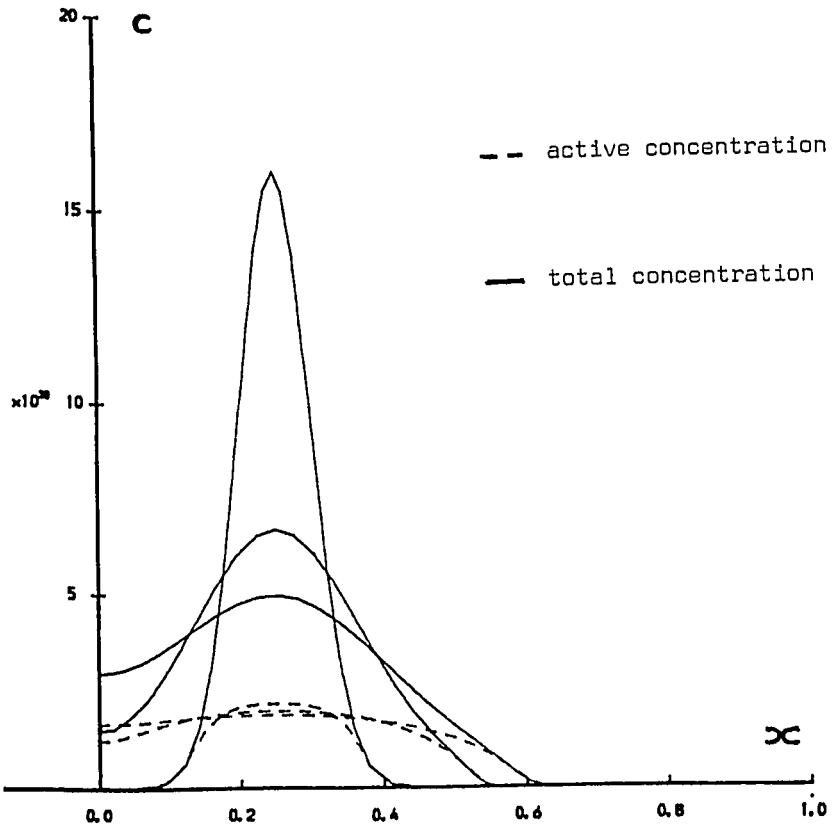
Figure 4   The active and total arsenic concentration for
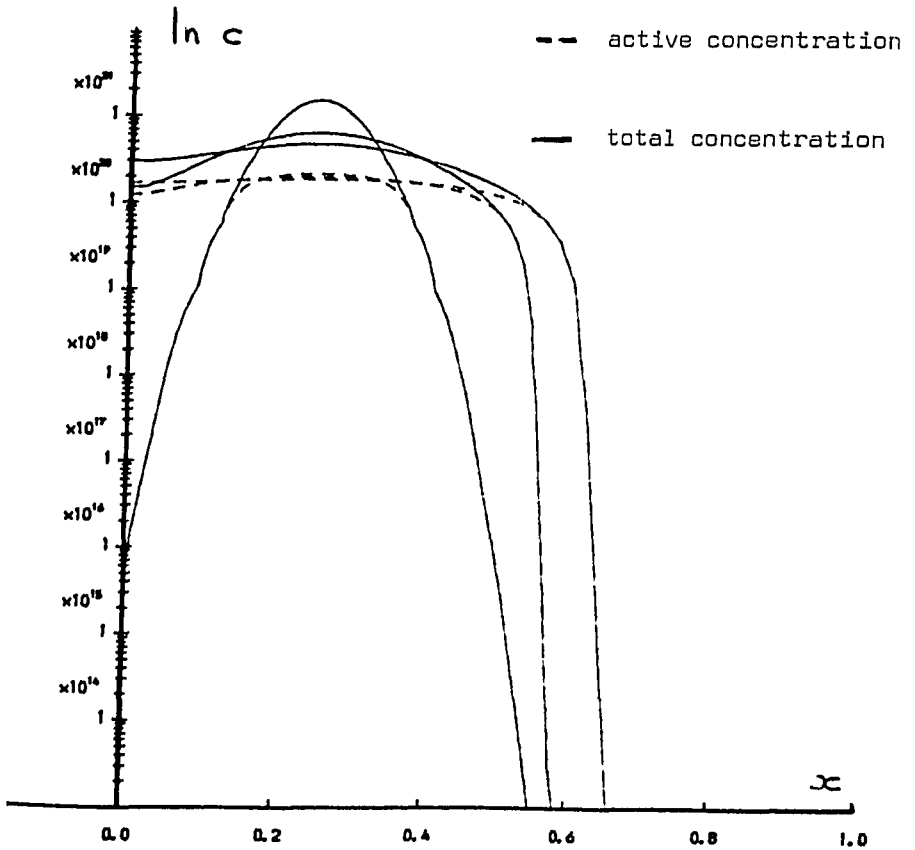   the dopant diffusion problem.

Figure 5   The log of the active and total concentrations for the dopant diffusion problem.

Note that the transformed variable is more uniform and easier to capture than c with rather few moving finite element nodes.

Results compare favourably with those produced by standard finite difference codes.

4. CONCLUSION

In this paper we have presented two new ideas of use in the numerical simulation of dopant diffusion in silicon. The first is a change of dependent variable to smooth the severe steep fronts which occur in the solution of the highly non-linear diffusion equation for the concentration.

The second (independent) idea has been to solve the equation numerically by the method of moving finite elements, a relatively new technique which has been partly developed by the authors. The results on a one-dimensional test problem are competitive using comparatively few elements, but the principal benefit is likely to come when the approach is extended to similar problems in two dimensions. In addition it is possible to deal with moving boundaries using the moving finite element technique which will allow the incorporation of oxide growth into the model.

5. ACKNOWLEDGEMENTS

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