Finite Element Formulation

i.Surface diffusion equations

Surface diffusion leaves solid mass conserved. As matter diffuses on the surface, the solid recedes where matter depletes, and protrudes where matter accumulates. The change is purely kinematic.

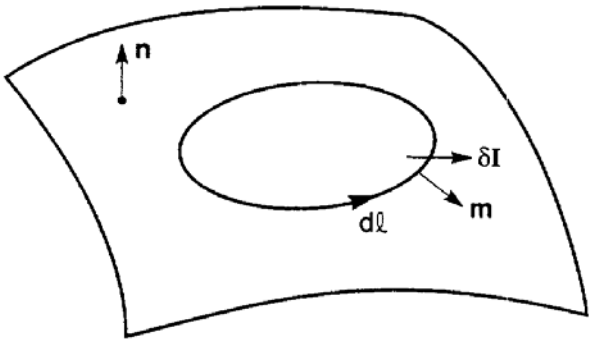

Fig. 1. A surface in three dimensions.

Here, we assume that the free energy consists of surface energy only, and the surface tension γ, is isotropic. For a polycrystalline particle, γ can take different values on the surface and on the grain boundaries.
The free energy of the particle is

$$G = \sum \gamma A \qquad (1)$$

The sum extends over all the surface and grain boundary areas, collectively denoted by A.
Based on Herring's classical theory, the flux of surface diffusion J is proportional to the driving force F.

$$J = M.F \qquad (2)$$

Where,
M is the diffusion mobility of atoms on the surface
F is the driving force defined by the amount of free energy decrease associated wth a unit volume of matter moving a unit distance on the surface.
The flux of surface diffusion **J** can also be written as

$$J = \frac{D\gamma\delta}{kT}\frac{\partial\kappa}{\partial s} \qquad (3)$$

Where,

the surface curvature $_K$ is positive when the surface is convex

∂ s is the element of arc length.

γ is the surface energy

The difference in chemical potential between a point of curvature $_K$ and a point of zero curvature on the surface of the microcrack is given by

$$\Delta\mu = \Omega\, \boldsymbol{\gamma}\, \kappa \qquad (4)$$

From the above equations, we get

$$-F = \nabla(\Delta\mu) = \nabla(\Omega\gamma\kappa) \qquad (5)$$

Where,

∇ represents the surface divergence

The atoms diffuse from a point with high chemical potential (low curvature) to a point with low chemical potential (high curvature).

Matter conservation requires that

$$V_{ns} = -\nabla.J \qquad (6)$$

$$\delta r_{ns} = -\nabla.(\delta I) \qquad (7)$$

Where,

V_{ns} is the normal velocity

∇ J is the divergence of the surface flux

δr_{ns} is the∫ virtual normal displacement

(δI) is the virtual mass displacement

ii.Controlling equations

a. Weak statement for surface diffusion.

Following the principle of virtual work, we get

$$\int \bar{F}.\delta\bar{I}\, dA = -\delta G \qquad (8)$$

Where,

δG is the increment of free energy

dA is the differential area.

Substituting J=M.F in eq.(8), we get the weak statement.

$$\int \frac{\bar{J}.\delta\dot{I}}{M} dA = \delta G \qquad (9)$$

Once J is solved using the above equation, the surface normal velocity can be obtained and used to update the solid shape.

b. Weak statement for combined surface diffusion and evaporation-condensation.

The surface diffusion problem of conserving solid mass as formulated is difficult to implement in a finite-element setting. However, evaporation condensation can be introduced to facilitate the finite element implementation.
The normal velocity of the interface, V_{nv}, is a function of the driving pressure p. For simplicity, we adopt a linear law:

$$V_{nv} = mp \qquad (10)$$

Where, m is the specific reaction rate or the interface mobility for the evaporation condensation process.

This equation is valid when the structure is not far from equilibrium, namely, when the free-energy reduction per adatom is small compared with the average thermal energy per atom.

Surface normal velocity: $V_n = V_{ns} + V_{nv}$ (11)
Surface virtual displacement: $\delta r_n = \delta r_{ns} + \delta r_{nv}$ (12)

Weak statement:

$$\int \{ \frac{\bar{J} . \delta \bar{I}}{M} + \frac{(v_n + \nabla . J)[\delta r_n + \nabla . (\delta \bar{I})]}{m} \} dA = -\delta G \qquad (13)$$

These are the equations due to combined action of evaporation condensation and surface diffusion.

c. Model

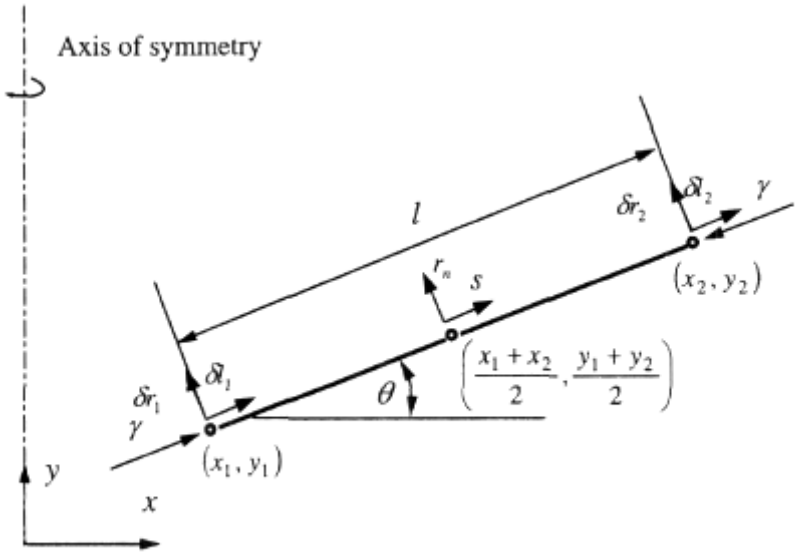

Fig. 2—An axisymmetric linear element.

The element, shown in figure 2 with nodes(x_1,y_1) and (x_2,y_2) with length l and slope θ, can be modeled with 4 degree of freedom (δx_1,δy_1,δx_2,δy_2), and surface diffusion is described by three degree of freedom(δl_1,δl_2,δl_m), where δl_1,δl_2 and δl_m are the virtual matter displacement of the two terminal nodes and the middle point of the element, respectively.

Generalized virtual displacement δq^e and virtual velocity q^e of the element can be expressed by

$$\delta q^e = [\delta x_1 \ \delta y_1 \ \delta I_1 \ \delta x_2 \ \delta y_2 \ \delta I_2 \ \delta I_m \ ]^T \qquad (14)$$

$$\dot{\bar{q}}^e = [\dot{x}_1 \quad \dot{y}_1 \quad J_1 \quad \dot{x}_2 \quad \dot{y}_2 \quad J_2 \quad J_m]^T \qquad (15)$$

Where J_1, J_2 and J_m are the matter flux of the two terminal nodes and the middle point of the element, respectively.

At a distance s from the matter flux of the two terminal nodes, the following relations hold for the virtual normal displacement, normal velocity, virtual matter displacement, and surface flux.

$$\delta r_n = N_1 \delta x_1 + N_2 \delta y_1 + N_3 \delta x_2 + N_4 \delta y_2 \qquad (16)$$

$$V_n = N_1 x_1 + N_2 y_1 + N_3 \delta x_2 + N_4 \delta y_2 \qquad (17)$$

$$\delta I = Q_1 \delta I_1 + Q_2 \delta I_2 + Q_m \delta I_m \qquad (18)$$

$$J = Q_1 J_1 + Q_2 J_2 + Q_m J_m \qquad (19)$$

Where the interpolation coefficients are given by

$$N_1 = -\left(\frac{1}{2} - \frac{s}{l}\right)\sin\theta$$
$$N_2 = \left(\frac{1}{2} - \frac{s}{l}\right)\cos\theta$$
$$N_3 = -\left(\frac{1}{2} + \frac{s}{l}\right)\sin\theta$$
$$N_4 = \left(\frac{1}{2} + \frac{s}{l}\right)\cos\theta$$

….(20)

$$Q_1 = -\frac{s}{l}\left(1 - \frac{2s}{l}\right)$$
$$Q_2 = \frac{s}{l}\left(1 + \frac{2s}{l}\right)$$
$$Q_m = 1 - \left(\frac{2s}{l}\right)^2$$

…..(21)

For each element, the displacement of the nodes can be divided into two components
δl – parallel to the element
δr – normal to the element
as shown if figure 2.

Variation of free energy due to displacement of nodes parallel to the element

$$\delta G_l^e = 2\gamma\pi x_1 \delta l_1 - 2\gamma\pi x_2 \delta l_2 \qquad (22)$$

Variation of free energy due to the displacement of nodes in the normal direction

$$\delta G_r^e = \gamma\pi l \sin\theta \delta r_1 + \gamma\pi l \sin\theta \delta r_2 \qquad (23)$$

Variation of the total free energy can be expressed in terms of virtual motion of the nodes

$$\delta G^e = -f_1 \delta x_1 - f_2 \delta y_1 - f_3 \delta x_2 - f_4 \delta y_2 \qquad (24)$$

Where, f_i are the force components acting on the two nodes due to surface tension and stress field. They can be written as

$$\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{bmatrix} = \begin{bmatrix} \gamma\cos\theta + \left[\frac{2}{3}w_1 + \frac{1}{3}w_2\right]\sin\theta \\ \gamma\sin\theta - \left[\frac{2}{3}w_1 + \frac{1}{3}w_2\right]\cos\theta \\ -\gamma\cos\theta + \left[\frac{1}{3}w_1 + \frac{2}{3}w_2\right]\sin\theta \\ -\gamma\sin\theta - \left[\frac{1}{3}w_1 + \frac{2}{3}w_2\right]\cos\theta \end{bmatrix} \qquad (25)$$

Where,

$$w_i = \frac{1}{2}\left[\sigma_{xi}\varepsilon_{xi} + \sigma_{yi}\varepsilon_{yi}\right] + \left[\tau_{xyi}\varepsilon_{xyi}\right]$$

and i is defined by the node.

Extending the integral for the weak statement, we can obtain the controlling equation of the finite element

$$H^e.q^e = f^e$$

Since the free energy depends on the solid shape, there are no forces associated with the nodal mass change. The force vector can be written as

$$f^e = [\, f_1\ f_2\ 0\ f_3\ f_4\ 0\ 0\,] \qquad (26)$$

The H matrix can be written as

$$\mathbf{H}^e = \frac{1}{6ml}\begin{bmatrix} 2l^2S^2 & -2l^2SC & 5lS & l^2S^2 & -l^2SC & -lS & -4lS \\ -2l^2SC & 2l^2C^2 & -5lC & -l^2SC & l^2C^2 & lC & 4lC \\ 5lS & -5lC & 14+4\mu & lS & -lC & 2-\mu & -16+2\mu \\ l^2S^2 & -l^2SC & lS & 2l^2S^2 & -2l^2SC & -5lS & 4lS \\ -l^2SC & l^2C^2 & -lC & -2l^2SC & 2l^2C^2 & 5lC & -4lC \\ -lS & lC & 2-\mu & -5lC & 5lC & 14+4\mu & -16+2\mu \\ -4lS & 4lC & -16+2\mu & 4lS & -4lC & -16+2\mu & 32+16\mu \end{bmatrix}$$