J Eng Math (2010) 66:87–102
DOI 10.1007/s10665-009-9332-9

Temperature-dependent surface diffusion near a grain boundary

P. Broadbridge · J. M. Goard

Received: 24 December 2008 / Accepted: 15 September 2009 / Published online: 8 October 2009

Abstract Metal surface evolution is described by a nonlinear fourth-order partial differential equation for curvature-driven flow. The standard boundary conditions for grain-boundary grooving, at a grain–grain–fluid triple intersection, involve a prescribed slope at the groove axis. The well-known similarity reduction is no longer valid when the dihedral angle and surface diffusivity depend on time due to variation of the surface temperature. We adapt a nonlinear fourth-order model that can be discerned from symmetry analysis to be integrable, equivalent to the fourth-order linear diffusion equation. The connection between classical symmetries and separation of variables allows us to develop the correction to the self-similar approximation as a power series in a time-like variable.

Keywords Free boundary · Generalized hypergeometric functions · Integrable model · Surface diffusion · Symmetry reductions

1 Introduction

For some metals such as gold, surface evolution occurs predominantly by surface diffusion, as described by the fourth-order Mullins equation [1]. In Cartesian coordinates,

$$y_t = -B\ \partial_x \left\{ \left(1 + y_x^2\right)^{-1/2} \partial_x \frac{y_{xx}}{\left(1 + y_x^2\right)^{3/2}} \right\}, \tag{1.1}$$

where B is constant. This is a conservation equation, of the form $y_t + J_x = 0$, where J is the surface-diffusive flux. By differentiating each side with respect to x, we obtain an evolution equation in the more standard nonlinear form

$$\theta_t = -\,\partial_x^2 \left\{ D(\theta)\partial_x \left[E(\theta)\theta_x \right] \right\}, \tag{1.2}$$

where $\theta = y_x = \arctan(\phi)$. For an anisotropic material, the coefficient functions $D(\theta)$ and $E(\theta)$ may be general when surface tension and diffusivity depend on the angle between the material surface and the crystal planes

P. Broadbridge (✉)
School of Engineering and Mathematical Sciences, La Trobe University, Bundoora, VIC 3086, Australia
e-mail: P.Broadbridge@latrobe.edu.au

J. M. Goard
School of Mathematics and Applied Statistics, University of Wollongong, Wollongong, NSW 2522, Australia

(e.g. [2,3]). For simplicity, we consider a grain boundary that is symmetric about the axis $x = 0$, where the groove root establishes an equilibrium dihedral angle $\pi - 2\phi$, determined by a balance between surface tension and grain boundary tension, $\gamma_b = 2\gamma_s \sin(\phi)$. Hence it is usual to impose an ideal boundary condition

$$y_x(0, t) = m(\text{constant}). \tag{1.3}$$

The standard boundary-value problem for a symmetric groove is completed by specifying flat initial conditions, zero-flux boundary condition, and a steady horizontal surface far from the groove:

$$y(x, 0) = 0, \quad x > 0 \tag{1.4}$$

$$J(0, t) = 0, \quad t \geq 0 \tag{1.5}$$

$$y(x, t) \to 0, \quad x \to \infty, \quad t \geq 0 \tag{1.6}$$

$$y_x(x, t) \to 0, \quad x \to \infty, \quad t \geq 0. \tag{1.7}$$

Exact unsteady solutions to (1.1) are notoriously hard to find [4]. Mullins [1] solved the grain-boundary grooving problem in the small-slope approximation that replaces (1.1) by a linear equation

$$y_t = -B y_{xxxx}.$$

In the mid 1990s, the exact similarity solution for the standard nonlinear boundary-value problem for grain-boundary evolution was constructed for an integrable model that agrees well with (1.1) for all positive values of the slope [5,6].

In reality, a polycrystalline metal first forms when a liquid cools. At that time, the surface temperature is approximately uniform in space but it may be rapidly decreasing in time due to contact with air. The surface diffusivity, the solid–fluid interfacial tension and the grain-boundary tension depend on temperature. Therefore, Eq. 1.1 should be extended to allow for transport coefficients to depend explicitly on time, as well as on slope. Due to temperature effects, not only the governing equation but also the boundary data must depend explicitly on time. The interfacial tension and the grain-boundary tension do not remain in fixed proportion as they vary with temperature. The dihedral angle is temperature-dependent and the prescribed groove slope $y_x(0, t) = m(t)$ must vary with time. The variation with time may in principle be controlled at will by either cooling or heating. Camel et al. [7] review three sets of experimental data, consistently showing that the dihedral angle of an Al-Sn system increases from zero to 70° as temperature varies from 880 to 500 K. At various temperatures and pressures, the dihedral angle of quartz grain boundaries in water is either decreasing or increasing [8].

In Sect. 2, we derive an integrable surface diffusion model with transport coefficients that depend on time in a general way, as well as depending on slope in a manner that approximates standard curvature-driven flow. The standard nonlinear boundary-value problem for grooving transforms to a linear fourth-order diffusion equation with time-dependent linear boundary conditions at a free boundary. The location of the free boundary is equivalent to finding the depth of the groove as a function of time.

When the dihedral angle is constant, it is well known that there is a direct similarity reduction due to scaling invariance. However, a time-dependent groove slope $y_x(0, t)$ is incompatible with such a reduction. Fortunately, for linear equations there is a well known connection between a Lie point symmetry (a one-parameter Lie group of transformations on the original set of variables that leaves the equation invariant) and suitable coordinates for separation of variables [9]. In terms of canonical coordinates for the symmetry, one may construct a more general power series in time, where each term is a separated solution, the simplest being the similarity solution. We then investigate whether such a power series is sufficient to satisfy the boundary conditions. After transforming the integrable governing equation to a linear equation, this approach is applied to the time-dependent grooving problem. When the groove slope varies in time from a non-zero initial value, the leading term in the series is indeed the similarity solution that is already known. Each correction term in the power series may be constructed explicitly in terms of generalized hypergeometric functions. In Sect. 4, we proceed to construct the series approximation for $y(x, t)$.

2 An integrable nonlinear time-dependent model for surface diffusion

Areal flux for material transport on the surface [dimensions L^2T^{-1}] is given by

$$J = -\nu\Omega v, \tag{2.1}$$

where ν is the areal density of particles on the surface [L^{-2}], Ω is mean particle volume and v is the drift velocity. v may be regarded as a terminal velocity that gives a balance between mechanical resistance and driving force. Ideally, from the Nernst–Einstein relation of kinetic theory (e.g. [1]),

$$v = \frac{-D_s}{kT}\frac{\partial\Phi}{\partial s}, \tag{2.2}$$

where T is absolute temperature, Φ is the chemical potential per particle, k is Boltzmann's constant and D_s is a surface mobility parameter [L^2T^{-1}]. For anisotropic materials, D_s is a function of angle ϕ.

Now according to Herring [10], at the leading order in curvature κ,

$$\Phi = \Omega\left[\gamma_s(\phi) + \gamma_s''(\phi)\right]\kappa. \tag{2.3}$$

As the simplest generalization to allow for temperature dependence, we assume that $\gamma_s(\phi)$ may be extended to a separated product $\xi(T)\gamma_s(\phi)$, where $\xi(T)$ is a dimensionless temperature-dependent factor. Then the flux is

$$J = -\frac{D_s(\phi)}{kT}\nu\Omega^2\partial_s\left\{\xi(T)[\gamma_s(\phi) + \gamma_s''(\phi)]\kappa\right\}. \tag{2.4}$$

Again for simplicity, we assume that surface temperature is uniform in space but varying in time. Then the equation of mass conservation in normal and tangential coordinates is $\partial_t N + \partial_s J = 0$, where $\partial_t N$ is the rate of build-up normal to the surface due to transported particles. In Cartesian coordinates,

$$y_t = -\gamma_0\frac{\xi(T)}{\nu kT}\partial_x\{D(y_x)\partial_x\left[E(y_x)y_{xx}\right]\}, \tag{2.5}$$

where

$$E(\theta) = \gamma_0^{-1}[\gamma_s(\phi) + \gamma_s''(\phi)](1+\theta^2)^{-3/2} \text{ [dimensionless]}, \tag{2.6}$$

$$D(\theta) = (1+\theta^2)^{-1/2}D_s(\phi)\nu^2\Omega^2 \; [L^4T^{-1}], \tag{2.7}$$

$$\phi = \arctan(y_x);\;\; \theta = y_x, \tag{2.8}$$

and $\gamma_0 = \gamma_s(0)$, which is the surface tension on a horizontal flat surface at some reference temperature T_0 where $\xi(T_0)$ is defined to be one. Now we define a new time-like coordinate $\bar{t}$ that also has the dimensions of time,

$$\bar{t} = \frac{\gamma_0}{\nu k}\int_0^t \frac{\xi(T(t_1))}{T(t_1)}\mathrm{d}t_1. \tag{2.9}$$

Use of this variable simplifies (2.5) to an autonomous equation

$$y_{\bar{t}} = -\partial_x\{D(y_x)\partial_x\left[E(y_x)y_{xx}\right]\}. \tag{2.10}$$

There is a time scale $\bar{t}_s$ for significant variation of the groove slope $m(\bar{t})$. The length scale for diffusion during this time is $\ell_s = (D_s(0)\nu^2\Omega^2\bar{t}_s)^{1/4}$. Defining dimensionless variables $(x^*, y^*, t^*) = (x/\ell_s, y/\ell_s, \bar{t}/t_s)$, the relevant boundary-value problem is

$$y^*_{t^*} = -\partial_{x^*}\left[D^*(y^*_{x^*})\partial_{x^*}\left[E(y^*_{x^*})y^*_{x^*x^*}\right]\right]; \tag{2.11}$$

$$(x^*, t^*) \in [0, \infty)^2$$

$$y^*(x^*, 0) = 0 \tag{2.12}$$

$$y^*_{x^*}(0, t^*) = m(t^*) \tag{2.13}$$

$$J^*(0, t^*) = -D^*(y^*_{x^*})\partial_{x^*}\left[E(y^*_{x^*})y^*_{x^*x^*}\right]|_{x^*=0} = 0 \tag{2.14}$$

$$y(x^*, t^*) \to 0, \quad x^* \to \infty \tag{2.15}$$

$$y^*_{x^*}(x^*, t^*) \to 0, \quad x^* \to \infty, \tag{2.16}$$

where $D^*(\theta) = D(\theta)/D(0)$.

Differentiating each side of (2.10) with respect to x^*, we have

$$\theta_{t^*} = -\partial^2_{x^*}\{D^*(\theta)\partial_{x^*}[E(\theta)\theta_{x^*}]\}. \tag{2.17}$$

From (2.7), for an isotropic material, the nonlinear diffusivity $D^*(\theta)$ is simply a geometric factor

$$D^*(\theta) = \cos(\phi) = f(\theta) = 1/\sqrt{1+\theta^2}, \tag{2.18}$$

which originates from the Euclidean metric $\mathrm{d}s = (\mathrm{d}x^2 + \mathrm{d}y^2)^{1/2}$, so that $\mathrm{d}x = f(y_x)\mathrm{d}s$. Similarly, from (2.4,2.6) $E(\theta)$ is obtained from a geometric operator,

$$-\kappa/y_{xx} = |\mathrm{d}^2\mathbf{r}/\mathrm{d}s^2|/y_{xx} \tag{2.19}$$

$$= f(y_x)\{[f'(y_x)]^2 + [y_x f'(y_x) + f(y_x)]^2\}^{1/2}. \tag{2.20}$$

In the isotropic surface diffusion equation (1.1), the small-slope approximation $|y_x| << 1$ leads to the linear equation

$$y_t = -By_{xxxx}$$

that can be treated by standard transform methods. An alternative interpretation of the case with both $D^*(\theta)$ and $E(\theta)$ constant, is that from (2.6, 2.7), (2.17) is the exact surface diffusion equation of an anisotropic material with

$$D_s(\phi) = D_0\sec(\phi) \tag{2.21}$$

$$\gamma_s = \gamma_0\left[A_1\cos(\phi) + (1-A_1)\sec(\phi) + A_2\sin(\phi)\right], \tag{2.22}$$

with D_0, A_1 and A_2 constant. The appearance of the singularity in surface tension at $\phi = \pm\pi/2$ highlights the fact that the linear fourth-order diffusion equation arises as a small-slope approximation, invalid when slopes are large. Another class of models that is integrable [5], more useful when y_x can take large positive values, is given by

$$D^*(\theta) = \frac{\beta}{\beta+\theta}, \quad E(\theta) = E_0\frac{\beta^3}{(\beta+\theta)^3}, \tag{2.23}$$

with E_0 constant. For that case, Eq. 2.17 is the fourth-order member of a hierarchy of integrable evolution equations, identifiable as the very special equations that have higher-order Lie–Bäcklund symmetries [11] or as those whose potential symmetries contain a free solution of an equivalent linear equation [12] or as those equations that have a nonlinear superposition principle [13]. In fact, Tritscher [14] showed that this integrable model is simply related to the linear model by a rotation in the xy-plane.

If the anisotropic surface tension takes the form

$$\gamma_s = \frac{\gamma_0}{\cos(\phi_0)}\left[A_1\cos(\phi-\phi_0) + (1-A_1)\cos^2(\phi_0)\sec(\phi-\phi_0) + A_2\sin(\phi)\right], \tag{2.24}$$

then from (2.6), $E(\theta)$ takes the form (2.23) with

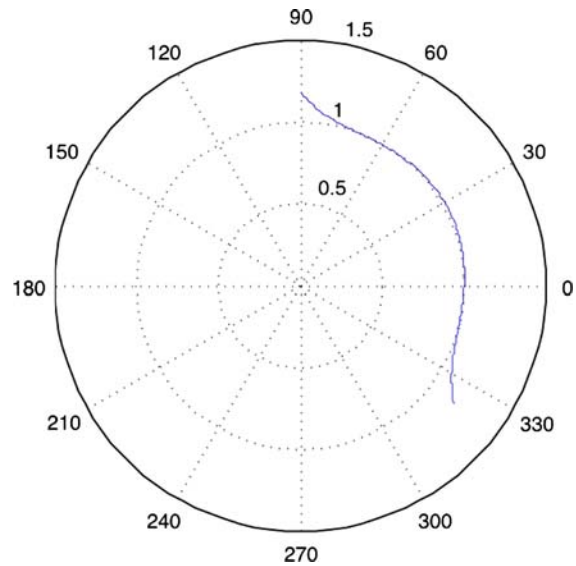
$$E_0 = 2(1-A_1)\frac{(1+\beta^2)}{\beta^2}, \tag{2.25}$$

where $\beta = \cot(\phi_0)$. Whereas the linear model corresponds to artificial singularities in surface tension at $\phi = \pm\pi/2$, in the integrable nonlinear model, these singularities are rotated to $\phi = \phi_0 \pm \pi/2$. If we intend to approximate an isotropic material, then following (2.18), $f(\theta)$ is approximated by $D^*(\theta)$, and the geometric relation (2.20) equates E_0 to be $\sqrt{1+\beta^{-2}}$. This agrees with (2.25) when

$$A_1 = 1 - \frac{\beta}{2\sqrt{1+\beta^2}} \tag{2.26}$$

and A_2 is arbitrary. In practice, isotropy of surface tension is best approximated when $A_2 = 0$. The integrable model (2.23) has the advantage that it agrees with the behaviour of the isotropic model $D(\theta) = O(\theta^{-1})$ and $E(\theta) = O(\theta^{-3})$ for large θ. The choice $\beta = 2.026$ minimizes the maximum difference of $D^*(\theta)$ from the isotropic

Fig. 1 Polar plot of model surface tension versus orientation of surface



model over the domain $0 \leq \theta < \infty$ [5]. Figure 1 shows that the model surface tension is almost isotropic for the wide range of surface orientations between -20 and $72°$. That range is likely to adequately describe the region $x > 0$. The singularities near orientations of 116 and $-64°$ are removed from the region of interest.

Using the model (2.23), the boundary-value problem (2.11)–(2.16) for slope $\theta(x^*, t^*)$ is:

$$\theta_{t^*} = -E_0 \partial^2_{x^*} \left[\frac{\beta}{\beta + \theta} \partial_{x^*} \left[\left(\frac{\beta}{\beta + \theta} \right)^3 \theta_{x^*} \right] \right], \quad (x^*, t^*) \in [0, \infty)^2 \tag{2.27}$$

$$\theta(x^*, 0) = 0, \tag{2.28}$$

$$\theta(0, t^*) = m(t^*), \tag{2.29}$$

$$x^* = 0, \partial_{x^*} \left[\left(\frac{\beta}{\beta + \theta(x^*, t^*)} \right)^3 \theta_{x^*}(x^*, t^*) \right] = 0, \tag{2.30}$$

$$\theta(x^*, t^*) \to 0, \quad x^* \to \infty, \tag{2.31}$$

$$\theta_{x^*}(x^*, t^*) \to 0, \quad x^* \to \infty. \tag{2.32}$$

It is expected that the solution $y^*(x^*, t^*)$ to (2.11–2.16) will have all derivatives rapidly approaching zero as x^* approaches ∞. In that case, $y^*(x^*, t^*)$ can be obtained by integrating the unique solution for $\theta(x^*, t^*)$. Now let

$$\mu = \frac{\beta}{\beta + \theta}, \tag{2.33}$$

$$z = \int_0^{x^*} \frac{\beta + \theta}{\beta} \mathrm{d}x^* = \int_0^{x^*} \frac{1}{\mu} \mathrm{d}x^*, \tag{2.34}$$

$$\tau = E_0 t^*. \tag{2.35}$$

This results in a linear equation

$$\mu_\tau = -\mu_{zzzz} - \frac{1}{\beta} R(\tau) \mu_z, \tag{2.36}$$

where

$$R(\tau) = -y^*_\tau(0, \tau). \tag{2.37}$$

The initial and boundary conditions are

$$\tau = 0, \quad \mu = 1, \tag{2.38}$$

$$z = 0, \quad \mu = \frac{\beta}{\beta + m(\tau)}, \quad \mu_{zz} = 0, \tag{2.39}$$

$$z \to \infty, \quad \mu \to 1, \quad \mu_z \to 0. \tag{2.40}$$

In addition, (2.11) and (2.37) imply a consistency relation

$$z = 0, \ \mu_{zzz} = \frac{-R(\tau)}{\beta + m(\tau)} \tag{2.41}$$

that will be needed in order to determine the unknown function $R(\tau)$.

In (2.36), the convective term can be set to 0 by a change of reference:

$$Z = z + \frac{1}{\beta} y^*(0, \tau), \tag{2.42}$$

$$\mu_\tau = -\mu_{ZZZZ}, \tag{2.43}$$

$$\tau = 0, \quad \mu = 1, \tag{2.44}$$

$$Z = \Sigma(\tau), \quad \mu = \frac{\beta}{\beta + m(\tau)}, \tag{2.45}$$

$$Z = \Sigma(\tau), \quad \mu_{ZZ} = 0, \tag{2.46}$$

$$Z \to \infty, \quad \mu \to 1, \tag{2.47}$$

$$Z \to \infty, \quad \mu_Z \to 0, \tag{2.48}$$

$$Z = \Sigma(\tau), \quad \mu_{ZZZ} = \frac{\beta \dot{\Sigma}(\tau)}{\beta + m(\tau)}, \tag{2.49}$$

where

$$\Sigma(\tau) = \frac{1}{\beta} y^*(0, \tau). \tag{2.50}$$

Solution of the free-boundary problem requires $\Sigma(\tau)$ as well as $\mu(Z, \tau)$.

In the next section, we use the fact that for a linear PDE with a Lie point symmetry, separation of variables is possible in terms of canonical symmetry coordinates.

3 Separation of variables

Neglecting linear superposition, a Lie point symmetry of a linear PDE $Qu(x, t) = 0$, may be represented as a linear first-order operator L, such that $Lu = 0$ is the invariant surface condition. The corresponding "vertical" extended symmetry transformation (e.g [9,15]) is

$$\tilde{\mu}(x, t, u, u_x, u_t) = Lu = v(x, t)u - X(x, t)u_x - T(x, t)u_t. \tag{3.1}$$

Following [9,16], one can choose a canonical coordinate system (y_1, y_2), where $y_2(x, t)$ is an invariant of the symmetry, $Ly_2 = 0$, and $L = \partial/\partial y_1$ so that $L(y_1(x, t)) = 1$. The symmetry theory of second-order linear equations [9] readily extends to higher-order equations. An equation that is invariant under symmetry L always admits separation of variables in the canonical coordinate system, $u(y_1, y_2) = \mathrm{e}^{ky_1} F(y_2)$. The separation constant k may be any spectral value of symmetry operator L, since the separated solution $u = \mathrm{e}^{ky_1} F(y_2)$ satisfies $Lu = ku$.

The separated solutions of (2.43) from its simple scaling symmetry are of the form

$$\tau^{k/4} F(Y), \tag{3.2}$$

with k arbitrary real and $Y = y_2 = Z\tau^{-1/4}$.

After replacing independent variables (Z, τ) by canonical coordinates, the governing equation (2.43) is equivalent to

$$\tau\mu_\tau = Y\mu_Y - 4\mu_{YYYY}. \tag{3.3}$$

The Y-dependent factor in the separated solutions satisfies the linear ordinary differential equation

$$4F''''(Y) - YF'(Y) = -kF, \tag{3.4}$$

for which the general solution with free parameters $C_1, \ldots, C_4$, is expressed in terms of generalized hypergeometric functions,

$$F(Y) = C_1\,{}_1F_3\left(\left[\frac{-k}{4}\right], \left[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\right], \frac{Y^4}{256}\right) + C_2 Y_1 F_3\left(\left[\frac{1-k}{4}\right], \left[\frac{1}{2}, \frac{3}{4}, \frac{5}{4}\right], \frac{Y^4}{256}\right)$$
$$+C_3 Y_1^2 F_3\left(\left[\frac{2-k}{4}\right], \left[\frac{3}{4}, \frac{5}{4}, \frac{3}{2}\right], \frac{Y^4}{256}\right) + C_4 Y_1^3 F_3\left(\left[\frac{3-k}{4}\right], \left[\frac{5}{4}, \frac{3}{2}, \frac{7}{4}\right], \frac{Y^4}{256}\right).$$

In the known similarity solution [5,6] with constant groove slope $y_x(0, \tau) = m$, $y(0, \tau)$ is proportional to $\tau^{1/4}$. The series method can accommodate a generalization with $m(\tau)$ an analytic function of $\tau^{1/4}$ specified from experimental conditions,

$$Z = \Sigma(\tau);\ \ \mu = \frac{\beta}{\beta + m(\tau)} = \sum_{i=0}^{\infty} \epsilon_i \tau^{i/4}. \tag{3.5}$$

This includes the case of m varying more smoothly as an analytic function of time. However, to demonstrate the capability of the method, later we produce numerical examples when m is modified by an $O(\tau^{1/4})$ correction. Conceivably, such less smooth adjustments to groove slope could model the addition of surfactant rather than control of temperature. Then $y^*(0, \tau)\tau^{-1/4}$ will be assumed to be a power series in $\tau^{1/4}$:

$$\begin{aligned} x = 0 \iff & y^*(0, \tau) = \beta\tau^{1/4} \sum_{i=0}^{\infty} b_i \tau^{i/4} \\ \iff & Z = \Sigma(\tau) = \frac{1}{\beta} y^*(0, \tau) \\ \iff & Y = \Sigma(\tau)/\tau^{1/4} = \sum_{i=0}^{\infty} b_i \tau^{i/4}, \end{aligned} \tag{3.6}$$

with b_i real constants and $b_0 < 0$. In order for the solution to be consistent with the boundary conditions, we make another reasonable assumption that the slope $m(\tau)$ at the groove root and the solution $\mu(Z, \tau)$ can be formally developed as analytic functions of $\tau^{1/4}$. This means that the separation constant k is an arbitrary non-negative integer, so that the solution to (3.3) can be developed as a formal power series

$$\mu = \mu_0(Y) + \sum_{j=0}^{\infty} \tau^{j/4} \left[K_{1j}\,{}_1F_3\left(\left[\frac{-j}{4}\right], \left[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\right], \frac{Y^4}{256}\right) + K_{2j} Y\,{}_1F_3\left(\left[\frac{1}{4} - \frac{j}{4}\right], \left[\frac{1}{2}, \frac{3}{4}, \frac{5}{4}\right], \frac{Y^4}{256}\right)\right.$$
$$\left. + K_{3j} Y^2\,{}_1F_3\left(\left[\frac{1}{2} - \frac{j}{4}\right], \left[\frac{3}{4}, \frac{5}{4}, \frac{3}{2}\right], \frac{Y^4}{256}\right) + K_{4j} Y^3\,{}_1F_3\left(\left[\frac{3}{4} - \frac{j}{4}\right], \left[\frac{5}{4}, \frac{3}{2}, \frac{7}{4}\right], \frac{Y^4}{256}\right)\right]. \tag{3.7}$$

Each term of this power series in $\tau^{1/4}$ is an exact solution of the linear governing equation. The terms of order $\tau^{j/4}$ are recognizable as self-similar solutions under a scaling symmetry that depends on j,

$$\bar{\mu} = e^{0.5j\epsilon}\mu;\ \ \bar{\tau} = e^{2\epsilon}\tau;\ \ \bar{Y} = e^{\epsilon} Y.$$

Note that only the first term $\mu_0(Y)$, with $j = 0$, is invariant under the Boltzmann scaling symmetry, which is the scaling symmetry that also leaves the dependent variable invariant. The other terms in the series, obtained by separating canonical coordinates of the Boltzmann symmetry, provide a solution that is much more general than the similarity solution alone. Such a construction by separation of variables has been used before to solve Stefan problems with classical second-order heat diffusion equation, general initial conditions and general time-dependent temperature boundary conditions [17] and to solve a modified Stefan problem with an additional heat supply at the phase boundary [18].

4 Formal series solution

Given the series (3.7) and (3.6), it remains to deduce the coefficients K_{ij} and b_j from the boundary conditions. The boundary conditions at $x = 0 (\Longleftrightarrow \; Y = \tau^{-1/4}\Sigma(\tau))$ may be effected as relations among the coefficients after a straightforward but tedious substitution. The boundary conditions at $Y \to \infty$ are more difficult to implement using power series forms for the special functions involved. As in Mullins' [1] treatment of the small-slope model, we use the fact that the zero value of the solution at infinity halves the number the free parameters in the Laplace transform solution, which in turn leads to parameter restrictions on the power series solution at any convenient value of Y where both types of solution can be evaluated and compared. The boundary conditions at $x = 0$ cannot be implemented directly using Laplace transforms because this is a free boundary with Y depending on τ.

4.1 Boundary conditions

$$\begin{aligned}
&\text{(a) } Y = \sum_{i=0}^{\infty} b_i \tau^{\frac{i}{4}}, \quad \mu = \sum_{j=0}^{\infty} \epsilon_j \tau^{\frac{j}{4}} \\
&\text{(b) } Y = \sum_{i=0}^{\infty} b_i \tau^{\frac{i}{4}}, \quad \mu_{YY} = 0 \\
&\text{(c) } \tau = 0 (\Rightarrow Y \to \infty), \quad \mu = 1 \\
&\text{(d) } Y \to \infty, \quad \mu \to 1 \\
&\text{(e) } Y \to \infty, \quad \mu_Y \to 0 \\
&\text{(f) } Y = \sum_{i=0}^{\infty} b_i \tau^{\frac{i}{4}}, \quad \mu_{YYY} = \sum_{l=0}^{\infty} \eta_l \tau^{\frac{l}{4}} = \sum_{i=0}^{\infty} b_i \frac{(i+1)}{4} \tau^{i/4} \sum_{j=0}^{\infty} \epsilon_j \tau^{j/4}.
\end{aligned} \tag{4.1}$$

The boundary conditions are correct at the leading order in τ if and only if the leading term in the expansion for μ is the known [5] similarity solution $\mu_0(Y)$ with constant groove slope $m = (\beta/\epsilon_0) - \beta$. Hence,

$$\begin{aligned}
\mu = \mu_0(Y) + \sum_{j=1}^{\infty} \tau^{j/4} \Bigg[& K_{1j}\, {}_1F_3\left(\left[\frac{-j}{4}\right], \left[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\right], \frac{Y^4}{256}\right) + K_{2j} Y\, {}_1F_3\left(\left[\frac{1}{4} - \frac{j}{4}\right], \left[\frac{1}{2}, \frac{3}{4}, \frac{5}{4}\right], \frac{Y^4}{256}\right) \\
& + K_{3j} Y^2\, {}_1F_3\left(\left[\frac{1}{2} - \frac{j}{4}\right], \left[\frac{3}{4}, \frac{5}{4}, \frac{3}{2}\right], \frac{Y^4}{256}\right) + K_{4j} Y^3\, {}_1F_3\left(\left[\frac{3}{4} - \frac{j}{4}\right], \left[\frac{5}{4}, \frac{3}{2}, \frac{7}{4}\right], \frac{Y^4}{256}\right) \Bigg].
\end{aligned} \tag{4.2}$$

For the case of variable $m(\tau)$, we have satisfied the boundary conditions to orders $\tau^{j/4}$ for $j = 0$ to 3. However, for the sake of brevity, details of the calculations are given only for $j = 1$, shown in Appendix A.

In Fig. 2, exact coefficients of the first five terms of the series solution have been used to construct an exact solution of the governing PDE. Similarity variables are used as coordinates so that the solution can be seen to evolve away from the similarity solution as the groove slope changes. The solution for $\theta(x, t)$ has been integrated from the calculated depth $y(0, t)$ to obtain $y(x, t)$. The approach of y to 0 as x tends to ∞ is a test of the solution accuracy. We have found that if the 5-term series is extended to $\tau = 10$, then $y/(B\tau)^{1/4}$ appears to approach a value near -0.04 as x increases.

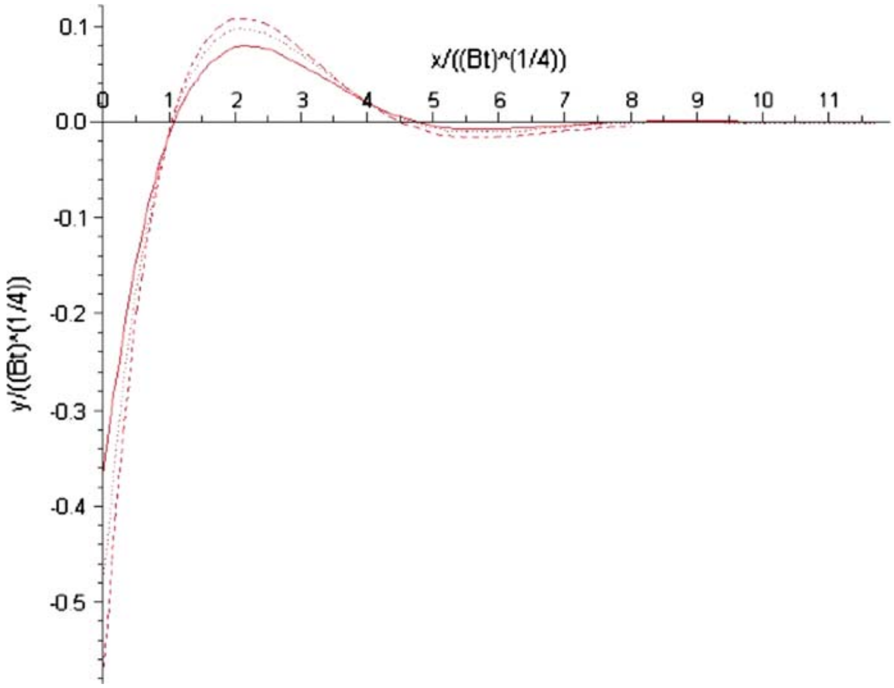


Fig. 2 Plot of surface in terms of dimensionless similarity coordinates at output times $\tau = 0.0002$ (*solid*), 0.01 (*dotted*), 1.0 (*dashed*), given prescribed slope $m(\tau) = 0.5 + 0.5\tau^{0.25}$ at groove root $x = 0$. Exact coefficients have been calculated for the first five terms of the series

5 Conclusion

For a linear partial differential equation, a Lie symmetry leads algorithmically, through separation of variables, to a solution that is much more general than the habitual similarity solution obtained by symmetry reduction. This allows one to formally solve free-boundary problems that have an approximate symmetry at early times. In the application given above, we have made use of a simple scaling symmetry but in other applications, the method of separation of variables could be developed from any symmetry (except for linear superposition) of any linear PDE. We have applied this method here to a complicated practical boundary-value problem for fourth-order surface diffusion near a grain boundary at changing temperature. Firstly we transform an integrable model to a linear governing equation. To solve (3.3) we find the values of the constants $K_{1j},\ K_{2j},\ K_{3j},\ K_{4j}$ in (4.2) as well as $\mu_0(y)$ and the constants $b_i = -4\gamma_i/\beta$ which give the free boundary. Then we invert the change of variables to get $y(x, t)$.

As discussed in Sect. 2, the integrable fourth-order diffusion equation (2.27) exactly describes surface diffusion on a material with a particular kind of crystal anisotropy. However, since for a wide range of surface orientations, the model material is close to isotropic (Fig. 1), Eq. 2.27 also approximates (1.1) for surface diffusion on an isotropic material. Tritscher [3] used an accurate numerical model to solve (1.1) for the grain-boundary problem and for evolution of a ramp dislocation when initial slopes were as large as 2. In each case the solution was within 2% of the solution of the anisotropic integrable model.

A number of significant questions about the rigour of the solution method remain unanswered. However, some indications of the answers are given by studies on simpler PDEs that have been solved by the same method. The integrable equation (2.27) is the fourth-order member of an integrable hierarchy of n'th order nonlinear PDE, each of which can be solved by essentially the same transformations given here [19,11,5].

After an additional change of variable, essentially the same formal series expansion method was applied to a second-order integrable diffusion-convection equation [18],

$$\theta_t = \partial_x[(\beta - \theta)^{-2}\theta_x] - [(\beta - \theta)^{-2} + \gamma]\theta_x,$$

subject to Dirichlet boundary conditions. Explicit recurrence relations were found for the series coefficients; up to 180 terms were calculated in examples. There is no evidence that the partial sums do not approach a limit. However, convergence of the formal series has not yet been proven.

Unlike in our method, in perturbation-series methods, partial sums do not give exact solutions to the governing equation. Unlike standard second-order diffusion problems, fourth-order diffusion problems do not in general obey a maximum principle and they do not have increasing Shannon information [20]. Solutions $\theta(x,t)$ to standard fourth-order diffusion problems are not one-to-one functions of x (e.g. Fig. 2) so that x cannot be a single valued function of (θ, t) and Philip's perturbation series approach [21] cannot be applied. Hence there are few, if any, rival methods for producing analytical solutions to nonlinear boundary-value problems with fourth-order diffusion.

A (Appendix): Evaluation of series coefficients

A.1 Boundary conditions at $Y = \sum_{i=0}^{\infty} b_i \tau^{\frac{i}{4}}$

At this stage it is convenient to define functions

$$\begin{aligned}
&f0_j(z) = {}_1F_3\left(\left[\frac{-j}{4}\right], \left[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\right], z\right), \quad f1_j(z) = {}_1F_3\left(\left[\frac{-j}{4}+2\right], \left[\frac{9}{4}, \frac{5}{2}, \frac{11}{4}\right], z\right),\\
&f2_j(z) = {}_1F_3\left(\left[1-\frac{j}{4}\right], \left[\frac{5}{4}, \frac{3}{2}, \frac{7}{4}\right], z\right), \quad f3_j(z) = {}_1F_3\left(\left[\frac{5}{4}-\frac{j}{4}\right], \left[\frac{3}{2}, \frac{7}{4}, \frac{9}{4}\right], z\right),\\
&f4_j(z) = {}_1F_3\left(\left[\frac{9}{4}-\frac{j}{4}\right], \left[\frac{5}{2}, \frac{11}{4}, \frac{13}{4}\right], z\right), \quad f5_j(z) = {}_1F_3\left(\left[\frac{1}{2}-\frac{j}{4}\right], \left[\frac{3}{4}, \frac{5}{4}, \frac{3}{2}\right], z\right),\\
&f6_j(z) = {}_1F_3\left(\left[\frac{3}{2}-\frac{j}{4}\right], \left[\frac{7}{4}, \frac{9}{4}, \frac{5}{2}\right], z\right), \quad f7_j(z) = {}_1F_3\left(\left[\frac{5}{2}-\frac{j}{4}\right], \left[\frac{11}{4}, \frac{13}{4}, \frac{7}{2}\right], z\right),\\
&f8_j(z) = {}_1F_3\left(\left[\frac{3}{4}-\frac{j}{4}\right], \left[\frac{5}{4}, \frac{3}{2}, \frac{7}{4}\right], z\right), \quad f9_j(z) = {}_1F_3\left(\left[\frac{7}{4}-\frac{j}{4}\right], \left[\frac{9}{4}, \frac{5}{2}, \frac{11}{4}\right], z\right),\\
&f10_j(z) = {}_1F_3\left(\left[\frac{11}{4}-\frac{j}{4}\right], \left[\frac{13}{4}, \frac{7}{2}, \frac{15}{4}\right], z\right), \quad f11_j(z) = {}_1F_3\left(\left[\frac{-j}{4}\right], \left[\frac{1}{2}, \frac{3}{4}, \frac{5}{4}\right], z\right),\\
&f12_j(z) = {}_1F_3\left(\left[3-\frac{j}{4}\right], \left[\frac{13}{4}, \frac{7}{2}, \frac{15}{4}\right], z\right), \quad f13_j(z) = {}_1F_3\left(\left[\frac{13}{4}-\frac{j}{4}\right], \left[\frac{7}{2}, \frac{15}{4}, \frac{17}{4}\right], z\right),\\
&f14_j(z) = {}_1F_3\left(\left[\frac{7}{2}-\frac{j}{4}\right], \left[\frac{15}{4}, \frac{17}{4}, \frac{9}{2}\right], z\right), \quad f15_j(z) = {}_1F_3\left(\left[\frac{15}{4}-\frac{j}{4}\right], \left[\frac{17}{4}, \frac{9}{2}, \frac{19}{4}\right], z\right).
\end{aligned} \tag{A.1}$$

The boundary conditions can be written in terms of these functions evaluated at $z = \bar{b} = b_0^4/256$. From boundary condition (4.1a), on equating powers of τ we obtain expressions for ϵ_i, $i = 0, 1, 2 \ldots$. For example, by balancing terms of degree $\tau^{\frac{1}{4}}$, we have

$$\epsilon_1 = K_{11} f0_1\left(\bar{b}\right) + K_{21} b_0 + K_{31} b_0^2 f5_1\left(\bar{b}\right) + K_{41} b_0^3 f8_1\left(\bar{b}\right) + \mu_0'(b_0) b_1. \tag{A.2}$$

For boundary condition (4.1b), we first expand μ_{YY}:

$$\begin{aligned}
\mu_{YY} = \mu_0''(Y) + \sum_{j=1}^{\infty} \tau^{\frac{j}{4}} \Bigg[&\left(-\frac{Y^6}{5040} j \left(1-\frac{j}{4}\right) f1_j\left(\frac{Y^4}{256}\right) - \frac{Y^2}{8} j f2_j\left(\frac{Y^4}{256}\right)\right) K_{1j}\\
&+ K_{2j}\left(\frac{Y^3}{6}\left(\frac{1}{4}-\frac{j}{4}\right) f3_j\left(\frac{Y^4}{256}\right) + \frac{Y^7}{11340}\left(\frac{1}{4}-\frac{j}{4}\right)\left(\frac{5}{4}-\frac{j}{4}\right) f4_j\left(\frac{Y^4}{256}\right)\right)
\end{aligned}$$

$$+K_{3j}\left(2f5_j\left(\frac{Y^4}{256}\right)+\frac{7Y^4}{90}\left(\frac{1}{2}-\frac{j}{4}\right)f6_j\left(\frac{Y^4}{256}\right)+\frac{Y^8}{56700}\left(\frac{1}{2}-\frac{j}{4}\right)(\frac{3}{2}-\frac{j}{4})f7_j\left(\frac{Y^4}{256}\right)\right)$$
$$+K_{4j}\left(6yf8_j\left(\frac{Y^4}{256}\right)+\frac{3Y^5}{70}\left(\frac{3}{4}-\frac{j}{4}\right)f9_j\left(\frac{Y^4}{256}\right)+\frac{Y^9}{207900}\left(\frac{3}{4}-\frac{j}{4}\right)\left(\frac{7}{4}-\frac{j}{4}\right)f10_j\left(\frac{Y^4}{256}\right)\right)\Bigg].$$

Balancing terms of degree 0 and 1 in $\tau^{1/4}$ for boundary condition (4.1b), we get

$$\begin{aligned}0&=\mu_0''(b_0)\\0&=K_{11}\left[\frac{-b_0^6}{6720}f1_1\left(\bar{b}\right)-\frac{b_0^2}{8}f2_1\left(\bar{b}\right)\right]+K_{31}\left[\frac{b_0^8}{181440}f7_1\left(\bar{b}\right)+2f5_1\left(\bar{b}\right)+\frac{7b_0^4}{360}f6_1\left(\bar{b}\right)\right]\\&\quad+K_{41}\left[\frac{3b_0^5}{140}f9_1\left(\bar{b}\right)+\frac{b_0^9}{277200}f10_1\left(\bar{b}\right)\ +6b_0f8_1(\bar{b})\right]+\mu_0'''(b_0)b_1.\end{aligned}\tag{A.3}$$

For boundary condition (4.1f), we need an expression for μ_{YYY}:

$$\begin{aligned}\mu_{YYY}=\mu_0'''(Y)+\sum_{j=1}^{\infty}\tau^{\frac{j}{4}}\Bigg[&K_{1j}\left(-\frac{Y^9}{4989600}j\left(1-\frac{j}{4}\right)\left(2-\frac{j}{4}\right)f12_j\left(\frac{Y^4}{256}\right)\right.\\&\left.-\frac{Y^5}{560}j\left(1-\frac{j}{4}\right)f1_j\left(\frac{Y^4}{256}\right)-\frac{Y}{4}f2_j\left(\frac{Y^4}{256}\right)\right)\\&+K_{2j}\left(\frac{Y^6}{945}\left(\frac{1}{4}-\frac{j}{4}\right)\left(\frac{5}{4}-\frac{j}{4}\right)f4_j\left(\frac{Y^4}{256}\right)+\frac{Y^2}{2}\left(\frac{1}{4}-\frac{j}{4}\right)f3_j\left(\frac{Y^4}{256}\right)\right.\\&\left.+\frac{Y^{10}}{16216200}\left(\frac{1}{4}-\frac{j}{4}\right)\left(\frac{5}{4}-\frac{j}{4}\right)\left(\frac{9}{4}-\frac{j}{4}\right)f13_j\left(\frac{Y^4}{256}\right)\right)\\&+K_{3j}\left(\frac{Y^3}{3}\left(\frac{1}{2}-\frac{j}{4}\right)f6_j\left(\frac{Y^4}{256}\right)+\frac{Y^7}{3780}\left(\frac{1}{2}-\frac{j}{4}\right)\left(\frac{3}{2}-\frac{j}{4}\right)f7_j\left(\frac{Y^4}{256}\right)\right.\\&\left.+\frac{Y^{11}}{113513400}\left(\frac{1}{2}-\frac{j}{4}\right)\left(\frac{3}{2}-\frac{j}{4}\right)\left(\frac{5}{2}-\frac{j}{4}\right)f14_j\left(\frac{Y^4}{256}\right)\right)\\&+K_{4j}\left(6f8_j+\frac{17Y^4}{70}\left(\frac{3}{4}-\frac{j}{4}\right)f9_j\left(\frac{Y^4}{256}\right)+\frac{Y^8}{11550}\left(\frac{3}{4}-\frac{j}{4}\right)\left(\frac{7}{4}-\frac{j}{4}\right)f10_j\left(\frac{Y^4}{256}\right)\right.\\&\left.+\frac{Y^{12}}{567567000}\left(\frac{3}{4}-\frac{j}{4}\right)\left(\frac{7}{4}-\frac{j}{4}\right)\left(\frac{11}{4}-\frac{j}{4}\right)f15_j\left(\frac{Y^4}{256}\right)\right)\Bigg].\end{aligned}\tag{A.4}$$

Balancing powers of τ for boundary condition (4.1f), we obtain expressions for η_i $i=0,1,2,\ldots$ In particular, by balancing terms of degree $\tau^{1/4}$, we obtain

$$\begin{aligned}\eta_1=\mu_0''''(b_0)b_1&+K_{11}\left[-\frac{3b_0^5}{2240}f1_1\left(\bar{b}\right)\ -\frac{b_0}{4}f2_1\left(\bar{b}\right)-\frac{b_0^9}{3801600}f12_1\left(\bar{b}\right)\right]\\&+K_{31}\left[\frac{b_0^3}{12}f6_1\left(\bar{b}\right)+\frac{b_0^{11}}{363242880}f14_1\left(\bar{b}\right)\ +\frac{b_0^7}{12096}f7_1\left(\bar{b}\right)\right]\\&+K_{41}\left[\frac{17b_0^4}{140}f9_1\left(\bar{b}\right)+6f8_1\left(\bar{b}\right)+\frac{b_0^8}{15400}f10_1\left(\bar{b}\right)+\frac{b_0^{12}}{302702400}f15_1\left(\bar{b}\right)\right]\end{aligned}\tag{A.5}$$

By equating terms of the same degree $\tau^{j/4}(j = 0, 1, 2 \ldots)$ in boundary conditions (4.1a, b,f), we obtain sets of determining equations, the first three of which are of the form:

$$\epsilon_0 = \mu_0(b_0), \quad 0 = \mu_0''(b_0), \quad \eta_0 = \mu_0'''(b_0), \tag{A.6}$$

$$\epsilon_1 = F_1(K_{11}, K_{21}, K_{31}, K_{41}, b_0, b_1), \quad 0 = G_1(K_{11}, K_{31}, K_{41}, b_0, b_1), \quad \eta_1 = H_1(K_{11}, K_{31}, K_{41}, b_0, b_1), \tag{A.7}$$

$$\begin{aligned} \epsilon_2 &= F_2(K_{11}, K_{21}, K_{31}, K_{41}, K_{12}, K_{22}, K_{32}, K_{42}, b_0, b_1, b_2) \\ 0 &= G_2(K_{11}, K_{31}, K_{41}, K_{12}, K_{22}, K_{32}, K_{42}, b_0, b_1, b_2) \\ \eta_2 &= H_2(K_{11}, K_{31}, K_{41}, K_{12}, K_{22}, K_{32}, K_{42}, b_0, b_1, b_2), \end{aligned} \tag{A.8}$$

where the η_i are in terms of $b_0, b_1, \ldots b_i$.

From (A.6) we can find b_0. From (A.7) we can express K_{21}, K_{41}, b_1 in terms of K_{11}, K_{31}. From (A.8), we can find K_{22}, K_{42}, b_2 in terms of $K_{11}, K_{31}, K_{12}, K_{32}$. Continuing in this way, we can derive linear equations that eliminate K_{2j}, K_{4j} and b_j for $j = 1, 2, 3, \ldots$

$$K_{2j} = \sum_{i=1}^{j} [\psi_{1i} K_{1i} + \psi_{3i} K_{3i} + \phi_i], \quad K_{4j} = \sum_{i=1}^{j} [v_{1i} K_{1i} + v_{3i} K_{3i} + M_i],$$

$$b_j = \sum_{i=1}^{j} [w_{1i} K_{1i} + w_{3i} K_{3i} + E_i]. \tag{A.9, 10, 11}$$

It remains then to determine $K_{1i}, K_{3i}, \phi_i, M_i, E_i$.

A.2 Matching power series and Laplace transform solutions with correct boundary conditions at $Y \to \infty$

Applying the Laplace transform with respect to τ, we obtain the general transformed solution to (2.43) with initial value 1 and boundary value 1 as $Z \to \infty$ as follows:

$$\bar{\mu} = \exp\left(\frac{-p^{\frac{1}{4}} Z}{\sqrt{2}}\right)\left[C_3(p)\cos\left(\frac{p^{\frac{1}{4}} Z}{\sqrt{2}}\right) + C_4(p)\sin\left(\frac{p^{\frac{1}{4}} Z}{\sqrt{2}}\right)\right] + \frac{1}{p}. \tag{A.12}$$

We now match the Laplace transform of power series solution (4.2) with that of the exact Laplace transform (A.12) at the convenient value $Z = 0$ ($\iff$ $Y = 0$) to find expressions for K_{1j} and K_{3j}.

A.2.1 Matching solution values:

Taking Laplace transforms with respect to τ, through (4.2), at $Y = 0$, we have

$$\tilde{\mu} = \frac{\mu_0(0)}{p} + \sum_{j=1}^{\infty} K_{1j} \frac{\Gamma(\frac{j}{4} + 1)}{p^{\frac{j}{4}+1}}. \tag{A.13}$$

Then from (A.12) at $Z = 0$:

$$\tilde{\mu} = \frac{1}{p} + C_3(p). \tag{A.14}$$

Equating (A.13) and (A.14) gives

$$C_3(p) = \sum_{j=1}^{\infty} \left[K_{1j} \frac{\Gamma(\frac{j}{4} + 1)}{p^{\frac{j}{4}+1}}\right] + \left(\frac{\mu_0(0) - 1}{p}\right). \tag{A.15}$$

A.2.2 Matching first derivatives:

Noting firstly that $\frac{\partial\mu}{\partial Z} = \tau^{-1/4}\frac{\partial\mu}{\partial Y}$, at $Z = 0(\iff Y = 0)$, from (4.2),

$$\frac{\partial\mu}{\partial Z} = \mu_0'(0)\tau^{-1/4} + \sum_{j=1}^{\infty} K_{2j}\tau^{\frac{j}{4}-\frac{1}{4}}.$$

Taking Laplace transforms with respect to τ, then at $Z = 0$,

$$\frac{\partial\tilde{\mu}}{\partial Z} = \frac{\mu_0'(0)\Gamma\left(\frac{3}{4}\right)}{p^{\frac{3}{4}}} + \sum_{j=1}^{\infty} K_{2j}\frac{\Gamma\left(\frac{j}{4}+\frac{3}{4}\right)}{p^{\frac{j}{4}+\frac{3}{4}}}. \tag{A.16}$$

From (A.12) at $Z = 0$,

$$\frac{\partial\tilde{\mu}}{\partial\bar{z}} = \frac{1}{\sqrt{2}}p^{\frac{1}{4}}[C_4(p) - C_3(p)]. \tag{A.17}$$

From (A.16) and (A.17), we deduce

$$C_4(p) - C_3(p) = \sqrt{2}\sum_{j=1}^{\infty} K_{2j}\frac{\Gamma\left(\frac{j}{4}+\frac{3}{4}\right)}{p^{\frac{j}{4}+1}} + \sqrt{2}\frac{\mu_0'(0)\Gamma\left(\frac{3}{4}\right)}{p}. \tag{A.18}$$

A.2.3 Matching second derivatives:

From (4.2) we have at $Z = 0$ $(\iff Y = 0)$,

$$\mu_{ZZ} = \mu_0''(0)\tau^{-1/2} + 2\sum_{j=1}^{\infty} K_{3j}\tau^{(j-2)/4}. \tag{A.19}$$

Taking Laplace transforms with respect to τ gives at $Z = 0$,

$$\frac{\partial^2\tilde{\mu}}{\partial Z^2} = \frac{\mu_0''(0)\Gamma\left(\frac{1}{2}\right)}{p^{\frac{1}{2}}} + 2\sum_{j=1}^{\infty} K_{3j}\frac{\Gamma\left(\frac{j}{4}+\frac{1}{2}\right)}{p^{\frac{j}{4}+\frac{1}{2}}}. \tag{A.20}$$

From (A.12) at $Z = 0$,

$$\frac{\partial^2\tilde{\mu}}{\partial Z^2} = -p^{\frac{1}{2}}C_4(p). \tag{A.21}$$

Therefore from (A.20) and (A.21), we have

$$C_4(p) = -\frac{\mu_0''(0)\Gamma\left(\frac{1}{2}\right)}{p} - 2\sum_{j=1}^{\infty} K_{3j}\frac{\Gamma\left(\frac{j}{4}+\frac{1}{2}\right)}{p^{\frac{j}{4}+1}}. \tag{A.22}$$

A.2.4 Matching third derivatives:

From (4.2) at $Z = 0$ $(\iff Y = 0)$,

$$\mu_{ZZZ} = \mu_0'''(0)\tau^{-3/4} + 6\sum_{j=1}^{\infty} K_{4j}\tau^{\frac{j}{4}-\frac{3}{4}}. \tag{A.23}$$

Taking Laplace transforms with respect to τ, we get at $Z = 0$,

$$\frac{\partial^3\tilde{\mu}}{\partial Z^3} = \frac{\mu_0'''(0)\Gamma\left(\frac{1}{4}\right)}{p^{\frac{1}{4}}} + 6\sum_{j=1}^{\infty} K_{4j}\frac{\Gamma\left(\frac{j}{4}+\frac{1}{4}\right)}{p^{\frac{j}{4}+\frac{1}{4}}}. \tag{A.24}$$

From (A.12), at $Z = 0$ we have

$$\frac{\partial^3 \tilde{\mu}}{\partial Z^3} = \frac{1}{\sqrt{2}} p^{\frac{3}{4}} [C_3(p) + C_4(p)]. \tag{A.25}$$

From (A.24) and (A.25), matching the third derivatives at $Z = 0$ gives

$$C_3(p) + C_4(p) = \frac{\sqrt{2}\mu'''(0)\Gamma\left(\frac{1}{4}\right)}{p} + 6\sqrt{2}\sum_{j=1}^{\infty} K_{4j} \frac{\Gamma\left(\frac{j}{4}+\frac{1}{4}\right)}{p^{\frac{j}{4}+1}}. \tag{A.26}$$

In the following, using (A.15), (A.18), (A.22), (A.26), we find K_{1j} and K_{3j}. Equations (A.26,A.18) imply

$$C_4(p) = \frac{1}{2}\left[\sqrt{2}\sum_{j=1}^{\infty} K_{2j}\frac{\Gamma\left(\frac{j}{4}+\frac{3}{4}\right)}{p^{\frac{j}{4}+1}} + 6\sqrt{2}\sum_{j=1}^{\infty} K_{4j}\frac{\Gamma\left(\frac{j}{4}+\frac{1}{4}\right)}{p^{\frac{j}{4}+1}}\right] + \frac{1}{2}\left[\frac{\sqrt{2}\mu_0'(0)\Gamma\left(\frac{3}{4}\right)}{p} + \frac{\sqrt{2}\mu_0'''(0)\Gamma\left(\frac{1}{4}\right)}{p}\right]. \tag{A.27}$$

Comparing (A.27) with (A.22), we have

$$-2\Gamma\left(\frac{j}{4}+\frac{1}{2}\right)K_{3j} = \frac{K_{2j}}{\sqrt{2}}\Gamma\left(\frac{j}{4}+\frac{3}{4}\right) + 3\sqrt{2}\Gamma\left(\frac{j}{4}+\frac{1}{4}\right)K_{4j} \tag{A.28}$$

and

$$-\mu_0''(0)\Gamma\left(\frac{1}{2}\right) = \frac{\sqrt{2}}{2}\left[\mu_0'(0)\Gamma\left(\frac{3}{4}\right) + \mu_0'''(0)\Gamma\left(\frac{1}{4}\right)\right], \tag{A.29}$$

so that using (A.9) and (A.10), (A.28) implies

$$-2\Gamma\left(\frac{j}{4}+\frac{1}{2}\right)K_{3j} = \frac{1}{\sqrt{2}}\Gamma\left(\frac{j}{4}+\frac{3}{4}\right)\sum_{i=1}^{j}(\psi_{1i}K_{1i} + \psi_{3i}K_{3i} + \phi_i)$$
$$+3\sqrt{2}\Gamma\left(\frac{j}{4}+\frac{1}{4}\right)\sum_{i=1}^{j}(v_{1i}K_{1i} + v_{3i}K_{3i} + M_i). \tag{A.30}$$

This equation is of the form

$$(A_{11}K_{11} + A_{12}K_{12} + \cdots + A_{1j}K_{1j}) + (A_{31}K_{31} + A_{32}K_{32} + \cdots + A_{3j}K_{3j}) = X_j, \tag{A.31}$$

where the $A_{1p}, A_{3p}, p = 1\ldots j$ and X_j are constants. Hence for

$$j = 1 \text{ and } 2,\ \ A_{11}K_{11} + A_{31}K_{31} = X_1, \tag{A.32}$$
$$j = 2,\ \ A_{11}K_{11} + A_{31}K_{31} + A_{12}K_{12} + A_{32}K_{32} = X_2. \tag{A.33}$$

Further, by subtraction, Eqs. A.18, A.26 give

$$2C_3(p) = \frac{\sqrt{2}\mu_0'''(0)\Gamma\left(\frac{1}{4}\right) - \sqrt{2}\mu_0'(0)\Gamma\left(\frac{3}{4}\right)}{p} + 6\sqrt{2}\sum_{j=1}^{\infty}\frac{\Gamma\left(\frac{j}{4}+\frac{1}{4}\right)}{p^{\frac{j}{4}+1}}K_{4j} - \sqrt{2}\sum_{j=1}^{\infty}\frac{\Gamma\left(\frac{j}{4}+\frac{3}{4}\right)}{p^{\frac{j}{4}+1}}K_{2j}. \tag{A.34}$$

Comparing (A.34) with (A.15) gives

$$\mu_0(0) - 1 = \frac{\sqrt{2}}{2}\left[\mu_0'''(0)\Gamma\left(\frac{1}{4}\right) - \mu_0'(0)\Gamma\left(\frac{3}{4}\right)\right] \tag{A.35}$$

and

$$K_{1j}\Gamma\left(\frac{j}{4}+1\right) = 3\sqrt{2}\Gamma\left(\frac{j}{4}+\frac{1}{4}\right)K_{4j} - \frac{\sqrt{2}}{2}K_{2j}\Gamma\left(\frac{1}{4}+\frac{3}{4}\right). \tag{A.36}$$

The general similarity solution $\mu_0(Y)$ contains four arbitrary constants that may be determined from (A.29, A.36) as well as (A.6). Using (A.9) and (A.10), (A.36) implies

$$K_{1j}\Gamma\left(\frac{j}{4}+1\right)=3\sqrt{2}\Gamma\left(\frac{j}{4}+\frac{1}{4}\right)\sum_{i=1}^{j}(v_{1i}K_{1i}+v_{3i}K_{3i}+M_i)$$

$$-\frac{\sqrt{2}}{2}\Gamma\left(\frac{j}{4}+\frac{3}{4}\right)\sum_{i=1}^{j}(\psi_{1i}K_{1i}+\psi_{3i}K_{3i}+\phi_i)\,. \tag{A.37}$$

This is again of the form

$$(T_{11}\ K_{11}+T_{12}\ K_{12}+\cdots+T_{1j}\ K_{1j})+(T_{31}\ K_{31}+T_{32}\ K_{32}+\cdots+T_{3j}\ K_{3j})=Z_j, \tag{A.38}$$

where the $T_{1m}, T_{3m}, m = 1\ldots j$ and Z_j are constants.

Hence for example when

$$j=1,\ T_{11}\ K_{11}\ +T_{31}\ K_{31}=Z_1, \tag{A.39}$$

$$j=2,\ T_{11}\ K_{11}\ +T_{31}\ K_{31}+T_{12}\ K_{12}+T_{32}\ K_{32}=Z_2. \tag{A.40}$$

Using (A.32) and (A.39) (values with $j = 1$) we can find K_{11} and K_{31}. Then on inserting these values into (A.33) and (A.40) we can solve for K_{12} and K_{32}. Continuing with successive values of j in (A.31) and (A.38) we can find the values of K_{1j} and K_{3j} for all natural numbers j.

In summary, *to find the constants*:

1. From (A.29, A.35, A.6) we have b_0 as well as the constants in the similarity solution $\mu_0(y)$ found at the leading order [5].
2. By successively equating powers of τ from boundary conditions (4.1a, b, f) at $y = \dfrac{-4}{\beta}\sum_{i=0}^{\infty}\gamma_i\tau^{(i+1)/4}$ find $K_{2j}, K_{4j}, b_j, j = 1 = 1, 2, \ldots$ in the forms (A.9–A.10), i.e., find $\psi_{1i}, \psi_{3i}, v_{1i}, v_{3i}, w_{1i}, w_{3i}, \phi_i, M_i, E_i$.
3. Construct a system of linear equations (A.31) and (A.38). Starting with $j = 1$, solve for K_{11}, K_{31}, then using $j = 2$ solve for K_{12}, K_{32} and with each successive j, solve for K_{1j}, K_{3j}.
4. Find $K_{2j}, K_{4j}, b_j, j = 1, 2, \ldots$, using (A.9), (A.10), (A.11).

References

1. Mullins WW (1957) Theory of thermal grooving. J Appl Phys 28:333–339
2. Defay R, Prigogine I (1966) Surface tension and adsorption. Longmans, London
3. Tritscher P (1996) Integrable nonlinear evolution equations applied to solidification and surface redistribution. PhD Thesis, University of Wollongong
4. Cahn JW, Taylor JE (1994) Surface motion by surface diffusion. Acta Metall Mater 42:1045–1063
5. Broadbridge P, Tritscher P (1994) An integrable fourth-order nonlinear evolution equation applied to thermal grooving of metal surfaces. IMA J Appl Math 53:249–265
6. Tritscher P, Broadbridge P (1995) Grain boundary grooving by surface diffusion: an analytic nonlinear model for a symmetric groove. Proc R Soc Lond A 450(1940):569–587
7. Camel D, Eustathopoulos N, Desré P (1980) Chemical adsorption and temperature dependence of the solid–liquid interfacial tension of metallic binary alloys. Acta Metall 28:239–247
8. Holness MB (1993) Temperature and pressure dependence of quartz-aqueous fluid dihedral angles: the control of adsorbed H_2O on the permeability of quartzites. Earth Planet Sci Lett 117(3–4):363–377
9. Miller W Jr (1977) Symmetry and separation of variables. Addison-Wesley, Reading
10. Herring C (1951) Surface tension as a motivation for sintering. In: Kingston WE (ed) The physics of powder metallurgy. McGraw-Hill, New York
11. Bluman GW, Kumei S (1980) On the remarkable nonlinear diffusion equation $\frac{\partial}{\partial x}\left[a(u+b)^{-2}\frac{\partial u}{\partial x}\right]-\frac{\partial u}{\partial t}=0$. J Math Phys 21:1019–1023
12. Bluman GW, Kumei S (1990) Symmetry-based algorithms to relate partial differential equations, II. Linearization by nonlocal symmetries. Euro J Appl Math 1:217–223

13. Goard JM, Broadbridge P (1997) Nonlinear superposition principles obtained by Lie symmetry methods. J Math Anal Appl 214:633–657
14. Tritscher P (1999) Thermal grooving by surface diffusion for an extended bicrystal abutting a half-space. Proc R Soc Lond A 455:1957–1977
15. Bluman GW, Kumei S (1989) Symmetries and differential equations. Springer Verlag, New York
16. Ibragimov NH (ed) (1994) CRC handbook of Lie group analysis of differential equations, vol 1. CRC Press, Boca Raton
17. Tao LN (1979) On free boundary problems with arbitrary initial and flux conditions. Z Angew Math Phys (ZAMP) 30(3):416–426
18. Broadbridge P, Triadis D, Hill JM (2009) Infiltration from supply at constant water content: an integrable model. J Eng Math 64(2):193–206
19. Rogers C (1983) Application of reciprocal B acklund transformations to a class of nonlinear boundary value problems. J Phys A 16:L493–L495
20. Broadbridge P (2008) Entropy diagnostics for fourth order partial differential equations in conservation form. Entropy 8:295–311
21. Philip JR (1969) Theory of infiltration. Adv Hydrosci 5:215–296