Atomic Diffusion from a Material Surface into a Grain Boundary

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Abstract

A model problem of stress induced atomic diffusion from the surface of a material into a semi-infinite grain boundary orthogonal to the surface is analysed. The governing equation is shown to be a singular integro-differential equation. An algorithm for exact solution to this problem is proposed. It involves reduction to a functional-difference equation in a strip and then to a Riemann-Hilbert boundary-value problem for an open contour that admits solution by quadratures. Analytical continuation of the solution of the difference equation in the strip is constructed. The continuation is a meromorphic function in the exterior of the strip. Its poles form a countable set and are not periodic. In addition to a closed-form solution of the integro-differential equation, a procedure of finding a rapidly convergent series representation and an asymptotic expansion for large arguments are proposed. Asymptotic analysis and numerical results for the grain boundary traction, the atomic flux in the boundary and the displacement rate are reported and discussed.

1 Introduction

Atomic diffusion from a material surface into grain boundaries has been proposed (Thouless et al., 1993; Vinci et al., 1995; Keller et al., 1998; Kobrinsky and Thompson, 1998; Gao et al., 1999; Weiss et al., 2001) as an important mechanism for stress relaxation and deformation in thin metal films that are now widely used in microelectronics, integrated optoelectronics, data storage technologies and micro-electro-mechanical systems. Recently, Gao et al. (1999) have investigated the problem of constrained diffusional creep in thin films with columnar grains. For the first time, this problem has been solved for the constraint of perfect film adhesion with no sliding and no diffusion at the film/substrate interface. In the solution method adopted by Gao et al. (1999), the coupled elasticity and grain-boundary diffusion problem was first reduced to an eigenvalue problem with a 1-d-integro-differential operator and then numerically solved by the method of orthogonal polynomials. Such analysis has indicated that the surface atoms, after being transported into the grain boundaries by directed diffusion under tensile stress, give rise to the formation of so called grain boundary diffusion wedges which exhibit crack-like singular stress behaviours near the film/substrate interface. As a result of perfect film adhesion, the stress is relaxed more efficiently at the grain boundaries and at the film surface than at the grain interior and at the film/substrate interface. Weiss et al. (2001) have made comparisons between theoretical predictions and experimental data and successfully described the stress-temperature curves of UHV synthesised Cu films by the constrained diffusional creep model.

The above studies have clearly demonstrated that atomic diffusion along surfaces and grain boundaries is a problem of significant technological importance. There is still a general lack of rigorous mathematical modelling of this important class of materials phenomena. In this paper, we develop a rigorous study of the problem of atomic diffusion from a material surface into a semi-infinite grain boundary, partly motivated by the need to understand the initial stage of atomic diffusion in thin films. Antipov & Gao (2000) have derived integro-differential equations for an infinite and a semi-infinite grain boundaries, both of which admit the following representation

$$-u^k f^{(p)}(u) = \int_0^\infty h\left(\frac{u}{v}\right) f^{(m)}(v)\frac{dv}{v}, \quad 0 < u < \infty \tag{1.1}$$

with $k = 1, p = 1, m = 3$. We mention that some cases of another class of integro-differential equations

$$-f(u) = \int_0^\infty h\left(\frac{u}{v}\right) f^{(m)}(v)\frac{dv}{v} + g(u), \quad 0 < u < \infty \tag{1.2}$$

(m is positive and integer) which arise in classical elasticity problems, have been studied by Koiter (1955), Bantsuri (1974), Popov & Tikhonenko (1974), Atkinson (1977), Atkinson & Craster (1994).

Antipov & Gao proposed a procedure for solution of the integro-differential equation (1.1) for the case of an infinite grain boundary. The main steps of the technique are:

(i) establish the class of solutions;

(ii) apply the Mellin transform and derive a functional-difference equation in a strip of a complex variable;

(iii) use conformal mapping to reduce the difference equation to a Riemann-Hilbert boundary-value problem on an open contour (a_1, a_2) with the coefficient that behaves at the ends as $c_j \log^2(s - a_j)$, where c_j are constants, s is a complex variable, $j = 1, 2$;

(iv) use inverse Mellin transform to obtain a closed form-solution to the integro-differential equation;

(v) construct an analytical continuation of the solution of the difference equation;

(vi) derive a series-form solution and an asymptotic expansion for large arguments.

Implementation of steps (iii) and (v) is based on the results of Čerskiĭ (1970), Mel'nik (1959) and Popov & Tikhonenko (1974). In addition to the complete analysis of the case of an infinite grain boundary, Antipov & Gao (2000) outlined the procedure for a semi-infinite grain boundary. However, to construct a series representation of the solution and an asymptotic expansion for that case, one needs to generalise the method for the case when the analytical continuation of the solution of the difference equation has a countable set of non-periodic poles. The main aims of this paper are:

(i) to construct an exact solution of the integro-differential equation for a semi-infinite grain boundary;

(ii) to develop a procedure for numerically efficient series-form solution and also an asymptotic expansion for large arguments;

(iii) to analyse the behaviour of the grain boundary traction (and therefore, the chemical potential along the grain boundary), the flux and the displacement rate as $t \to 0$ and $t \to \infty$.

The structure of the paper is as follows. Section 2 models atomic diffusion from the surface of a material along a semi-infinite grain boundary in terms of a one-dimensional singular integro-differential equation. In section 3, we present the main steps of the algorithm and write down a solution in integral form. An analytical continuation into the whole complex plane of the solution of a difference equation, is constructed in section 4. We derive a rapidly convergent series representation of the solution in section 5. It is established that $f(u) = O(u^2 \log u)$ as $u \to 0$, and $f'''(u) \sim cu^{-1}$ and it is also checked that the singular integral in (1.1) converges as $u \to 0$. Section 6 provides an asymptotic expansion of the solution for large arguments. It is found out that $-uf'(u) \sim 16u^{-3}$ as $u \to \infty$ and it is proved that the right-hand side of equation (1.1) has the same behaviour at infinity: $h * f''' \sim 16u^{-3}$, $u \to \infty$. Asymptotic formulae for the grain boundary traction, the atomic flux and the displacement rate are derived in section 7. Numerical results are also reported in that section. Concluding remarks are given in the final section.

2 Problem formulation

We consider atomic diffusion from the surface $\{-\infty < x < \infty, z = 0\}$ of a material $\{|x| < \infty, 0 < z < \infty\}$ into a semi-infinite grain boundary $\{x = \pm 0, 0 < z < \infty\}$, in response to an applied stress σ_0 as shown in Fig.1. The atomic diffusion causes a wedge of material to spread along the grain boundary. The opening displacement of the diffusion wedge determines the amount of material that must be transported. We model the crack-like diffusion wedge as a continuous array of climb-edge dislocations. The normal traction on the boundary σ_{gb} due to the material wedge with the opening

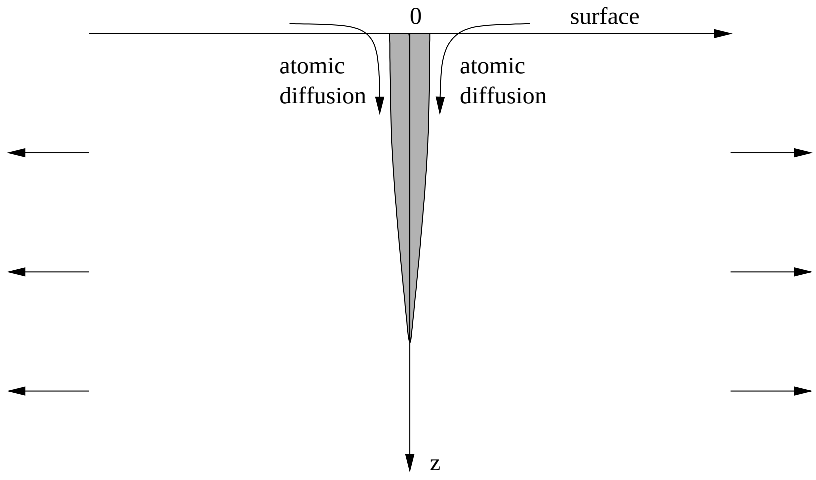

Figure 1: Atomic diffusion along a semi-infinite grain boundary

normal displacement function $2u_{gb}(z,t)$ is defined by (see, for example, Eshelby, 1979; Gao et al., 1999)

$$\sigma_{gb}(z,t) = \sigma_0 - \frac{E^*}{2\pi} \int_0^\infty S(z,\zeta) \frac{\partial u_{gb}(\zeta,t)}{\partial \zeta} d\zeta, \tag{2.1}$$

where

$$E^* = \frac{E}{1-\nu^2}, \quad S(z,\zeta) = \frac{1}{z-\zeta} - \frac{1}{z+\zeta} - \frac{2\zeta(z-\zeta)}{(z+\zeta)^3}, \tag{2.2}$$

E is the Young modulus, ν is Poisson's ratio. The singular integral here and and further is understood in the sense of the principal value. Due to mass conservation, the flux divergence at any point on the boundary is related to the displacement rate at that point through

$$2\frac{\partial u_{gb}(z,t)}{\partial t} = -\Omega \frac{\partial j(z,t)}{\partial z}, \tag{2.3}$$

where Ω is the atomic volume, and the atomic flux $j(z,t)$ in the boundary per unit out-of-plane thickness is

$$j(z,t) = -\frac{\delta_{gb} D_{gb}}{kT\Omega} \frac{\partial \mu(z,t)}{\partial z}. \tag{2.4}$$

Here $\mu(z,t)$ is the chemical potential along the grain boundary, δ_{gb} is the boundary thickness, D_{gb} is the atomic diffusivity in the boundary and kT is the product of Boltzmann's constant and temperature. Relative to a flat, free surface, the chemical potential along the grain boundary is proportional to the grain boundary traction (Rice & Chuang, 1981)

$$\mu(z,t) = -\sigma_{gb}(z,t)\Omega. \tag{2.5}$$

The system of partial differential equations (2.3), (2.4) and (2.5) with the integral representation (2.1) can be reduced to the following 2-d-integro-differential equation

$$\frac{\partial \sigma_{gb}(z,t)}{\partial t} = \frac{E^* D_{gb} \delta_{gb} \Omega}{4\pi kT} \int_0^\infty S(z,\zeta) \frac{\partial^3 \sigma_{gb}(\zeta,t)}{\partial \zeta^3} d\zeta \tag{2.6}$$

subject to the initial condition

$$\sigma_{gb}(z,0) = \sigma_0 \tag{2.7}$$

and the boundary conditions

$$\sigma_{gb}(\infty,t) = \sigma_0, \quad \sigma_{gb}(0,t) = 0. \tag{2.8}$$

The partial differential equation with the integral operator (2.6) admits reduction to a 1-d-integro-differential equation for the function

$$\sigma_{gb}(z,t) = \sigma_0 f(u), \tag{2.9}$$

where

$$u = \frac{z}{(at)^{1/3}}, \quad a = \frac{3E^* \delta_{gb} D_{gb} \Omega}{4\pi kT}. \tag{2.10}$$

Finally, the resulting equation becomes

$$uf'(u) + 8u \int_0^\infty \frac{v^2 f'''(v) dv}{(u-v)(u+v)^3} = 0, \quad 0 < u < \infty \tag{2.11}$$

with the additional conditions

$$f(0) = 0, \qquad f(\infty) = 1. \tag{2.12}$$

3 Solution of the integro-differential equation by quadratures

In this section we outline a procedure that leads to a closed-form solution of the integro-differential equation

$$uf'(u) + \int_0^\infty h\left(\frac{u}{v}\right) f'''(v) \frac{dv}{v} = 0, \quad 0 < u < \infty. \tag{3.1}$$

In the case of equation (2.11), the kernel-function $h(s)$ has the form

$$h(t) = \frac{8t}{(t-1)(t+1)^3}. \tag{3.2}$$

The procedure consists of several steps.

Step 1: Class of solutions. At the first stage we need to define a class of solutions that should be in agreement with the physical sense of the unknown function.

Let $f(u) \in \mathcal{H}^{2-\delta,0}(0,\infty)$, where $\delta \in (0,1)$ and the class $\mathcal{H}^{\alpha,\beta}(0,\infty)$ is identified as follows. A function $\phi(u)$ is said to belong to the class $\mathcal{H}^{\alpha,\beta}(0,\infty)$ if

(i) $\phi(u)$ is a Hölder function on (a,b) for any a,b such that $0 < a < b < \infty$,

(ii) At zero and at infinity, the function $\phi(u)$ is estimated by

$$|\phi(u)| < Au^{\alpha}, \quad u \to 0, \qquad |\phi(u)| < Bu^{\beta}, \quad u \to \infty.$$

In addition, we assume that

$$f'(u) \in \mathcal{H}^{1-\delta,0}(0,\infty), \quad f''(u) \in \mathcal{H}^{-\delta,-1}(0,\infty), \quad f'''(u) \in \mathcal{H}^{-1-\delta,-2}(0,\infty). \tag{3.3}$$

Step 2: A functional-difference equation in a strip. We introduce the Mellin transform of the density of the singular integral in (3.1)

$$F(s) = \int_0^\infty f'''(u)u^{s-1}du. \tag{3.4}$$

Because of the choice of the class (3.3), the function $F(s)$ is analytic in the strip $1+\delta < \Re(s) < 2$. Integrating by parts and using the Mellin convolution theorem (Titchmarsh, 1948) transform equation (3.1) as follows

$$\frac{1}{2\pi i}\int_\Omega \frac{F(s)u^{3-s}ds}{(s-1)(s-2)} = -\frac{1}{2\pi i}\int_\Omega F(s)H(s)u^{-s}ds, \quad 0 < u < \infty, \tag{3.5}$$

where

$$H(s) = \int_0^\infty h(t)t^{s-1}dt = -\pi\cot\pi s\left(1 + \frac{4s-2s^2-1}{\cos\pi s}\right), \quad -1 < \Re(s) < 3. \tag{3.6}$$

The last equation is meaningful if the function

$$\Phi(s) = -H(s)F(s) \tag{3.7}$$

is analytic in the strip $\Pi = \{-3+c < \Re(s) < c\}$ with $c \in (1+\delta, 2)$, and uniformly with respect to $x \in [-3+c, c]$

$$\int_{-\infty}^{\infty} |\Phi(x+it)|^2 dt \le const. \tag{3.8}$$

It also follows that another function $\Phi^*(s) = [(s-1)(s-2)]^{-1}F(s)$ is analytic in the strip $\Pi^* = \{c < \Re(s) < c+3\}$. On equal grounds, both functions $\Phi(s)$ and $\Phi^*(s)$ can be used in the algorithm. For definiteness, we choose the first function $\Phi(s)$. By the Cauchy theorem, equation (3.5) can be written in terms of the function $\Phi(s)$ as follows

$$\frac{1}{2\pi i}\int\limits_{\Omega}\left[\Phi(s-3)+\frac{\Phi(s)}{(s-1)(s-2)H(s)}\right]u^{-s+3}ds=0, \quad 0<u<\infty. \tag{3.9}$$

This means that the original integro-differential equation (2.11) is equivalent to the following problem:
Find a function $\Phi(s)$, that is analytic in the strip $\Pi=\{-3+c<\Re(s)<c\}$, satisfies the condition (3.8) and the boundary condition:

$$\Phi(\sigma)+D(\sigma)\Phi(\sigma-3)=0, \quad \sigma\in\Omega, \tag{3.10}$$

with

$$D(s)=(s-1)(s-2)H(s). \tag{3.11}$$

Step 3: A Riemann-Hilbert boundary-value problem and its solution. At this stage, we reduce problem (3.10) to a Riemann-Hilbert problem which can be solved exactly for any coefficient $D(\sigma)$. For this, we introduce a new function

$$\varphi(w)=\frac{1}{1+w}\left(i\frac{1-w}{1+w}\right)^{-1/2}\Phi(s), \tag{3.12}$$

where

$$w=i\tan\left\{\pi\left(\frac{1}{4}+\frac{s-c}{3}\right)\right\}, \quad s=c+\frac{3i}{2\pi}\log\left(i\frac{1-w}{1+w}\right). \tag{3.13}$$

We emphasise, that the functions

$$\zeta_1(w)=\log\left(i\frac{1-w}{1+w}\right) \quad \text{and} \quad \zeta_2(w)=\left(i\frac{1-w}{1+w}\right)^{1/2} \tag{3.14}$$

are defined and analytic in the w-plane with the cut $\gamma=\{|w|=1, \quad \Im(w)\geq 0\}$. Further, let

$$\gamma^+=\{|w|=1-0,\ \Im(w)>0\},\ \gamma^-=\{|w|=1+0, \quad \Im(w)>0\}. \tag{3.15}$$

On the contour γ^+, the logarithmic function $\zeta_1(\eta)$ is real and the function $\zeta_2(\eta)$ is positive. The contour Ω of the s-plane is mapped by the function w onto the contour γ^+ and the contour $\Omega_{-1}=\{\Re(s)=c-3\}$ is mapped onto γ^-. The starting point of the contour γ, the point $w=1$, corresponds to the point $s=c-i\infty$ of the contour Ω and the terminal point $w=-1$ corresponds to the point $s=c+i\infty$. Let $\varphi^\pm(\eta)$ be the limit values of the function $\varphi(w)$ as $w\to\eta\in\gamma^\pm$. Then

$$(1+\eta)\varphi^+(\eta)=e^{-\frac{\pi i}{3}(c-\sigma)}\Phi(\sigma),$$

$$(1+\eta)\varphi^-(\eta) = -e^{-\frac{\pi i}{3}(c-\sigma)}\Phi(\sigma-3), \quad \eta\in\gamma, \;\; \sigma\in\Omega. \tag{3.16}$$

In terms of the limit values of the function $\varphi(\zeta)$, the condition (3.8) can be written as follows

$$\left|\int_\gamma |\varphi^\pm(\eta)|^2 d\eta\right| \le \text{const}, \tag{3.17}$$

that is $\varphi^\pm(\eta)\in L_2(\gamma)$. From (3.12), the new unknown function $\varphi(w)$ behaves at infinity as $c_0 w^{-1}$, c_0 =const. Thus, we arrive at the following case of the Riemann-Hilbert boundary-value problem:

Find a function $\varphi(w)$ analytic in the w-plane with the cut γ, subject to the boundary condition

$$\varphi^+(\eta) = G(\eta)\varphi^-(\eta), \quad \eta\in\gamma, \tag{3.18}$$

where

$$G(\eta) = D\left(c + \frac{3i}{2\pi}\log\left(i\frac{1-\eta}{1+\eta}\right)\right). \tag{3.19}$$

The function $\varphi(w)$ vanishes at infinity as $c_0 w^{-1}$, $\varphi^\pm(\eta)\in L_2(\gamma)$ and $\varphi(w)$ is representable by a Cauchy integral.

Here and further we fix the branches of the logarithmic functions $\log(\eta-1)$ and $\log(\eta+1)$ by stipulating the inequalities

$$0<\arg(\eta+1)<\pi, \quad 0<\arg(\eta-1)<\pi, \quad \eta\in\gamma. \tag{3.20}$$

The coefficient $G(\eta)$ of the problem (3.18) grows at the ends $\eta=1$ and $\eta=-1$ of the contour γ as $\log^2(\eta-1)$ and $\log^2(\eta+1)$, respectively.

The exact solution of the problem (3.18) is given by Antipov & Gao (2000)

$$\varphi(w) = C_0(w+1)^{-1}\exp\left\{\frac{1}{2\pi i}\int_\gamma \frac{\log G(\eta)}{\eta-w}d\eta\right\}. \tag{3.21}$$

The function $\varphi(w)$ possesses the power-logarithmic singularities at the ends

$$\varphi(w) \sim A_1(w-1)^{-1/4}\{\log(w-1)\}^{1/2+2c/3}, \quad w\to 1,$$
$$\varphi(w) \sim A_2(w+1)^{-1/4}\{\log(w+1)\}^{-1/2+2c/3}, \quad w\to -1, \tag{3.22}$$

where A_1, A_2 are constants. The branch of the logarithmic function $\log G(\tau)$ in the Cauchy integral (3.21) is defined by the inequality

$$\frac{\pi}{2}\le \arg G(\tau)\le\frac{3\pi}{2} \quad \text{as} \quad \tau\in\gamma. \tag{3.23}$$

In particularly, $\arg G(1)=\pi/2$ and $\arg G(-1)=3\pi/2$.

Step 4: Integral representation of the solution to the integro-differential equation. Now it is easy to write down the solution of the original equation (2.11) by quadratures.

This is the last step of the algorithm. By integration by parts and by the inverse Mellin formula, we have from (3.4)

$$f(u) = -\frac{1}{2\pi i}\int_{\Omega} \frac{F(s)u^{3-s}ds}{(s-1)(s-2)(s-3)}, \tag{3.24}$$

where

$$F(s) = -\frac{\Phi(s)}{H(s)}. \tag{3.25}$$

Using the inverse map (3.13) and formulae (3.12), (3.21) we obtain the expression for the potential $\Phi(s)$:

$$\Phi(s) = C_0 \exp\left\{\frac{\pi i}{3}(c-s)\right\} Q(s), \quad s \in \Pi. \tag{3.26}$$

This formula is valid for inner points of the strip Π. If $s = \sigma \in \Omega$ or $s = \sigma \in \Omega_{-1}$, then by the Sokhotski-Plemelj formulae

$$\Phi(\sigma) = C_0 \exp\left\{\frac{\pi i}{3}(c-\sigma) + \frac{1}{2}\log D(\sigma)\right\} Q(\sigma), \quad \sigma \in \Omega,$$

$$\Phi(\sigma-3) = -C_0 \exp\left\{\frac{\pi i}{3}(c-\sigma) - \frac{1}{2}\log D(\sigma)\right\} Q(\sigma), \quad \sigma \in \Omega, \tag{3.27}$$

where

$$Q(s) = \exp\left\{-\frac{i+\exp(\frac{2\pi i}{3}(c-s))}{3}\int_{\Omega} \frac{\log D(\sigma)d\sigma}{[1-\exp\{\frac{2\pi i}{3}(\sigma-s)\}][i+\exp\{\frac{2\pi i}{3}(c-\sigma)\}]}\right\}. \tag{3.28}$$

Direct analysis shows that the function $\Phi(s)$ is analytic everywhere in the strip Π and satisfies the condition (3.8). This is because the function $\varphi(w) \in L_2(\mathbb{C} \setminus \gamma)$ ($\mathbb{C}$ is the w-plane) and $\varphi^{\pm}(\eta) \in L_2(\gamma)$. Finally, we mention that the solution, we have constructed, has an arbitrary constant that will be determined from the additional condition $f(\infty) = 1$.

4 Analytical continuation of the potential $\Phi(s)$

We have found a closed-form solution of the integro-differential equation, the function $f(u)$. However, this form is inconvenient for analysis of the behaviour of the function $f(u)$ at zero and at infinity, which we need to satisfy the additional conditions (2.12). Moreover, it is not efficient for numerical purposes. In order to construct a series representation and asymptotic expansion for large u, we have to define the function $\Phi(s)$ in the whole complex plane. We emphasise that the formulae (3.26)-(3.28) are valid in the strip Π only. In this section we construct the analytical continuation of the function

$\Phi(s)$, the solution to functional-difference equation (3.10). First, we mention that the function $\Phi(s)$, defined by (3.26), is analytic in each strip

$$\Pi_m = \{s \in \mathbb{C} : c + 3m - 3 < \Re(s) < c + 3m\}, \quad m = 0, \pm 1, \pm 2, \ldots$$

and is discontinuous when s crosses each contour

$$\Omega_m = \{s \in \mathbb{C} : \Re(s) = c + 3m\}, \quad m = 0, \pm 1, \pm 2, \ldots.$$

In order to show this, we introduce notations for the limit values of the function $\Phi(s)$

$$\Phi_-(s_m) = \lim_{\varepsilon \to +0} \Phi(3m + it + c - \varepsilon),$$

$$\Phi_+(s_m) = \lim_{\varepsilon \to +0} \Phi(3m + it + c + \varepsilon), \quad s_m = 3m + \sigma, \quad \sigma \in \Omega \tag{4.1}$$

on each contour Ω_m, $(m = 0, \pm 1, \pm 2, \ldots.)$ Analysis of formulae (3.27) and (3.28) gives the following relations for the functions $\Phi_-(s_m)$ and $\Phi_+(s_m)$:

$$\Phi_-(s_m) = (-1)^m \Phi(\sigma), \quad \Phi_+(s_m) = (-1)^{m+1}\Phi(\sigma - 3), \quad s_m \in \Omega_m, \quad \sigma \in \Omega_0 = \Omega. \tag{4.2}$$

By substituting these two results into the boundary condition (3.10), we get (see, also, Popov & Tikhonenko (1974))

$$\Phi_-(s_m) = D(s_m - 3m)\Phi_+(s_m), \quad s_m \in \Omega_m, \quad m = 0, \pm 1, \pm 2, \ldots. \tag{4.3}$$

Therefore the function $\Phi(s)$ is discontinuous on each contour Ω_m and its jumps are described by (4.3). This formula, in addition, allows to construct an analytical continuation of the function $\Phi(s)$ from the strip Π into the strips $\Pi_1, \Pi_2, \ldots$ (to the right) and $\Pi_{-1}, \Pi_{-2}, \ldots$ (to the left):

$$\mathfrak{F}_1(s) = \Phi(s)D(s), \quad s \in \Pi_1, \qquad \mathfrak{F}_2(s) = \Phi(s)D(s)D(s-3), \quad s \in \Pi_2, \ldots$$

$$\mathfrak{F}_{-1}(s) = \frac{\Phi(s)}{D(s+3)}, \quad s \in \Pi_{-1}, \qquad \mathfrak{F}_{-2}(s) = \frac{\Phi(s)}{D(s+3)D(s+6)}, \quad s \in \Pi_{-2}, \ldots \tag{4.4}$$

Thus, the analytical continuation of the function $\Phi(s)$ to the half-planes $\Re(s) > c$ and $\Re(s) < c - 3$ is given by

$$\mathfrak{F}_n(s) = \Phi(s) \prod_{m=0}^{n-1} D(s - 3m), \quad s \in \Pi_n, \quad n = 1, 2, \ldots,$$

$$\mathfrak{F}_{-n}(s) = \frac{\Phi(s)}{\prod_{m=1}^{n} D(s + 3m)}, \quad s \in \Pi_{-n}, \quad n = 1, 2, \ldots, \tag{4.5}$$

where

$$\Phi(s) = C_0 \exp\left\{\frac{\pi i}{3}(c - s)\right\} Q(s), \quad s \in \Pi_n \quad (n = 0, \pm 1, \ldots) \tag{4.6}$$

and $Q(s)$ is the integral (3.28) for $s \in \Pi_n$ $(n = 0, \pm 1, \ldots)$.

5 Series representation for the function $f(u)$

The analytical continuation of the function $\Phi(s)$, the function $\mathfrak{F}(s) = \mathfrak{F}_n(s),\ s \in \Pi_n$ ($n = 0, \pm1, \ldots$), is now constructed. We aim to write down a series-form solution in terms of the powers of the argument u. The theorem of residues and the analytical continuation of the function $\Phi(s)$ enable us to find such a representation. In contrast to the situation described by Antipov & Gao (2000), the zeros of the function $H(s)$ are not periodic. It makes the algorithm different. We start with the formula

$$f(u) = \frac{1}{2\pi i} \int_{\Omega} \frac{\Phi(s) u^{3-s} ds}{(s-1)(s-2)(s-3)H(s)} \tag{5.1}$$

that follows from (3.4) and (3.7). By the boundary condition (3.10)

$$f(u) = -\frac{1}{2\pi i} \int_{\Omega} \frac{\Phi(s-3) u^{3-s} ds}{s-3} = -\frac{1}{2\pi i} \int_{\Omega_{-1}} \frac{\Phi_+(s)}{s} u^{-s} ds. \tag{5.2}$$

Here we used the analyticity of the function $\Phi(s)$ in the strip Π. Next, applying the formula of the analytical continuation (4.4) we get

$$f(u) = -\frac{1}{2\pi i} \int_{\Omega_{-1}} \mathfrak{F}_{-1}(s) \frac{u^{-s} ds}{s} = \frac{1}{2\pi i} \int_{\Omega_{-1}} \frac{\sin \pi s \Phi_-(s) u^{-s} ds}{\pi s(s+1)(s+2)R(s)}, \tag{5.3}$$

where

$$R(s) = \cos \pi s + 2s^2 + 8s + 7. \tag{5.4}$$

The function $\mathfrak{F}_{-1}(s)$ has only one pole in the strip Π_{-1}, namely, $s = -2$, which is that of the second order. Working out the residue of the integrand at this point we get

$$\operatorname*{res}_{s=-2} \frac{\sin \pi s \Phi(s) u^{-s}}{\pi s(s+1)(s+2)R(s)} = u^2 \operatorname*{res}_{t=0} \frac{[\Phi(-2) + t\Phi'(-2)](1 - t\log u)}{(2-3t)[R(-2) + tR'(-2) + \frac{1}{2}t^2 R''(-2) + \frac{1}{6}t^3 R'''(-2)]}$$

$$= \frac{u^2}{\pi^2 - 4} \left[\left(\frac{3}{2} - \log u \right) \Phi(1) + \Phi'(1) \right]. \tag{5.5}$$

Here we used

$$R(-2) = R'(-2) = R'''(-2) = 0, \quad R''(-2) = 4 - \pi^2. \tag{5.6}$$

By the Cauchy theorem and the analytical continuation (4.4)

$$f(u) = -\frac{u^2}{\pi^2 - 4} \left[\Phi(1) \left(\log u - \frac{3}{2} \right) - \Phi'(1) \right]$$

$$+ \frac{1}{2\pi i} \int_{\Omega_{-2}} \frac{\sin^2 \pi s \Phi_-(s) u^{-s} ds}{\pi^2 s(s+1)(s+2)(s+4)(s+5)R(s)R(s+3)}. \tag{5.7}$$

Note that due to periodicity of the function $Q(s)$ that follows from the definition (3.28): $Q(s) = Q(s+3m),\ s \in \Pi,\ m = 0, \pm 1, \pm 2, \ldots,$ the potential $\Phi(s)$ satisfies the relations

$$\Phi(s) = (-1)^m \Phi(s+3m), \quad \Phi'(s) = (-1)^m \Phi'(s+3m),\ s \in \Pi,\ m = 0, \pm 1, \pm 2, \ldots. \tag{5.8}$$

In the strip $\Pi_{-2} = \{s \in \mathbb{C} : c-9 < \Re(s) < c-6\}$ $(1 < c < 2)$, there are five poles of the function $\mathfrak{F}_{-2}(s)$. They coincide with the roots of the function $R(s)$ in the strip Π_{-2} : s_2, s_2', s_2'', $\bar{s}_2'$, $\bar{s}_2''$. These poles are simple and their values are

$$s_2 = -5, \quad s_2' \approx -4.73959 - i1.11902, \quad s_2'' \approx -6.80825 - i1.46392$$

and $\bar{s}_2', \bar{s}_2''$ are the conjugates of s_2', s_2'', respectively. By the residues theorem,

$$f(u) = -\frac{u^2}{\pi^2 - 4}\left[\Phi(1)\left(\log u - \frac{3}{2}\right) - \Phi'(1)\right] + \frac{\Phi(1)u^5}{480(4-\pi^2)}$$

$$+V_{20}(s_2', u)\Phi(s_2') + V_{20}(s_2'', u)\Phi(s_2'') + V_{20}(\bar{s}_2', u)\Phi(\bar{s}_2') + V_{20}(\bar{s}_2'', u)\Phi(\bar{s}_2'') + W_3(u), \tag{5.9}$$

where

$$V_{20}(s,u) = \frac{\sin^2 \pi s u^{-s}}{\pi^2 s(s+1)(s+2)(s+4)(s+5)R(s+3)R'(s)},$$

$$W_3(u) = -\frac{1}{2\pi i}\int_{\Omega_{-3}} \frac{\sin^3 \pi s \Phi_-(s) u^{-s} ds}{\pi^3 s(s+1)(s+2)(s+4)(s+5)(s+7)(s+8)R(s)R(s+3)R(s+6)}. \tag{5.10}$$

In the next strip Π_{-3}, there are six simple poles of the integrand. Two of them, $s_3 \approx -8.84513 - i1.68163$ and $\bar{s}_3$ are zeros of the function $R(s)$ and the other four poles $-3+s_2', -3+\bar{s}_2', -3+s_2'', -3+\bar{s}_2''$ are zeros of the function $R(s+3)$. Thus,

$$W_3(s) = -V_{30}(s_3, u)\Phi(s_3) - V_{30}(\bar{s}_3, u)\Phi(\bar{s}_3) - V_{31}(-3+s_2', u)\Phi(-3+s_2')$$

$$-V_{31}(-3+\bar{s}_2', u)\Phi(-3+\bar{s}_2') - V_{31}(-3+s_2'', u)\Phi(-3+s_2'') - V_{31}(-3+\bar{s}_2'', u)\Phi(-3+\bar{s}_2'') + W_4(s), \tag{5.11}$$

where

$$V_{30}(s,u) = \frac{\sin^3 \pi s u^{-s}}{\pi^3 s(s+1)(s+2)(s+4)(s+5)(s+7)(s+8)R(s+6)R(s+3)R'(s)},$$

$$V_{31}(s,u) = \frac{\sin^3 \pi s u^{-s}}{\pi^3 s(s+1)(s+2)(s+4)(s+5)(s+7)(s+8)R(s+6)R'(s+3)R(s)},$$

$$W_4(u) = -\frac{1}{2\pi i}\int_{\Omega_{-3}} \frac{\sin^4 \pi s \Phi_-(s)}{\pi^4 s(s+1)(s+2)(s+4)(s+5)(s+7)(s+8)(s+10)(s+11)}$$

$$\times \frac{u^{-s} ds}{R(s)R(s+3)R(s+6)R(s+9)}. \tag{5.12}$$

We repeat this procedure again and again and finally

$$f(u)=-\frac{u^2}{\pi^2-4}\left[\Phi(1)\left(\log u-\frac{3}{2}\right)-\Phi'(1)\right]+\frac{\Phi(1)u^5}{480(4-\pi^2)}+W(u)+\overline{W}(u), \quad (5.13)$$

where

$$W(u)=\sum_{k=1}^{\infty}(-1)^k\left[\Phi(s'_{2k})\sum_{j=1}^{\infty}(-1)^{E[(j+1)/2]}V_{j+2k-1,j-1}(s'_{2k}-3j+3,u)\right.$$

$$+\Phi(s''_{2k})\sum_{j=1}^{\infty}(-1)^{E[(j+1)/2]}V_{j+2k-1,j-1}(s''_{2k}-3j+3,u)$$

$$\left.+\Phi(s_{2k+1})\sum_{j=1}^{\infty}(-1)^{E[j/2]}V_{j+2k,j-1}(s_{2k+1}-3j+3,u)\right], \quad (5.14)$$

where $E[a]$ is the integer part of a and

$$V_{mn}(s,u)=\frac{\pi^{-m}\sin^m\pi s u^{-s}}{s(s+1)(s+2)(s+4)(s+5)(s+7)(s+8)\cdot\ldots\cdot(s+3m-2)(s+3m-1)}$$

$$\times\frac{1}{R(s)R(s+3)\ldots R(s+3n-3)R'(s+3n)R(s+3n+3)\ldots R(s+3m-3)},$$

$$m=2,3,\ldots;\quad n=0,1,\ldots,m-2. \quad (5.15)$$

The series converges absolutely for all u: $|u|<\infty$. It is easy now to write down the expressions for the derivatives of the function $f(u)$:

$$f'(u)=\frac{2u}{\pi^2-4}\left[\Phi(1)\left(1-\log u\right)+\Phi'(1)\right]+\frac{\Phi(1)u^4}{96(4-\pi^2)}+W'(u)+\overline{W'}(u),$$

$$f''(u)=\frac{2}{\pi^2-4}\left[-\Phi(1)\log u+\Phi'(1)\right]+\frac{\Phi(1)u^3}{24(4-\pi^2)}+W''(u)+\overline{W''}(u),$$

$$f'''(u)=-\frac{2\Phi(1)}{(\pi^2-4)u}+\frac{\Phi(1)u^2}{8(4-\pi^2)}+W'''(u)+\overline{W'''}(u). \quad (5.16)$$

To compute the derivatives of the function $W(u)$, we need the following relations

$$\frac{\partial}{\partial u}V_{mn}(s,u)=-\frac{s}{u}V_{mn}(s,u),\quad \frac{\partial^2}{\partial u^2}V_{mn}(s,u)=\frac{s(s+1)}{u^2}V_{mn}(s,u),$$

$$\frac{\partial^3}{\partial u^3}V_{mn}(s,u)=-\frac{s(s+1)(s+2)}{u^3}V_{mn}(s,u). \quad (5.17)$$

Formulae (5.13)-(5.15) indicate that behaviour of the solution in a vicinity of the point $u=0$ is similar to that in the case of an infinite grain boundary (Antipov & Gao, 2000), namely,

$$f(u)\sim\frac{u^2\log u}{4-\pi^2}\Phi(1),\quad u\to 0 \quad (5.18)$$

and, therefore, $f(0)=0$, that is the first additional condition in (2.12) is automatically satisfied. The behaviour at zero of the derivatives of the function $f(u)$ is described by

$$f'(u)\sim\frac{2\Phi(1)}{4-\pi^2}u\log u,\quad f''(u)\sim\frac{2\Phi(1)}{4-\pi^2}\log u,$$

$$f'''(u)\sim\frac{2\Phi(1)}{(4-\pi^2)u},\quad u\to 0. \tag{5.19}$$

At the first glance, the integral (2.11) does not exist at the point $u=0$ since $f'''(v)=O(v^{-1}),\ v\to 0$. To prove the convergence of that integral as $u\to 0$, we rewrite it in another manner

$$I(u)=\int\limits_0^\infty\left(\frac{1}{u-v}+\frac{v^2-u^2-4uv}{(u+v)^3}\right)f'''(v)dv \tag{5.20}$$

and use the behaviour of the singular integrals in a vicinity of the point $u=0$

$$\int\limits_0^1\frac{v^\alpha}{u-v}dv=\frac{\pi u^\alpha}{\tan\pi\alpha}+B_1(u),\quad u\to+0,$$

$$\int\limits_0^1\frac{v^\beta}{(u+v)^3}dv=\frac{\pi\beta(1-\beta)u^{\beta-2}}{2\sin\pi\beta}+B_2(u),\quad u\to+0, \tag{5.21}$$

where $-1<\Re(\alpha)<0$; $-1<\Re(\beta)<2$ and $\beta\neq 0,1$. The functions $B_1(u)$, $B_2(u)$ are bounded as $u\to+0$. $|B_2(u)|\le C\max\{u^{\beta-1},1\}$ (C is a constant). Assume now that $f'''(v)\sim Av^\alpha, -1<\Re(\alpha)<0$, A is a constant. By comparing formulae (5.21) and (5.20), we get

$$I(u)=\frac{\pi Au^\alpha}{\sin\pi\alpha}(\cos\pi\alpha-2\alpha^2-4\alpha-1)+B(u),\quad u\to 0, \tag{5.22}$$

where $B(u)$ is bounded if $u\to 0$. Since

$$\lim_{\alpha\to-1}\frac{\cos\pi\alpha-2\alpha^2-4\alpha-1}{\sin\pi\alpha}=0, \tag{5.23}$$

the integral $I(u)$ converges as $u\to 0$ and $f'''(v)=O(v^{-1}),\ v\to 0$.

6 Asymptotic expansion for large u

Although the series representation (5.14) converges rapidly for all $u<\infty$, it does not allow to find the behaviour of the solution at infinity. We need it to satisfy the second additional condition in (2.12), namely, $f(\infty)=1$. To do this, we use the analytical continuation (4.5) to the right into the half-plane $\Re(s)>c$. First, use formula (4.3) for $m=0$

$$\Phi(\sigma)=\Phi_-(\sigma)=D(\sigma)\Phi_+(\sigma)=(\sigma-1)(\sigma-2)H(\sigma)\Phi_+(\sigma) \tag{6.1}$$

to continue analytically the function $\Phi(\sigma)$ into the strip Π_1. We obtain from (5.1)

$$f(u) = \frac{1}{2\pi i} \int\limits_{\Omega_0} \frac{\Phi_+(s)}{s-3} u^{-s+3} ds. \tag{6.2}$$

By the Cauchy theorem,

$$f(u) = -\Phi(3) - \frac{1}{2\pi i} \int\limits_{\Omega_1} \frac{\pi(s-4)(s-5)T(s)}{(s-3)\sin \pi s} \Phi_+(s) u^{-s+3} ds. \tag{6.3}$$

Here we used the analytical continuation $\mathfrak{F}_2(s)$ of the function $\Phi(s)$ into the strip Π_2 and

$$D(s-3) = -\frac{\pi(s-4)(s-5)}{\sin \pi s} T(s), \quad T(s) = \cos \pi s + 2s^2 - 16s + 31. \tag{6.4}$$

The integrand in (6.3) has two poles $s = 6$ and $s = 7$ in the strip Π_2. Therefore

$$f(u) = \Phi(0) + \frac{16}{3}\Phi(0)u^{-3} - 24\Phi(1)u^{-4}$$

$$-\frac{1}{2\pi i} \int\limits_{\Omega_2} \frac{\pi^2(s-4)(s-5)(s-7)(s-8)}{(s-3)\sin^2 \pi s} T(s)T(s-3)\Phi_+(s)u^{-s+3} ds. \tag{6.5}$$

We note that $T(6) = 8,\ T(7) = 16$ and $\Phi(3) = -\Phi(0),\ \Phi(6) = \Phi(0),\ \Phi(7) = \Phi(1)$. The theorem of residues enables us to find the next terms of the asymptotic expansion of the function $f(u)$. The integrand in (6.5) in the strip Π_3 has two poles: $s = 9$ and $s = 10$, both of the second order. (Since $T(5) = 0$, the point $s = 8$ is a removable singularity of the integrand.) The residue of the integrand at the point $s = 9$ is

$$-\frac{512}{u^6}(16 - 5\log u + 5\Phi'(0)). \tag{6.6}$$

Therefore, for large u, the function $f(u)$ admits the following asymptotic expansion

$$f(u) = 1 + \frac{16}{3u^3} - \frac{24}{u^4}\Phi(1) + \frac{2560}{u^6}\log u$$

$$-\frac{512}{u^6}(16 + 5\Phi'(0)) + O\left(\frac{\log u}{u^7}\right), \quad u \to \infty. \tag{6.7}$$

Here we used the additional condition (2.12), namely, $f(\infty) = 1$ to fix the constant C_0, that is $\Phi(0) = 1$ and hence

$$C_0 = \frac{e^{-\pi i c/3}}{Q(0)}. \tag{6.8}$$

Proceeding as before, we may find the next terms of the asymptotic expansion. However, the order of the poles $s = 12$ and $s = 13$ in the next strip Π_4 is equal to three. The third pole $s = 11$ is of the second order. This means that to write down the terms of order u^{-9}, for instance, we have to work out the residue of the integrand at the pole $s = 12$ of the third order. The order of poles $s = k$ $(k = 14, 15, 16, \ldots)$ in the corresponding strip Π_n increases with the increase of n.

By direct differentiation of the expansion (6.7) we can find asymptotic expansions for the derivatives of the function $f(u)$:

$$f'(u) = -\frac{16}{u^4} + \frac{96}{u^5}\Phi(1) - \frac{15360}{u^7}\log u + \frac{512(101 + 30\Phi'(0))}{u^7} + O\left(\frac{\log u}{u^8}\right), \quad u \to \infty \quad (6.9)$$

and

$$f''(u) = \frac{64}{u^5} - \frac{480}{u^6}\Phi(1) + \frac{107520}{u^8}\log u + O\left(\frac{1}{u^8}\right), \quad u \to \infty,$$
$$f'''(u) = -\frac{320}{u^6} + \frac{2880}{u^7}\Phi(1) - \frac{860160}{u^9}\log u + O\left(\frac{1}{u^9}\right), \quad u \to \infty. \quad (6.10)$$

Let us prove that the behaviour of the integral in equation (2.11) as $u \to \infty$ is consistent with the behaviour of the function $uf'(u)$ for large u. Analysis of the integral in (2.11) shows that

$$I(u) = 8u \int_0^\infty \frac{v^2 f'''(v)dv}{(u-v)(u+v)^3} = \frac{8}{u^3}F(3) + O\left(\frac{1}{u^4}\right), \quad u \to \infty, \quad (6.11)$$

where $F(3)$ is defined by (3.7) and (4.5)

$$F(3) = \int_0^\infty v^2 f'''(v)dv = -\lim_{s\to 3}\frac{\mathfrak{F}_1(s)}{H(s)} = -\lim_{s\to 3}\frac{D(s)\Phi(s)}{H(s)} \quad (6.12)$$

since $s = 3 \in \Pi_1$. Therefore, by (3.11)

$$F(3) = -\lim_{s\to 3}(s-1)(s-2)\Phi(s) = -2\Phi(3) = 2\Phi(0) = 2. \quad (6.13)$$

This means that

$$I(u) = \frac{16}{u^3} + O\left(\frac{1}{u^4}\right), \quad u \to \infty. \quad (6.14)$$

On the other hand, from (6.9)

$$-uf'(u) = \frac{16}{u^3} + O\left(\frac{1}{u^4}\right), \quad u \to \infty. \quad (6.15)$$

This is reconciled with the asymptotics (6.14) of the integral $I(u)$ as $u \to \infty$.

7 Physical quantities and numerical results

To compute the numerical values of the function $f(u)$, we use the series representation (5.13) and the asymptotic expansion (6.7) for large u. The poles s'_{2k}, s''_{2k} and s_{2k+1} ($k = 1, 2, \ldots$) are defined by the following procedure. Let $s = -iz$ be a root of the function $R(s)$. Then from (5.4)

$$e^{\pi z} = 4z^2 + 16iz - 14 - e^{-\pi z}. \tag{7.1}$$

Denote by $z_n^{(k)}$ the k-th approximation of the root z_n. From (7.1) we get

$$z_n^{(1)} = -2ni,$$
$$z_n^{(k)} = -2ni + \frac{1}{\pi}\log\chi(z_n^{(k-1)}), \quad k = 2, 3, \ldots, \tag{7.2}$$

where

$$\chi(z) = -e^{-\pi z} + 4z^2 + 16iz - 14. \tag{7.3}$$

The recurrence procedure (7.2) yields good results for all roots z_n ($n = 2, 3, \ldots$). The poles s'_{2k}, s''_{2k}, s_{2k+1} are expressed in terms of the roots z_n as follows

$$s'_{2k} = -iz_{3k-1}, \quad s''_{2k} = -iz_{3k}, \quad s_{2k+1} = -iz_{3k+1} \quad (k = 1, 2, \ldots). \tag{7.4}$$

The series representation (5.13) and the asymptotic expansion (6.7) involve the following values of the potential and its first derivative

$$\Phi(s) = \frac{Q(s)}{e^{\pi is/3}Q(0)}, \quad \text{as} \quad s = 1,\, s'_{2k},\, s''_{2k},\, s_{2k+1},\ (k = 1, 2, \ldots)$$
$$\Phi'(0) = -\frac{\pi i}{3} + Q_0(0), \quad \Phi'(1) = \Phi(1)\left[-\frac{\pi i}{3} + Q_0(1)\right], \tag{7.5}$$

where

$$Q(s) = \exp\left\{\frac{1}{2\pi}\int_0^\pi \frac{\log G_0(\theta)}{e^{i\theta} - w}e^{i\theta}d\theta\right\}, \quad w \notin \gamma,$$
$$Q_0(s) = \frac{w^2 - 1}{6i}\int_0^\pi \frac{\log G_0(\theta)}{(e^{i\theta} - w)^2}e^{i\theta}d\theta. \tag{7.6}$$

and

$$G_0(\theta) = D(\sigma), \quad \sigma = c + \frac{3i}{2\pi}\log\left(\tan\frac{\theta}{2}\right),$$
$$w = i\tan\left\{\pi\left(\frac{1}{4} + \frac{s - c}{3}\right)\right\}. \tag{7.7}$$

The unique branch of the function $\log G_0(\theta)$ is defined by

$$\log G_0(\theta) = |\log G_0(\theta)| + i\tan^{-1}\left(\frac{\Im\{G_0(\theta)\}}{\Re\{G_0(\theta)\}}\right) + i\pi. \tag{7.8}$$

Note that the function $\log G_0(\theta)$ slowly grows at the ends:

$$\log G_0(\theta) = O(\log\log\theta), \quad \theta \to 0,$$
$$\log G_0(\theta) = O(\log\log(\pi - \theta)), \quad \theta \to \pi. \tag{7.9}$$

In the table bellow, we list the values of the potential $\Phi(s)$ which are involved in formulae (5.13) and (6.7).

Strip	$\Re(s)$	$\Im(s)$	$\Re\Phi(s)$	$\Im\Phi(s)$
Π_{-2}	-4.739593	-1.119024	1.520193	-0.621598
Π_{-2}	-6.808250	-1.463928	0.446549	0.032571
Π_{-3}	-8.845135	-1.681634	-0.567066	0.416293
Π_{-4}	-10.868825	-1.842383	0.803440	-1.240380
Π_{-4}	-12.885552	-1.970199	0.271592	-0.056018
Π_{-5}	-14.898090	-2.076415	-0.349547	0.452333
Π_{-6}	-16.907890	-2.167332	0.364906	-1.306177
Π_{-6}	-18.915790	-2.246828	0.197012	-0.086937
Π_{-7}	-20.922311	-2.317464	-0.221910	0.448796
Π_{-8}	-22.927799	-2.381025	0.079103	-1.270866
Π_{-8}	-24.932487	-2.438804	0.151764	-0.100090
Π_{-9}	-26.936546	-2.491767	-0.135667	0.433659
Π_{-10}	-28.940098	-2.540657	-0.122240	-1.205617
Π_{-10}	-30.943235	-2.586056	0.120334	-0.105791

In addition, we need the following constants:

$$\Phi(1) = 1.210107, \quad \Phi'(0) = 0.1053885, \quad \Phi'(1) = 0.1680426.$$

Numerical computations show that the asymptotic expansion (6.7) with just the five terms starts to work for $u \geq 8$. On the other hand, to obtain the values of the function $f(u)$ with good accuracy for $u \in (7, 8)$ we have to carry on continuing the function $\Phi(s)$ to the left at least until Π_{-10}. In Fig.2, we present the graph of the function $f(u)$. It is very close to that for the case of an infinite grain boundary (Antipov & Gao, 2000). However, for a semi-infinite grain boundary

$$\max f(u) = 1.06975 \quad \text{at} \quad u = 4.02$$

and for the infinite case $\max f(u) = 1.04027 \quad \text{at} \quad u = 4.33$.

Let us analyse the situation when a point z (Fig.1) is fixed and time t varies. The Fig.3 illustrates the grain boundary traction $\sigma_0^{-1}\sigma_{gb}(z,t)$ for some points z. Since $\sigma_{gb}(z,t) = \sigma_0 f(z(at)^{-1/3})$, we can establish the asymptotic behaviour of the function $\sigma_{gb}(z,t)$ for small and large at (z is fixed)

$$\sigma_{gb}(z,t) = \frac{\sigma_0 z^2}{(at)^{2/3}(\pi^2 - 4)}\left[\Phi'(1) + \left(\frac{3}{2} - \log z + \frac{1}{3}\log at\right)\Phi(1)\right] + O\left(\frac{1}{(at)^{5/3}}\right), \quad at \to \infty,$$

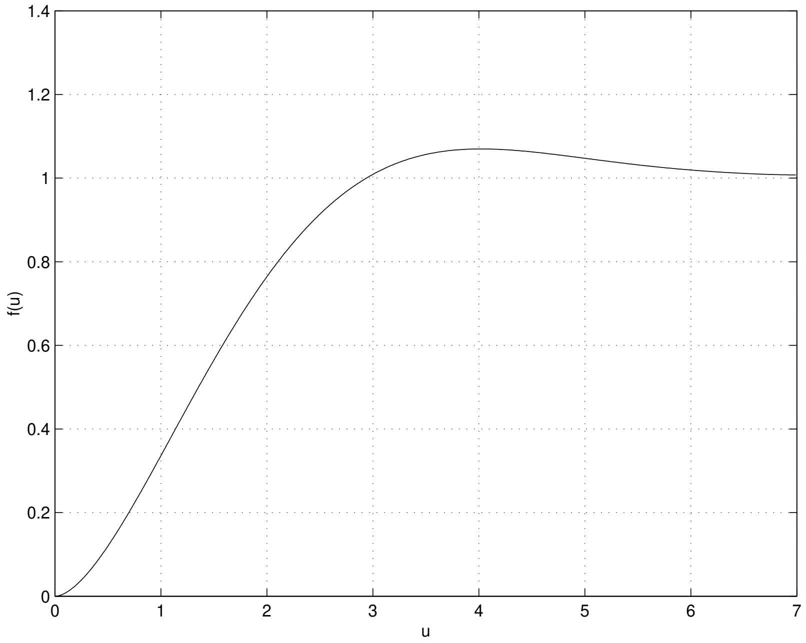

Figure 2: Function $f(u)$.

$$\sigma_{gb}(z,t)=\sigma_0\left[1+\frac{16at}{3z^3}-\frac{24(at)^{4/3}}{z^4}\Phi(1)\right]+O\left((at)^2\log at\right),\quad at\to 0. \tag{7.10}$$

The atomic flux in the boundary $j(z,t)$ is defined by (2.4) and (2.5) and (2.9), that is

$$j(z,t)=\frac{\Lambda\sigma_0}{(at)^{1/3}}f'\left(\frac{z}{(at)^{1/3}}\right),\quad \Lambda=\frac{\delta_{gb}D_{gb}}{kT}. \tag{7.11}$$

We present the graphs of the function $(\Lambda\sigma_0)^{-1}j(z,t)$ versus t for some points z in Fig.4. Analysis of relations (5.16) and (6.10) enables us to derive formulae for the atomic flux for small and large time (as before z is fixed)

$$j(z,t)=\frac{2\Lambda\sigma_0 z}{(at)^{2/3}(\pi^2-4)}\left[\Phi'(1)+\left(1-\log z+\frac{1}{3}\log at\right)\Phi(1)\right]+O\left(\frac{1}{(at)^{5/3}}\right),\quad at\to\infty,$$

$$j(z,t)=\Lambda\sigma_0\left[-\frac{16at}{z^4}+\frac{96(at)^{4/3}}{z^5}\Phi(1)\right]+O\left((at)^2\log at\right),\quad at\to 0. \tag{7.12}$$

Finally, we compute the displacement rate

$$\frac{\partial u_{gb}}{\partial t}(z,t)=-\frac{\Omega}{2}\frac{\partial j(z,t)}{\partial z}=-\frac{M}{(at)^{2/3}}f''\left(\frac{z}{(at)^{1/3}}\right), \tag{7.13}$$

where $M=\frac{1}{2}\Omega\Lambda\sigma_0$. The graphs of the function $M^{-1}\frac{\partial u_{gb}}{\partial t}(z,t)$ versus at for some values z are shown in Fig.5. For fixed z, the displacement rate decreases as $at\to 0$ or $at\to\infty$:

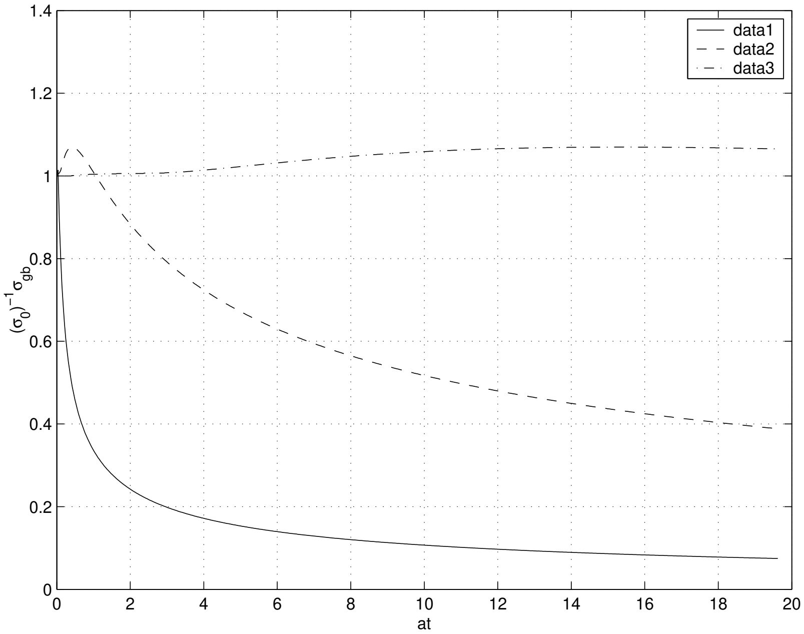

Figure 3: The grain boundary traction $\sigma_0^{-1}\sigma_{gb}(z,t)$ vs at for $z = 1$ (data1), $z = 3$ (data2) and $z = 10$ (data3).

$$\frac{\partial u_{gb}}{\partial t}(z,t) = -\frac{2M}{(at)^{2/3}(\pi^2-4)}\left[\Phi'(1) - \left(\log z - \frac{1}{3}\log at\right)\Phi(1)\right] + O\left(\frac{1}{(at)^{5/3}}\right), \quad at \to \infty,$$

$$\frac{\partial u_{gb}}{\partial t}(z,t) = -M\left[\frac{64at}{z^5} - \frac{480(at)^{4/3}}{z^6}\Phi(1)\right] + O\left((at)^2 \log at\right), \quad at \to 0. \qquad (7.14)$$

Analysis of the asymptotic expansion for the displacement rate indicates a rapid growth of $|\frac{\partial u_{gb}}{\partial t}|$ in a vicinity of the point $at = 0$. Indeed,

$$\frac{\partial^2 u_{gb}}{\partial t^2}(z,t) \sim -M\frac{64a}{z^6}, \quad at \to 0.$$

This is confirmed by the numerical experiment (Fig.5).

8 Conclusion

A model problem of atomic diffusion from the surface of a material into a semi-infinite grain boundary has been analysed. It was shown that the coupled elasticity and grain-boundary diffusion problem is equivalent to a 1-d-singular integro-differential equation on a semi-infinite axis with two additional conditions. The symbol of the integro-differential equation is a meromorphic function whose poles form a countable set and they are not periodic in contrast to the case of an infinite grain boundary analysed before. In this paper, the procedure of exact solution described by Antipov & Gao (2000) for an infinite grain boundary has been generalised for the case of non-periodic poles.

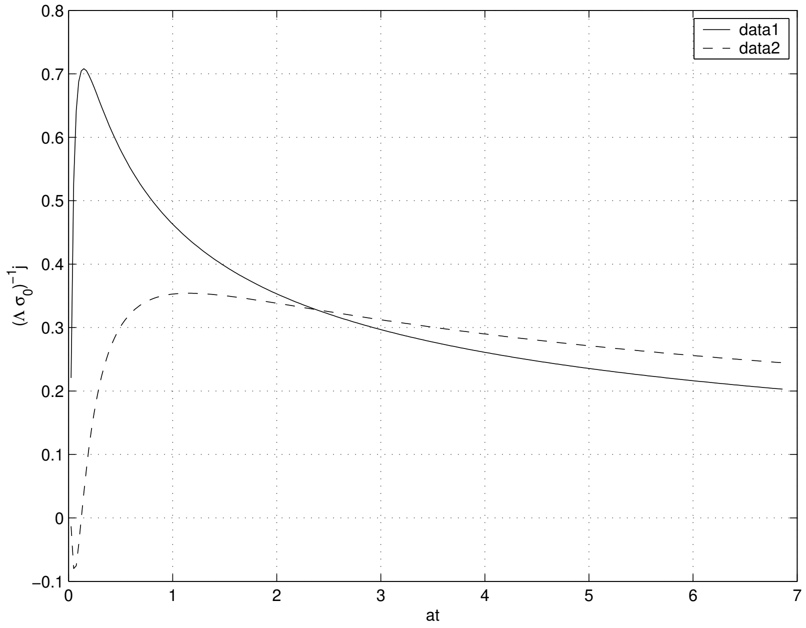

Figure 4: The atomic flux in the boundary $(\Lambda\sigma_0)^{-1}j(z,t)$: vs at for $z=1$ (data1) and $z=2$ (data2).

The procedure of solution consists of several steps. First, one needs to introduce a class of solutions. Second, by the Mellin transformation, we derive a functional-difference equation in a strip, reduce it to a scalar Riemann-Hilbert boundary-value problem on an open contour and solve it. Inverse Mellin transformation gives a solution by quadratures. To satisfy the conditions at zero and at infinity, one needs to continue the potential, the solution of the difference equation, that is analytic in a strip, to the next strip to the left and to the right. Also, to derive formulae efficient for numerical purposes, it is desirable to obtain a series representation. To do this, we constructed the analytical continuation of the potential to the strips $\Pi_{-1}, \Pi_{-2}, \ldots$ which lie to the left from the basic strip Π_0 where the the potential is analytic. This continuation and the residue theorem give rise to a rapidly convergent series representation of the solution. The same trick applied to the strips $\Pi_1, \Pi_2, \ldots$ which lie to the right from the strip Π_0, leads to an asymptotic expansion for large arguments.

The asymptotic behaviour of the grain boundary traction σ_{gb}, the atomic flux $j(z,t)$ and the displacement rate $\frac{\partial u_{gb}}{\partial t}$ for small and large time t as z is fixed, has been studied. The leading term of the asymptotic expansions as $t \to \infty$ (z is fixed) for the functions σ_{gb}, $j(z,t)$ and $\frac{\partial u_{gb}}{\partial t}$ coincide up to a constant factor. As $t \to 0$, the flux and the displacement rate tend to zero. However, the displacement rate grows rapidly for small time.

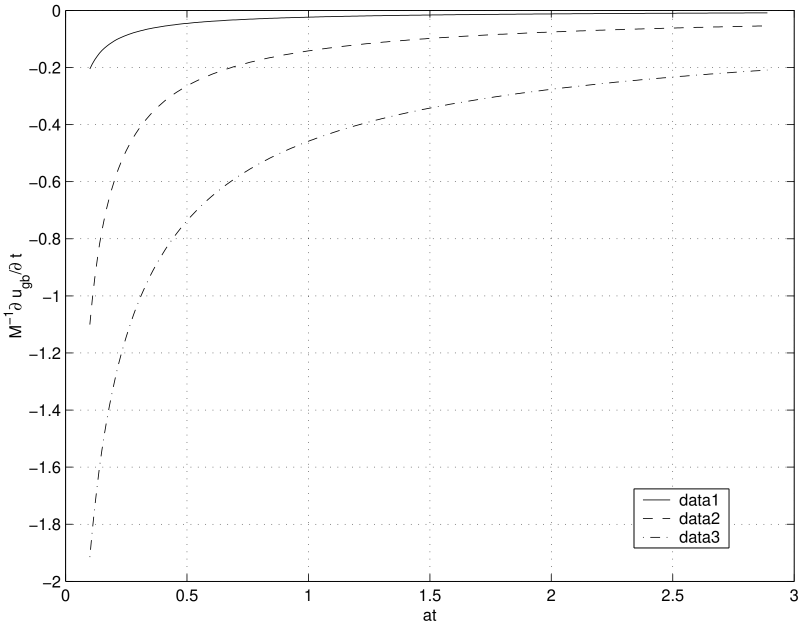

Figure 5: The rate of the displacement $M^{-1}\frac{\partial u_{gb}}{\partial t}(z,t)$: vs at for $z = 0.01$ (data1), $z = 0.1$ (data2) and $z = 1$ (data3).

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