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Groove growth by surface subdiffusion

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HIGHLIGHTS

- The problem of the groove growth is solved in the case of the surface subdiffusion.
- An exact self-similar solution is obtained.
- Basic properties of the solution are described.
- Geometrical properties of the groove profile are calculated.

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ABSTRACT

The investigation of the grain-boundary groove growth by normal surface diffusion was first done by Mullins. However, the diffusion on a solid surface is often anomalous. Recently, the groove growth in the case of surface superdiffusion has been analyzed. In the present paper, the problem of the groove growth is solved in the case of the surface subdiffusion. An exact self-similar solution is obtained and represented in terms of the Fox H-function. Basic properties of the solution are described.

1. Introduction

The time dependent profile of a groove surface which develops on the surface of a hot polycrystal was first investigated by Mullins [1] in two special cases, (i) when the evaporation-condensation mechanism is dominant, and (ii) when the surface diffusion is dominant. In the latter case, the equation governing the temporal evolution of a small-slope surface deflection $z = h(x, t)$ has the form,

$$\partial_t h = -B\partial_x^4 h, \tag{1}$$

where B is a coefficient proportional to the surface diffusivity. The analysis of the groove surface evolution due to the surface diffusion mechanism was extended in [2,3] where grooves with finite surface slopes were considered, and in [4], where multigroove solutions were obtained. In the above-mentioned works the diffusion process is normal diffusion, which describes the macroscopic limit of a Markovian random walk characterized by a linear relation between the mean square displacement of atoms and time, $\langle x^2(t)\rangle = Dt$, where D is the diffusion coefficient. In the case of the normal diffusion, the flux of atoms along the surface at each point and at any time instant is proportional to the gradient of the chemical potential at the same point and at the same time instant.

However, a detailed analysis of the diffusion on solid surfaces led to a clear understanding that the deviation from the standard law of the linear time dependence of the mean squared displacement (anomalous diffusion) is a typical phenomenon [5]. If $\langle x^2(t)\rangle \sim t^a$, the process is called superdiffusion, if $a > 1$, and subdiffusion, if $a < 1$. Several approaches for modeling anomalous diffusion were employed, among them fractional differential equations. In [6], possible implications of the surface superdiffusion for the grain boundary dynamics were investigated using the evolutionary equation,

$$\partial_t h = -BD_{|x|}^{\beta}\partial_x^2 h, \quad 1 < \beta < 2, \tag{2}$$

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where $D^{\beta}_{|x|}$ is the fractional Riesz derivative [7]. Here the limit $\beta \to 2$ corresponds to the normal diffusion, and the limit $\beta \to 1$ corresponds to the ballistic growth. That approach allows to find an exact self-similar solution, which is characterized by an algebraic power law decay in the self-similar variable with the power exponent depending on the fractional parameter, while the decay is exponential in the normal diffusion case. Therefore, a measurement of the shape of the groove tail may be a basis for distinguishing between the normal and anomalous surface diffusion.

In some cases, both superdiffusive and subdiffusive spreading of surface particles takes place [5,8,9]. Specifically, a subdiffusive behavior was predicted for an overdamped Brownian motion of particles in random potentials [10], and, under some conditions, for a bulk-mediated surface diffusion [11].

In the present paper, we consider the influence of the surface subdiffusion on the growth of a one-dimensional symmetric groove on a grain boundary. The mathematical formulation of the problem is given in Section 2. Section 3 contains the exact solution of the problem. Some conclusions are drawn in Section 4.

2. Problem formulation

First, let us remind the description of the grain-boundary groove growth by normal surface diffusion [1]. The Brownian motion of particles on the surface is influenced by the gradient of the chemical potential μ along the surface, which acts like an external force,

$$\mathbf{F} = -\nabla\mu. \tag{3}$$

In fact, the only relevant factor, which determines the inhomogeneity of the chemical potential, is the local curvature of the surface K:

$$\mu = \mu(K); \quad \frac{d\mu}{dK} = \gamma\Omega, \tag{4}$$

where γ is the surface free energy per unit area, and Ω is the molecular volume. The average drift velocity $\mathbf{v}$ of particles is determined by the relation

$$\mathbf{v} = b\mathbf{F}; \tag{5}$$

due to the Nernst–Einstein relation, the mobility

$$b = \frac{D_s}{kT}, \tag{6}$$

where D_s is the coefficient of surface diffusion, k is the Boltzmann constant, and T is the absolute temperature. The number flux of particles is

$$\mathbf{j} = -bn\nabla\mu, \tag{7}$$

where n is the number of particles per unit area, and the evolution equation for the surface deflection is

$$\partial_t h = -\Omega\nabla\cdot\mathbf{j}. \tag{8}$$

In the case of a symmetric, one-dimensional, small-slope groove, the latter equation is reduced to

$$\partial_t h(x,t) = -B\partial_x^4 h(x,t), \quad 0 < x < \infty, \ t > 0, \tag{9}$$

where $B = D_s\gamma\Omega^2 n/kT$, which is solved with the boundary conditions

$$h_x(0,t) = m, \qquad h_{xxx}(0,t) = 0, \qquad h(\infty,t) = 0, \qquad t > 0 \tag{10}$$

where m is the tangent of the equilibrium contact angle, and the initial condition

$$h(x,0) = 0, \quad 0 < x < \infty. \tag{11}$$

The classical relation (5) between the instantaneous values of the particle velocity and the force acting on the particle is violated in the case of subdiffusion. The fractional Fokker–Planck equation for the particle distribution function $P(\mathbf{x},t)$, which can be derived from the CTRW model with a long-tailed waiting time probability density function (pdf) [7], differs from its normal counterpart by the presence of a memory operator:

$$\partial_t P = {}_0D_t^{1-\alpha}[-b\nabla\cdot(\mathbf{F}P) + K_\alpha\nabla^2 P], \quad 0 < \alpha < 1, \tag{12}$$

where

$${}_0D_t^{1-\alpha} f(t) = \frac{1}{\Gamma(\alpha)}\partial_t \int_0^t \frac{f(\tau)}{(t-\tau)^{1-\alpha}} d\tau \tag{13}$$

is the Riemann–Liouville fractional derivative, and K_α is a constant coefficient. Under reasonable assumptions on the behavior of $P(\mathbf{x},t)$ on the infinity, one obtains that the temporal evolution of first moment $\langle\mathbf{x}\rangle$ is governed by the equation

$$\frac{d}{dt}\langle\mathbf{x}\rangle = b\ {}_0D_t^{1-\alpha}\langle\mathbf{F}\rangle. \tag{14}$$

In the macroscopic limit, we find a non-standard relation between the flux and force,

$$\mathbf{j} = -bn\ {}_0D_t^{1-\alpha}\nabla\mu, \tag{15}$$

which replaces relation (7). Under the assumptions listed above [1], the following evolution equation for the surface deflection is obtained:

$$\partial_t h(x,t) = -B\ {}_0D_t^{1-\alpha}\partial_x^4 h(x,t), \quad 0 < x < \infty, \ t > 0. \tag{16}$$

Eq. (16) can be written in the equivalent forms [7,12],

$$\begin{aligned}&{}_0D_t^{\alpha} h(x,t) - \frac{t^{-\alpha}}{\Gamma(1-\alpha)} h(x,0)\\ &\quad = -B\partial_x^4 h(x,t), \quad 0 < x < \infty, \ t > 0.\end{aligned} \tag{17}$$

or

$$\partial_t^\alpha h(x,t) = -B\partial_x^4 h(x,t), \quad 0 < x < \infty, \ t > 0 \tag{18}$$

where ∂_t^α is the Caputo fractional derivative,

$$\partial_t^\alpha h(x,t) = \frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{\partial h(x,\tau)}{\partial\tau}\frac{d\tau}{(t-\tau)^\alpha}, \quad 0 < \alpha < 1. \tag{19}$$

The boundary and initial conditions (10) and (11) are retained.

3. Solution

3.1. Integral form of the solution

We use integral transforms for solving the problem formulated above. First, we apply the Laplace transform of the equation with respect to t, defined by

$$\tilde{h}(x,s) = \mathcal{L}\{h(x,t);s\} = \int_0^\infty h(x,t)e^{-st}dt.$$

Using the property [12],

$$\mathcal{L}\{\partial_t^\alpha h(x,t);s\} = s^\alpha\tilde{h}(x,s) - h(x,0^+)s^{\alpha-1}, \tag{20}$$

with initial condition (11) we obtain:

$$s^\alpha\tilde{h}(x,s) = -B\ \partial_x^4\tilde{h}(x,s) \tag{21a}$$

$$\tilde{h}_x(0,s) = m/s \tag{21b}$$

$$\tilde{h}_{xxx}(0,s) = 0. \tag{21c}$$