School of Physics and Astronomy

Interacting Diffusion in Metals
First Year Report and Literature Review

Joshua DM Hellier

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Abstract

There will eventually be an abstract here, when I've gotten round to writing it. Lol!

Signature: Date:

Supervisor: Professor Graeme Ackland

Contents

1 Background

looooooooooool [1, 2] [3, pp 151–152]

General background stuff here, for the scientific layman.

2 Review of Background Bibliography

This bit should be long, somehow.

3 Progress to Date

3.1 Solutions to the 1-D Transport Equation in Moving Frames

The experimental evidence presented in [1] suggests that the interface growth rate in Nb-alloyed Titanium is sublinear; therefore, the process is likely to be limited by diffusion. Thus, I briefly investigated the 1-D diffusion equation in frames moving with time according to a power law, which takes the form

$$\frac{\partial u}{\partial t} - n\nu t^{n-1}\frac{\partial u}{\partial x} = \kappa\frac{\partial^2 u}{\partial x^2}. \tag{1}$$

Here, the frame is moving as $x = t^n$, for some real n and hence we have used the convective derivative $\frac{\partial u}{\partial t} - n\nu t^{n-1}\frac{\partial u}{\partial x}$ to take account of this motion. My reason for doing this is to allow us to easily follow an interface which is being pushed forward by a diffusive process, as such an interface would be described by x being held constant (in particular at 0).

In the spirit of the Fluid Dynamicists [4], let us first switch from (x, t, u) to a set of dimensionless parameters, (ξ, η, u) [1]. We see straight away that the variable $\xi = \frac{x}{\sqrt{\kappa t}}$

[1]Note that the dimension of u is immaterial, as it appears once in every term.

is dimensionless, and indeed this is the same dimensionless quantity encountered when attempting similarity solution of the standard 1-D diffusion equation. In the moving frame, there is an additional dimensionless variable $\eta = \frac{x}{\nu t^n}$. In general, we would now transform into the new coordinates and seek $u(\xi, \eta)$ as the solution to the new PDE.

However, the case $n = \frac{1}{2}$ (which happens to be the case we are most interested in, as it represents sublinear "quadratic growth") is special, as ξ and η in this case are not independent; indeed, we can see that $\nu^2\eta^2 = \kappa\xi^2$. Thus, in the situation that there is no particular scale being imposed upon the system by the initial data, any solution may now be written as $u(\xi)$. Under these assumptions, the PDE reduces to the ODE

$$u'' + \frac{1}{2}\left(\xi + \nu\kappa^{-\frac{1}{2}}\right)u = 0 \tag{2}$$

where $'$ denotes differentiation with respect to ξ. This has the general solution

$$u(\xi) = A\,\mathrm{erf}\left[\frac{1}{2}\left(\xi + \frac{\nu}{\sqrt{\kappa}}\right)\right] + B \tag{3}$$

for A, B arbitrary real constants. Substituting in our definition of ξ, we see that the solution takes the form

$$u(x,t) = A\,\mathrm{erf}\left[\frac{1}{2}\left(\frac{x + \nu\sqrt{t}}{\kappa\sqrt{t}}\right)\right] + B \tag{4}$$

It is interesting to note that the particle current,

$$J = -\kappa - \frac{1}{2}\nu t^{-\frac{1}{2}} \tag{5}$$

passing through $x = 0$ varies in proportion to $t^{-\frac{1}{2}}$, which happens to be the rate of deposition required to build structure in quadratic growth. I intended to use this solution to build an Oxygen/Antioxygen model for the TiO_2/Ti interface, but have put this on hold as it would require detailed knowledge of the interface region, which presents quite a challenge; I will probably return to this question later, possibly armed with computational results. Meanwhile, I have recently turned my attentions to the diffusion of dilute Oxygen/Niobium mixtures in Titanium, which is the subject of the next section.

3.2 Deriving a Simple Interacting Multi-Species Diffusion Model

4 Proposal

What things I intend to do in the future.

5 Summary

Summary of stuff.

References

[1] BE Tegner, L Zhu, C Siemers, K Saksl, and GJ Ackland. High temperature oxidation resistance in titanium–niobium alloys. *Journal of Alloys and Compounds*, 643:100–105, 2015.

[2] Linggang Zhu, Qing-Miao Hu, Rui Yang, and Graeme J Ackland. Atomic-scale modeling of the dynamics of titanium oxidation. *The Journal of Physical Chemistry C*, 116(45):24201–24205, 2012.

[3] Paul M Chaikin and Tom C Lubensky. *Principles of condensed matter physics*, volume 1. Cambridge University Press, 2000.

[4] George Keith Batchelor. *An introduction to fluid dynamics*. Cambridge University Press, 2000.