# School of Physics and Astronomy

## Surface Layer Growth in Metal Corrosion
## First Year Summary

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**Abstract**

Corrosion is an important process, which may severely limit the utility of an alloy. In this PhD project, I intend to improve our theoretical understanding of this phenomenon.

Signature: Date:

**Supervisor:** Professor Graeme Ackland

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# 1 Project Outline

## 1.1 Background

The reader may be familiar with the fact that bulk metals tend corrode when exposed to Oxygen and other substances in the environment, often causing an oxide layer to form on the surface of the metal. The reader might not be familiar with how difficult it is to predict the rate at which this process occurs, particularly with regards to the dependence of the rate upon temperature and alloy composition. This difficulty arises from corrosion being a **multiscale** phenomenon, in the sense that a model for corrosion requires detailed knowledge of both microscopic and macroscopic processes. In this case, the **macroscopic** process in play is the bulk motion of Oxygen and other substances through the oxide layer and the metal, whilst the growth of the layer itself is probably driven by **microscopic** chemical processes occurring at the interfaces between layers. The large-scale diffusive phenomena determine how much of a substance is available to take part in the small-scale layer construction, whilst the rate of layer construction impacts the behaviour at the large scale by moving the boundary; thus one can see why we need a good description at both large and small scales to fully understand what is going on.

In this project, we wish to understand in particular the corrosion of Titanium that has been alloyed with Niobium. From experiment [1], it is known that there are in fact three layers near the surface of corroding Titanium: A $TiO_2$ layer, then an Nb-depleted Ti layer, then an Nb-rich Ti region which melds into the rest of the bulk metal; an SEM image of these surface layers is shown in Figure 1.1. In order to really understand how this Ti alloy corrodes, and predict the rate of corrosion, we need to know why these different regions exist (i.e. what is happening, quantitatively, at the interfaces), and what is happening within the different regimes. The direct application of such knowledge has obvious benefits, as it could allow us to make better alloys. However, more indirectly, it is yet another interesting nonequilibrium statistical system, and as such is of great scientific interest in its own right.

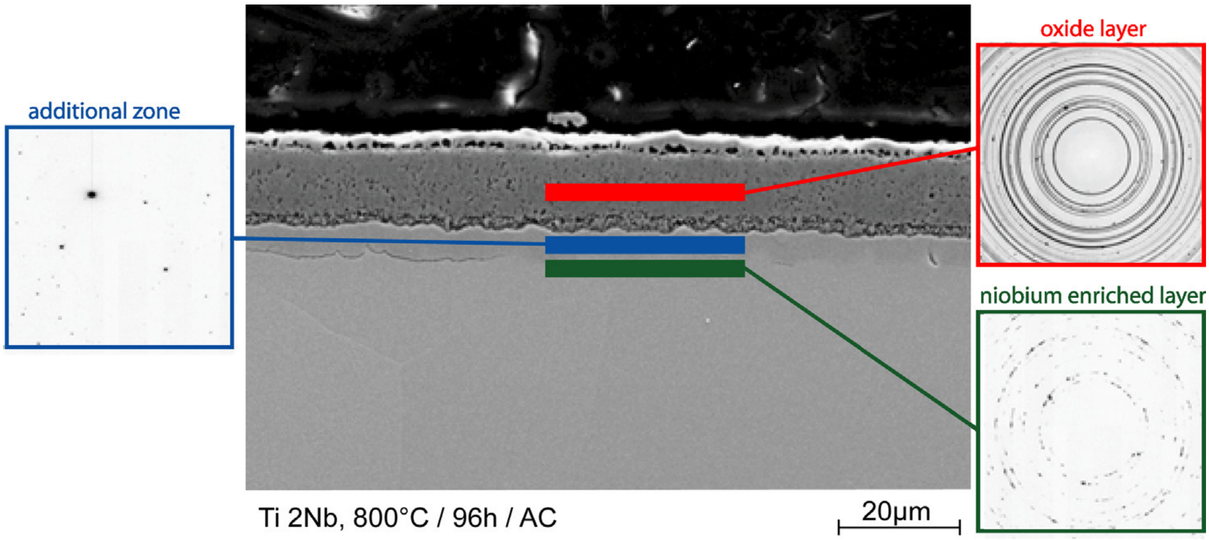


Figure 1: An SEM image of the surface layers of Nb-alloyed Ti, complete with microfocussed x-ray diffraction spectra. Courtesy of [1].

### 1.2 Progress So Far

This year, I have been getting up to speed with the literature and techniques of nonequilibrium statistical mechanics. I have found an exact solution to the 1-d diffusion equation in a frame comoving with the Ti/$TiO_2$ interface, which should help me later when I have a decent theory of interacting species diffusing through Titanium. Recently, I have tried to find such a theory, but analysis of my theory shows it to be flawed, so I need to make a better one.

## 2 SUPA Courses

| Name | Assessed |
|---|---|
| Advanced Data Analysis | Y |
| Advanced Statistical Physics | Y |
| Chaikin and Lubensky's Principles of Condensed Matter | Y |
| Computational Materials Physics | Y |
| Interacting Electron Problem in Solids | N |
| Non-equilibrium Statistical Mechanics | N |

## 3 Teaching

| Course | Hours |
|---|---|
| Thermodynamics | 40 |
| Physics of Fields and Matter | 49 |
| Symmetries of Classical Mechanics | 16 |

# 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.