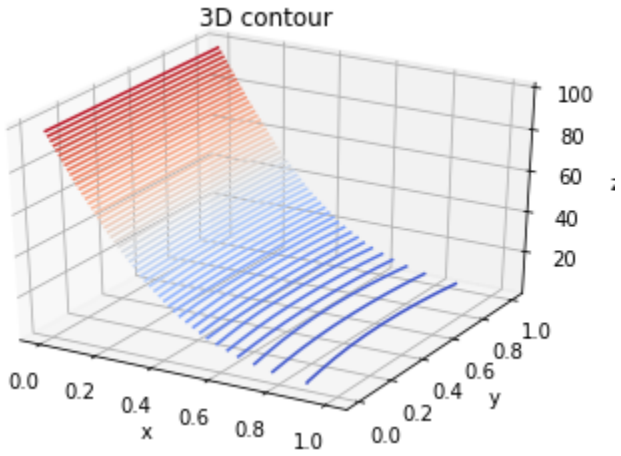
Progress Report

Name: Colton Dudley
CID: 01858493
Supervisor: Mike Finnis
Title: Simulating multi component diffusion through a film of oxide

Progress:

We started by looking into the theory of diffusion of Oxygen through aluminum oxide, through bulk and boundary layers. We familiarized ourselves with the work of Mishin and Borchardt who used Oxygen isotopes to model and experimentally understand this diffusion. We numerically solved the diffusion equation in one direction with moving boundary conditions to simulate this diffusion along a grain boundary. We then extended this diffusion into two dimensions to simulate diffusion into and along the grain bulk. To do this we used periodic boundary conditions in the ‘y’ direction. An arbitrary time into this diffusion is shown here:



Challenges:

The first thing to consider is that when using an isotope of oxygen in a system already saturated by oxygen it is necessary to use a more general diffusion model than the diffusion of ‘holes’ as they are replaced by oxygen. An equation has been found with effectively a diffusion coefficient that is dependent on position which we need to implement into our simulation. We then also need to include the moving boundary extended into 2 dimensions. Finally we need to use less arbitrary values in order to match our simulation to the real world application given by Mishin and Borchardt. After this we can consider the diffusion of Aluminum across the aluminum oxide which should be trivial.