Oxide dissolution and oxygen diffusion scenarios in niobium and implications on the Bean–Livingston barrier in superconducting cavities

Work presented is based on our paper in Journal of Applied Physics:
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Eric M. Lechner
**Introduction – Importance of Impurities**

- Impurities are effective for reducing the surface resistance.
- Reduction of $R_s$ arises from a competition of diminishing conductivity and lengthening penetration depth.
- Successfully implemented N-doping in LCLS-II

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**Ti impurities**

**N impurities**

**O impurities**

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Introduction – Nanostructuring For Boosting $E_{\text{acc}}$

Previously used to shift supercurrent away from the surface ($x=0$) to protect from possible hydrides, but is essentially a model that can be used instead to examine peak spatial supercurrent. More on this later...

Oxide Dissolution & O Diffusion

\[ \frac{\partial c(x, t)}{\partial t} = D(T) \frac{\partial^2 c(x, t)}{\partial x^2} + \sum_x q(x, t) \]

**Semi-infinite slab**

\[ \frac{\partial c}{\partial t} - D \frac{\partial c}{\partial x^2} = \sum_{k=-\infty}^{\infty} \sum_{n=1}^{m} \gamma_n(\delta(x + a_n - 2kd) + \delta(x - a_n - 2kd)) \]

**Finite thickness impermeable substrate**

\[ \frac{\partial c(x, t)}{\partial t} - D(T) \frac{\partial^2 c(x, t)}{\partial x^2} = \sum_{n=1}^{m} \gamma_n(t)(\delta(x + a_n) + \delta(x - a_n)) \]

**Semi-infinite Single Oxide Layer Dissolution (Nb_2O_5)**

\[ c(x, t) = \frac{V_0}{\sqrt{\pi D t}} \exp(-x^2/4Dt) + \int_0^t \frac{u_0 k_1 \exp(-k_1 t)}{\sqrt{\pi D(t-s)}} \exp(-x^2/4D(t-s)) ds \]

*Explicit Assumption:*

1. Diffusion lengths through oxides is larger than oxide thickness. Availability of O to the substrate is not limited by mass transport through the oxide. Otherwise boundary conditions at each oxide need to be considered.

**Semi-infinite Substrate**
- Develop homogeneous or deep O concentrations to explore the effect of O depth at constant O concentration.
- Tune interstitials to bend supercurrent density in the first 100 nm while maintaining a higher O content within the RF active region.

**Impermeable Substrate**
- Allow for “short” SIMS measurements to determine layer dissolution parameters. Instead on needing to many microns into the surface.
- Note: Easy to poison thin films with O if Nb is heated much at all.
Short heat treatment (ramp time is considerable)

\[ \frac{-dA}{dt} = k_1 A \]

\[ \frac{-dA}{dt} \propto q = u_0 k(T(t)) \exp\left(-\int_0^t k(T(s))ds\right) \delta(x) \]

\[ \frac{\partial c(x, t)}{\partial t} = D(T(t)) \frac{\partial^2 c(x, t)}{\partial x^2} + q(t, T(t)) \]

**TABLE I.** Model parameters used for theoretical O concentration profiles in Figs. 3 and 4.

<table>
<thead>
<tr>
<th>Ref. 31</th>
<th>NL298</th>
<th>NL321</th>
<th>NL324</th>
<th>NL563</th>
<th>NL564</th>
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</thead>
<tbody>
<tr>
<td>( u_0 ) (at. % nm)</td>
<td>200</td>
<td>200</td>
<td>257</td>
<td>187</td>
<td>155</td>
</tr>
<tr>
<td>( v_0 ) (at. % nm)</td>
<td>3.5</td>
<td>3.5</td>
<td>3.5</td>
<td>3.5</td>
<td>3.5</td>
</tr>
<tr>
<td>( A \times 10^7 ) (1/s)</td>
<td>0.9</td>
<td>0.994</td>
<td>0.959</td>
<td>0.993</td>
<td>0.986</td>
</tr>
<tr>
<td>( E_r ) (kJ/mol)</td>
<td>131</td>
<td>132</td>
<td>134</td>
<td>135</td>
<td>137</td>
</tr>
<tr>
<td>( D_0 ) (cm²/s)</td>
<td>0.075</td>
<td>0.077</td>
<td>0.067</td>
<td>0.073</td>
<td>0.059</td>
</tr>
<tr>
<td>( E_{AD} ) (kJ/mol)</td>
<td>119.9</td>
<td>118</td>
<td>120</td>
<td>119</td>
<td>118</td>
</tr>
</tbody>
</table>
Modified London Equation

\[ \lambda^2 B''(x) + 2\lambda' B'(x) - B(x) = 0 \]

\[ \lambda(x) = (\lambda_0 - \lambda_\delta) \text{Erfc} \left( \frac{x}{\delta} \right) + \lambda_0 \]

**Breakdown condition**

Hydride breakdown at surface

\[ B'(0) = \mu_0 I_H = -B_{EP}/\lambda_0, \]

Both models are critical field models

**Modified London Equation**

\[ \frac{\lambda^2 B''(x) + 2\lambda' B'(x) - B(x)}{\Delta \phi_0} = 0 \]

\[ l(x) = \frac{\sigma}{\lambda_0 \sqrt{1 + \frac{\phi_0}{l(x)}}} \]

**Breakdown condition**

Vortex Nucleation

\[ \max(J(x)) = J_d \]
What’s Been Done Previously?

Modified London Equation

\[ \lambda^2 B''(x) + 2 \lambda B'(x) - B(x) = 0 \]

\[ \lambda(x) = (\lambda_s - \lambda_0) \text{Erfc} \left[ \frac{x}{\delta} \right] + \lambda_0 \]

**Breakdown condition**

**Hydride breakdown at surface**

\[ B'(0) = \mu_0 J_H = -B_{EP}/\lambda_0, \]

**Consideration:**

In the present O diffusion model, strongest suppression of the supercurrent density at the surface occurs for short treatments. This means very short LTB times should produce the best result in the hydride breakdown model, in contradiction to LTB measurements.

Modified London Equation

\[ J^2 B''(x) + 2 \lambda J B'(x) - B(x) = 0 \]

\[ l(x) = \frac{\sigma}{\Delta \varphi_0} \lambda(x) = \lambda_0 \sqrt{1 + \frac{\xi_0}{l(x)}} \]

\[ c(x,t) = \frac{\mu_0}{\sqrt{\pi} \delta} \exp(-x^2/4D\delta) \]

\[ + \int_0^\infty \frac{\mu_0 k_0 \exp(-k_0 t)}{\sqrt{\pi} \delta} \exp(-x^2/4D\delta(t-s)) ds \]

**Breakdown condition**

**Vortex Nucleation**

\[ \max(J(x)) = J_d \]
Do Thin Impurity Profiles Play a Role In Low Temperature Baked Nb?

Major O contributor in LTB is the interstitial O at the oxide/metal interface

\[ \lambda(x)^2 B'' + 2\lambda(x)\lambda'(x)B' = B \]

\[ \lambda(x) = \lambda_0 \sqrt{1 + \frac{\xi_0}{l(x)}} \]

\[ l(x) = \frac{\sigma}{\Delta\rho_0} \]

\[ \sigma = 0.37 \times 10^{-15} \text{\Omega m}^2 \]

\[ \Delta\rho_0(x) = ac(x) \]

\[ a = 4.5 \times 10^{-8} \text{\Omega m} \]

\[ \lambda_0 = 39 \text{ nm} \]

\[ \xi_0 = 38 \text{ nm} \]

Reasonably describes the locations of HFQS ameliorating heat treatment times and temperatures.

\[ E_q = E_{q0}J_{\text{max}0} / \max(J(x, T, t)). \]
Quench Field Measurements

Best fit to Bafia et al.

\[ E_q = E_{q0}j_{\text{max}0} / \max (J(x, T, t)) \]

\[ E_{q0} = 29.2 \text{ MV/m} \]

\[ \nu_0 = 2.6 \pm 0.3 \text{ at. % nm} \]

Estimate from Lechner et al.

\[ E_{q0} = 29.2 \text{ MV/m} \]

\[ \nu_0 = 3.5\text{at. % nm} \]

Vortex Nucleation Scenarios


Topographically?

Weakened Superconductivity?

Maybe nano hydrides?
Conclusions

• Further developed a model to describe O migration in multi-component, multilayer decomposition.

• Time dependent temperature single layer dissolution and multistep processes model developed.

• A model for peak supercurrent suppression based on the modified London equation and O diffusion is proposed. It is found to reasonably describe the T-t distribution of HFQS ameliorating heat treatments. It is in reasonable agreement with the measurements of Bafia et al.
Acknowledgments

**Coauthors**
J.W. Angle
C.E. Reece
M.J. Kelley
F.A. Stevie
A.D. Palczewski

**Others**
C. Baxley
R. Overton
T. Harris