Analytical modeling of the evolution of the nonlinearity parameter of sensitized stainless steel.

Brian Fuchs[1], Graduate Research Assistant

Jin-Yeon Kim[2], Jianmin Qu,[3] and Laurence J. Jacobs[1,2]

[1]GW Woodruff School of Mechanical Engineering, Georgia Tech
[2]School of Civil and Environmental Engineering, Georgia Tech
[3]Department of Mechanical Engineering, Tufts University

Motivation

Precipitation in Stainless Steel

- Stainless steels have a wide range of uses in the energy industry due to their corrosion resistance.
- When exposed to high temperatures, carbon and chromium diffuse to the grain boundary, forming $M_{23}C_6$ carbides (sensitization).
- Chromium-depleted zones near the grain boundary become susceptible to corrosive attack, including stress corrosion cracking.

Nonlinear Ultrasonic Techniques (NLU)

- NLU has been shown to be sensitive to sensitization in stainless steel.
- There are few models relating the acoustic nonlinearity parameter, β, to a quantified amount of damage in stainless steel.

Objectives

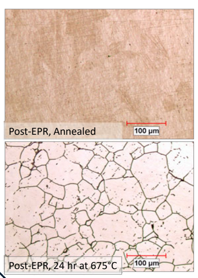
- Develop a diffusion model that accurately predicts $M_{23}C_6$ precipitate growth in thermally aged stainless steel.
- Develop an analytical model relating $M_{23}C_6$ growth to the increase in β. J.-Y. Kim2

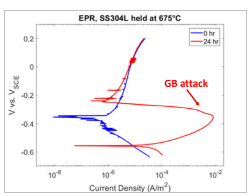
304L Stainless Steel

SS 304L (wt %)	C	Cr	Ni	Mn	Cu	Mo	Co
	0.019	18.37	8.13	1.66	0.39	0.39	0.119

Bar samples: 6" x 2" x 0.75" (152 x 50.4 x 17.1 mm)

Heat Treatment: Annealing (1080°C, 30 min, Air Cool), followed by Sensitization @ 675°C, for 0 hr, 24 hr)





EPR tests show that significant sensitization has occurred after 24 hours at 675°C. The pictures on the left show that the corrosion occurred at the grain boundaries.

This material is based upon work supported under an Integrated University Program Graduate Fellowship.

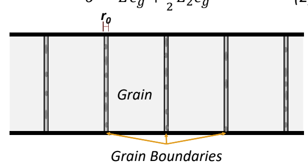
Methods

1-D Grain Boundary Separation Model

Stress in the material is modeled as a 1-D series of distributed nonlinear springs, described by:

Grain Boundary: $$\sigma = k\epsilon_b + \frac{1}{2}k_2\epsilon_b \quad (1)$$

Grain: $$\sigma = E\epsilon_g + \frac{1}{2}E_2\epsilon_g \quad (2)$$



The acoustic nonlinearity parameter is given by:

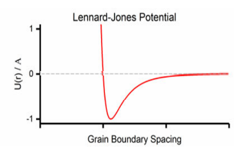
$$\beta = \frac{\delta^2\epsilon}{\delta\sigma^2}\left(\frac{\delta\epsilon}{\delta\sigma}\right)^{-2}\Big|_{\sigma=0} \quad (3)$$

Utilizing the relations described in (1) and (2), the contribution to the nonlinearity parameter from the grain, β_g and the grain boundary, β_b are determined:

$$\beta_g = -\frac{E_2}{E} \quad (4)$$

$$\beta_b = \frac{r_0}{d}\left(\frac{2E_2}{k} - \frac{E^2k_2}{k^3}\right) \quad (5)$$

We assume that grain boundary constants can be determined from a potential function, such as Lennard-Jones.



$$U(r) = 4A\left(\left(\frac{B}{r}\right)^{12} - \left(\frac{B}{r}\right)^{6}\right) \quad (6)$$

$$k = \frac{r_0\delta^2U(r)}{a^2\delta r^2} \qquad k_2 = \frac{r_0^2\delta^3U(r)}{a^2\delta r^3} \quad (7,8)$$

During thermal aging, grain-boundary precipitate radius grows:

$$r_p = r_0(1+\delta) \quad (9)$$

Under the assumption that r_0 is the equilibrium spacing dictated by the Lennard-Jones potential, the relative change in β is then

$$\frac{\beta(r_p)}{\beta(r_0)} = 1 + \frac{56\left(172^{\frac{1}{6}}a^2BE^2+54AE_2\right)\delta}{3\left(72^{\frac{1}{6}}a^2BE^2+48AE_2\right)}f \quad (10)$$

Given that the material properties are constants, β is then linearly related to the change in grain boundary thickness. In this work, we assume a linear relation between precipitate radius and *δ*, necessitating a scalar correction factor (f).

A[2]	B[2]	E[3]	E_2[3]	*f*
Energy well depth	Atom spacing at U = 0	1st-order Young's modulus, Fe	2nd -order Young's modulus, Fe	Linear fit parameter
0.7064 eV	2.02E-10 m	230 GPa	275 GPa	0.0037

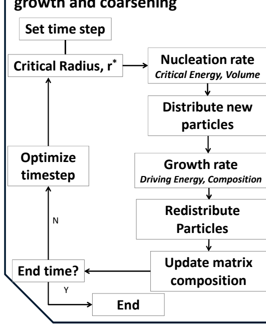
Grain Boundary Precipitate Modeling

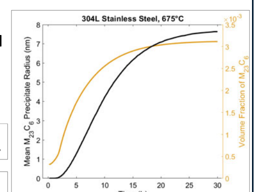
TC-PRISMA[4] Precipitate Growth Module (General) J.-Y. Kim1

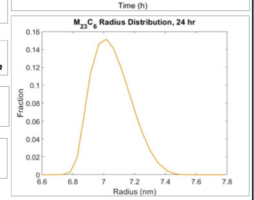
Assumptions

- Pseudo-steady state diffusion within each time step (based on matrix composition)
- $M_{23}C_6$ precipitates are spherical.

Based on Langer-Schwartz theory and Kampmann-Wagner numerical method to simulate nucleation, growth and coarsening



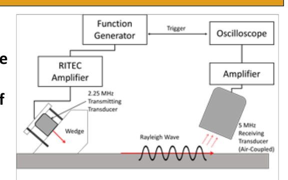


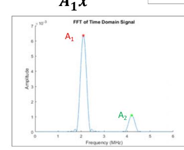


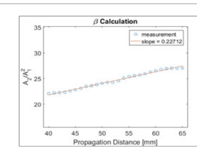
Nonlinear Ultrasound

As an ultrasonic wave interacts with microstructural damage in a material, it generates harmonics of the original wave. β is quantified as:

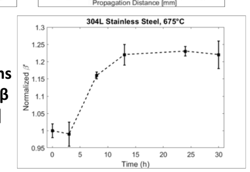
$$\beta \propto \frac{A_2}{A_1^2x}$$



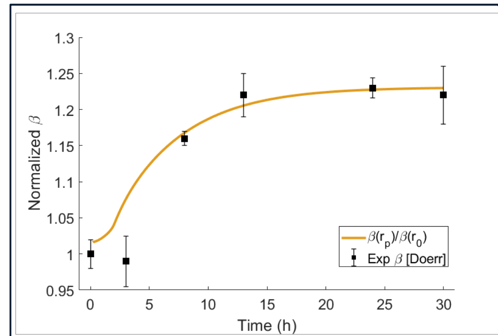




Measurements of thermally aged stainless steel specimens show a significant change in β with increasing time. [Doerr]



Results



The prediction of the 1D model follows experimental data between 8 and 30 hours of aging,[Doerr] coinciding to predicted mean precipitate radii of 5 – 7 nm.

Conclusions

A model describing evolution of acoustic nonlinearity of sensitized stainless steel 304L was developed. This model relates the radius of grain boundary $M_{23}C_6$ precipitates to the increase in β, demonstrating a linear relationship over a range of precipitate radii.

Future Work

- Assess the Lennard-Jones potential in the description of grain boundary energy.
- Determine the influence of precipitate distribution on β
- Optimize the correction factor and determine its order across alloys.
- Use SEM or other characterization to assess the accuracy of the Thermocalc software in the growth of grain boundary precipitates.
- Further tests on 304L stainless steel to assess repeatability and reliability of measurement.

Reference

[1] C Doerr, J-Y Kim, P Singh, J Wall, LJ Jacobs, *NDT&E Int.*, 88, p. 17-23 (2017)
[2] V Filipova, E Blinova, N Shurygina, *Inorg. Mat. Appl. Rsch*, 6, p. 402-406 (2015)
[3] C Cube, J Turner, *J. Acoust. Soc. Am.*, 138, p. 2613-2625 (2015)
[4] TC-PRISMA, https://www.thermocalc.com/

Slide 1

J.-Y. Kim1 in Thermo-Calc Software
Jin-Yeon Kim, 7/2/2019

J.-Y. Kim2 Quantify degree of sensitization (DOS) using measued acoustic nonliearity parameter

Brian, this will be the ultimate goal of the research!
Jin-Yeon Kim, 7/2/2019

M23C6 precipitates well before sigma phase
https://inis.iaea.org/collection/NCLCollectionStore/_Public/36/083/36083651.pdf?r=1&r=1