Numerical computation for prediction of grain growth on stainless steel 316L

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Numerical computation for prediction of grain growth on stainless steel 316L

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Abstract. This research aims to predict the grain size growth using numerical computation. The material to be investigated is stainless steel 316L (SS316L). The mathematical modeling is derived into two cases, namely with the absence of precipitate (free growth) and with the presence of growing precipitates. The numerical computation involves ordinary differential equation using Runge-Kutta 4th order written with FORTRAN language. The experimental verification is carried out by using quenching and deformation dilatometers. It can be concluded that modified kinetic constant (Mo*) should be defined differently for certain temperature range.

1. Introduction

SS316L is an austenitic chromium-nickel stainless steel that contains between 2% and 3% molybdenum. The molybdenum content increases the corrosion resistance, improves resistance to pitting in chloride ion solutions, and increases strength at high temperatures [1]. Hence, this material is most familiar used in high resistance application such as heat exchanger, jet engine parts and also suitable in marine applications, in petrochemical reactor as well as gas industries [2]. This type of low carbon austenitic alloy is made to keep away from the formation of chromium carbides which result in an exhaustion of chromium from the austenite matrix and a loss in the resistance against corrosion. SS316L has a small thermal conductivity and a large thermal expansion coefficient and hence it is prone to produce welding residual stress and deformation [3].

The grain size has an influence on the material properties and a considerable effect on the mechanical properties. For instance at room temperature, the yield strength, hardness, fatigue strength, tensile strength and impact strength are increased with decreasing of grain size [4]. On the other hand, one of the most important factors controlling austenite grain structure at the end of cold-working and annealing operations is the austenite stability with respect to strain induced transformation [5]. Grain growth in stainless steel is enhanced by boron and to be increased with the temperature [3]. Consequently, to improve the strength of a material is to make the grains as small as possible by

increasing the amount of grain boundary. Small grain sizes are accompanied by high volume of grain boundaries and as a result, the more grain boundaries that be present, the higher the strength becomes.

This research aim to predict the grain size using numerical computation of compiler Force 2.0 with Fortran programming languages by implementing the grain growth mathematical model. The grain growth for material SS316L was calculated in two cases with the absence of alloying elements or precipitates (free grain growth) and with the presence of growing precipitates. For comparison purpose, experimental investigation was carried out by using quenching and deformation dilatometers.

2. Numerical method for grain growth prediction

The flow process to calculate the grain size using numerical computation with Fortran programming languages is presented in figure 1. The input files contain input of temperature (T) and time (dt). The input data have heating and cooling temperatures while the condition of the temperature depends on the row that has been set by the user. The initial grain size used in this simulation is 20μm. In this programming, the grain size is considered as 20 μm during the heating temperature and the grain size will be calculated during the cooling temperature. The final grain size is calculated by using Ordinary Differential Equation (ODE)'s problem solving method.

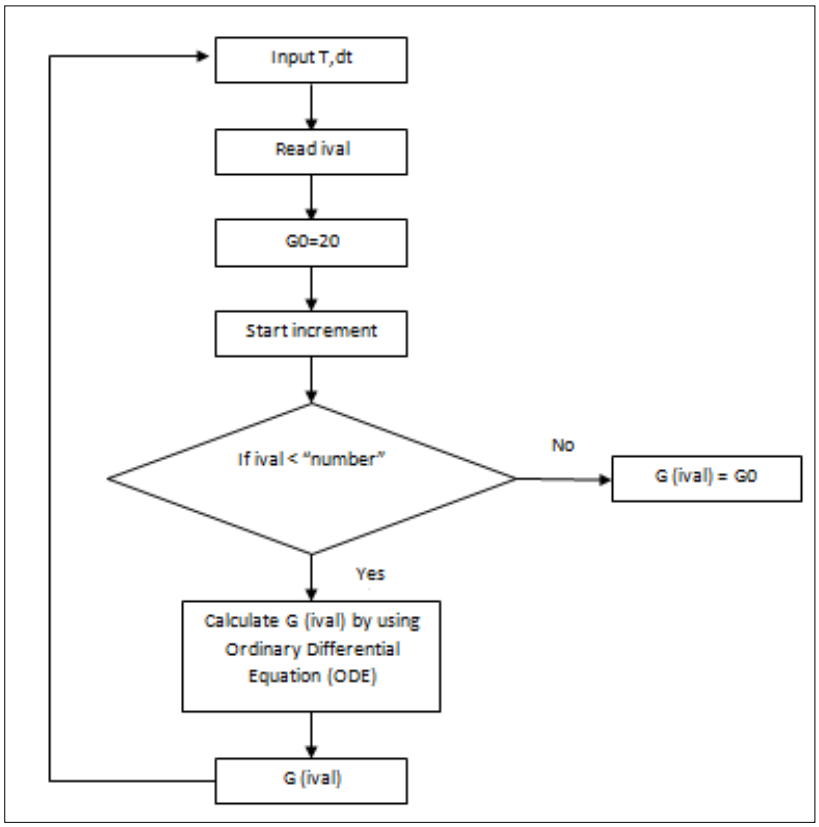


Figure 1. Flow chart for grain size calculation.

2.1. Basic equation for grain growth size calculation

In calculating the grain size for SS316L, there are two cases have been studied. Case 1 is a grain growth in the absence of alloying elements/precipitates (free grain growth) and case 2 is a grain growth in the presence of growing precipitates. A general formula for the grain growth as in equation (1) [6].

$$\frac{\partial \bar{g}}{\partial t} = M_0{}^* \exp\left[-\frac{Q_{app}}{RT(t)}\right]\left[\frac{1}{\bar{g}} - \frac{1}{\bar{g}_{lim}}\right]^{\left(\frac{1}{n}-1\right)} \quad (1)$$

Where;
$M_0{}^*$= Modified kinetic constant ($\mu m^2 s^{-1}$)
Q_{app}= Activation energy ($kJ\ mol^{-1}$)
R= Gas constant (8314 J $K^{-1}mol^{-1}$)
T= Absolute temperature (K)
$\bar{g}$= Average/initial grain size (μm) and $\bar{g}_{lim}$ depends on the cases.

The grain growth formula for the case 1 as in equation (2) below:

$$\frac{\partial \bar{g}}{\partial t} = M_0{}^* \exp\left[-\frac{Q_{app}}{RT(t)}\right]\left[\frac{1}{\bar{g}} - \frac{1}{\bar{g}_{lim}}\right]^{\left(\frac{1}{n}-1\right)} \quad (2)$$

Where;
$\bar{g}_{lim} = k\frac{r}{f}$

r = Radius of precipitate (μm)
f = Volume fraction of precipitate
k = Zener coefficient

The value of f = 0 due to absence of precipitate therefore $\bar{g}_{lim}$ will become ∞. As a result, the numerical equation for case 1 as in equation (3).

$$\frac{\partial \bar{g}}{\partial t} = M_0{}^* \exp\left[-\frac{Q_{app}}{RT(t)}\right]\left[\frac{1}{\bar{g}}\right]^{\left(\frac{1}{n}-1\right)} \quad (3)$$

The grain growth equation for the case 2 as in equation (4) below:

$$\frac{\partial \bar{g}}{\partial t} = M_0{}^* \exp\left[-\frac{Q_{app}}{RT(t)}\right]\left[\frac{1}{\bar{g}} - \frac{1}{\bar{g}_{lim}}\right]^{\left(\frac{1}{n}-1\right)} \quad (4)$$

Where;
$\bar{g}_{lim} = \left[\left(\overline{g_{lim}}^0\right) + \left(\frac{k}{f_0}\right)^3 I_2\right]^{\frac{1}{3}}$
$\overline{g_{lim}}^0 = k\frac{r_0}{f_0}$
$I_2 = C_5 \int_0^t \frac{1}{T(t)} exp\left[-\frac{Q_s}{RT(t)}\right] dt$
r_0 = Initial radius of precipitate (μm)
f_0 = Initial volume fraction of precipitate
I_2 = Kinetic strength of the thermal cycle particle coarsening (μm^3)
C_5 = Kinetic constant
Q_s = Activation energy for coarsening process ($kJ\ mol^{-1}$)

2.2. Ordinary differential equation (ODE)

In mathematics, ODE is a differential equation containing one or more functions of one independent variable and derivatives of those functions [7]. Since the equation for the grain size is a type of ODE equation, therefore the Runge-Kutta 4th order method was used to solve the grain size formula as in equation (5 – 9).

$$G_{i+1} = G_i + \frac{1}{6}(K_1 + 2\,K_2 + 2K_3 + K_4)h \quad (5)$$

$$K_1 = f(dt_i, T) \quad (6)$$

$$K_2 = f(dt_i + \frac{1}{2}h, G_i + \frac{1}{2}K_1 h) \quad (7)$$

$$K_3 = f(dt_i + \frac{1}{2}h, G_i + \frac{1}{2}K_2 h) \quad (8)$$

$$K_4 = f(dt_i + \frac{1}{2}h, G_i + K_3 h) \quad (9)$$

Where;
G_i = initial grain size
G_{i+1} = next grain size
h = time step
T = temperature
dt_i = time

3. Experimental validation of SS316L

In order to obtain the grain size of SS316L, experiment has been conducted using quenching and deformation dilatometers machine with model DIL 805A/D as in figure 2. The chemical composition of SS316L is tabulated in table 1. The specimen as presented in figure 3 had been through heat treatment process at temperature of 1000 ºC, 1100 ºC, and 1200 ºC with the holding time of 30 s. Afterward, the epoxy has been used to mount the specimens. After 12 hours, the specimens were grinded by using forcipol grinding machine in order to get a better surface. For metallographic observation, the specimens were etched with V2A solution for 10 minutes and consequently the grain size of the SS316L was defined.

Figure 2. Quenching and deformation dilatometers.

Table 1. Chemical composition of SS316L.

%C	%Mn	%Si	%Cr	%Ni	%Mo	%P	%S
0.05	2.0	1.0	19	11	2.3	0.045	0.03

Figure 3. Specimen of SS316L.

4. Result and discussions

The grain growth of SS316L was predicted using numerical computation with Fortran programming languages by implementing the grain growth mathematical model. In this simulation, the temperature used to predict the grain size were 1000 ºC, 1100 ºC, and 1200 ºC with the initial grain size was 20 μm. Other parameters for calculating the grain size such as activation energy, time exponent and gas constant were referred to Øystein G [6]. A simulation result in terms of grain size with the absence of alloying elements is presented in figure 4. From the graph, it can be seen that the grain grows from 20 μm to 27. 80 μm at temperature of 1000 ºC, it grows from 20 μm to 40.54 μm at temperature of 1100 ºC and grows bigger at temperature of 1200 ºC which is from 20 μm to 64.28 μm.

Figure 5 presents the grain growth simulation results with the presence of growing precipitates. From the graph, it shows that the grain grows from 20 μm to 27.57 μm, 20 μm to 39.52 μm and 20 μm to 63.18 μm for the temperature of 1000 ºC, 1100 ºC, and 1200 ºC respectively. Grain growth is a thermally activated process in which the grain size increases as temperature and time are increased [3], [8], [9]. This occurs when recovery and recrystallisation are complete and further reduction in the internal energy can only be achieved by reducing the total area of grain boundary. Thus, an easy way to improve the strength of a material is to make the grains as small as possible by increasing the amount of grain boundary. Smaller grains have better ratios of surface area to volume, which means a greater ratio of grain boundary to dislocations.

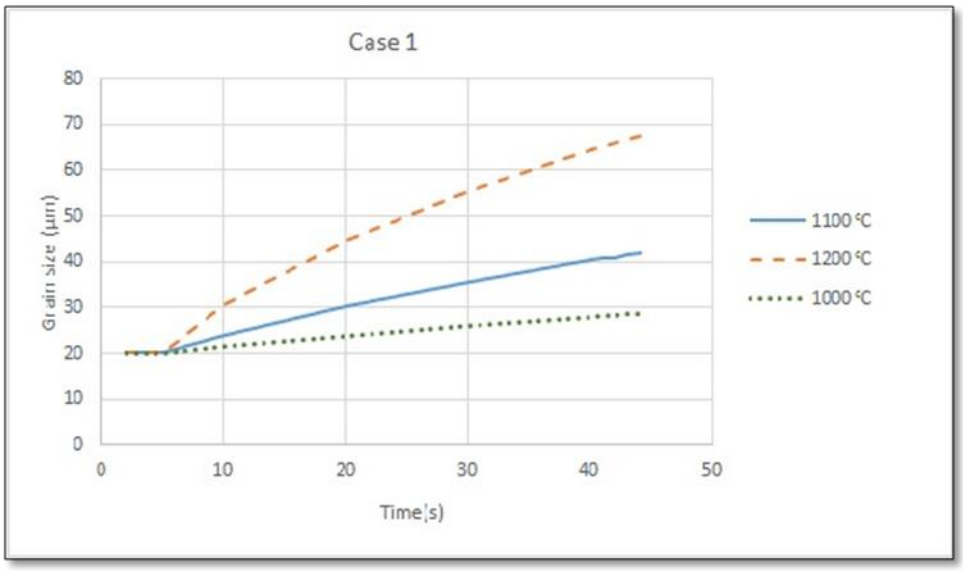


Figure 4. Grain growth with the absence of alloying elements.

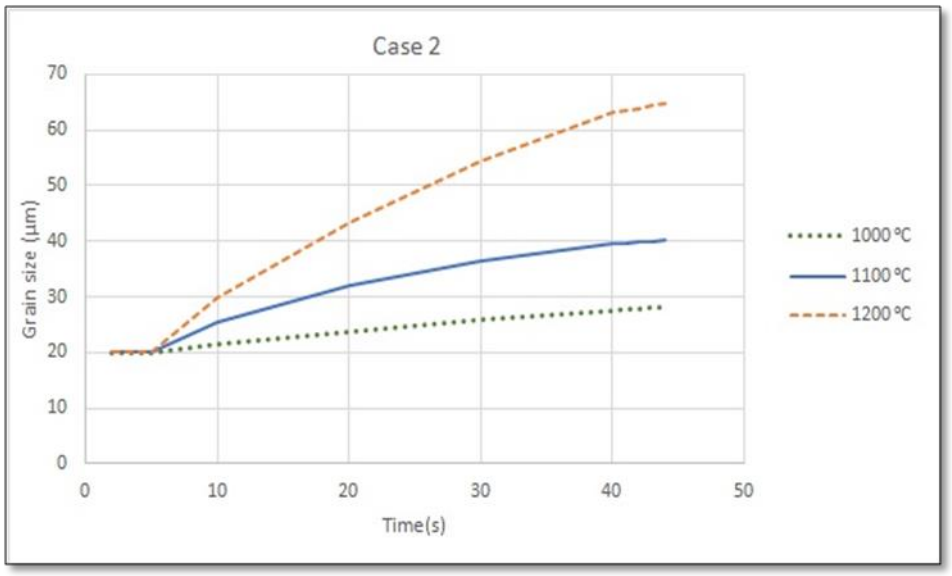


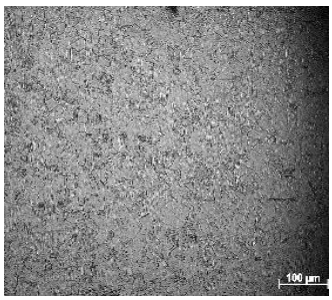
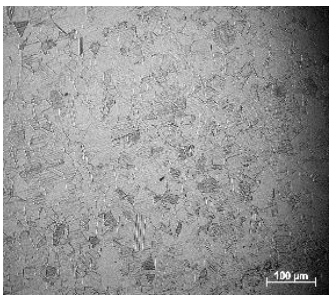
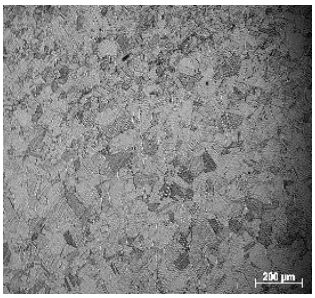
Figure 5. Grain growth with the presence of growing precipitates.

Grain growth occurs by boundary migration and the rate of boundary migration increases with driving force. The driving force for grain growth results from the decrease in the free energy of the system. The grain boundary area is the main source of energy in the austenitic microstructure. Consequently, during this process the system will evolved to reduce its grain boundary area. The larger grains will grow at the expense of the smaller ones. Microalloying elements such as vanadium, niobium and titanium have been employed in produce fine precipitation in the matrix. The austenite grain boundaries and dislocations are pinned by these precipitates, inhibiting their movement during the thermomechanical processing of steels [10]. The influence of these elements is shown by the way they delay the grain growth process and also the phase transformations, during subsequent cooling. As a result, their influence leads to fine-grained microstructures with improved the mechanical properties.

Table 2 displays the experimental result of the grain growth for SS316L. It was observed using optical microscope with 20X magnification. From the observation, it shows the grain size increases with increasing of the temperature. The grain growth is the increase of grains (crystallites) in a material at high temperature. The higher the temperature, the heating occur austenite grain size. When

the heating temperature increased it will result in increasing of the grains size formed [11]. This is due to the increase of holding time and heating temperature that will increase the activation energy of growth which will go against previous dislocations that exists on the grain boundaries, so the growth of grain boundaries is not deferred by dislocation for growing.

Table 2. Experimental results.

Temperature	1000 ºC	1100 ºC	1200 ºC
Grain size	28 μm	40 μm	63 μm
Micrograph			

Simulation and experimental results of the grain growth are depicted in Table 3. The results indicate the grain sizes increased with temperature, as predicted from the grain growth equations. An increase in temperature was found to have a larger effect on the grain size. Grain growth predicted with the presence of growing precipitates (case 2) is closed to experimental result. The approximate modified kinetic constant (Mo*) used in this simulation for the case 2 is tabulated in Table 4. The percentage error between simulation and experiment is presented in table 5. It was found out that the numerical computations of grain growth prediction are accurately correlated with the results of the experiment.

Table 3. Simulation and experimental results.

Temperature (ºC)	Grain size (μm)		
	Case 1	Case 2	Experiment
1000	27.80	27.57	28
1100	40.54	39.52	40
1200	64.28	63.18	63

Table 4. Approximate modified kinetic constant.

Temperature (ºC)	Mo* ($\mu m^2 s^{-1}$)
1000	$5000x10^9$
1100	$3000x10^9$
1200	$2000x10^9$

Table 5. Percentage error between simulation and experiment

Temperature (ºC)	Percentage error (%)	
	Case 1	Case 2
1000	0.71	1.54
1100	1.35	1.20
1200	2.03	0.29

5. Conclusion

The fundamental study on prediction of grain size growth of SS316L was conducted by using Fortran based numerical computation. The comparison between results of numerical computation and experiment show good agreement, since different modified kinetic constant (Mo*) are considered for different temperature. As further recommendation, a strategy for fitting the Mo* should be discuss before implementing this model on manufacturing application.

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