

D. Optimization of Johnson Mehl Avrami Equation Parameters for α -Ferrite to γ -Austenite Transformation in Steel Welds using a Genetic Algorithm
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Introduction

The non-isothermal Johnson-Mehl-Avrami (JMA) equation has been often used to represent phase transformation behavior in many systems involving nucleation and growth. However, the JMA equation contains three unknown parameters, i.e., the activation energy (Q), pre-exponential factor (k_0) and JMA exponent (n). At present there is no unified method to assign the values of these important parameters. Since the transformation rate is very sensitive to the values of all three JMA parameters, none of these parameters can be assumed to be known. The goal of the present work is to estimate all three parameters of the JMA equation through an inverse modeling approach. The approach involves a combination of a genetic algorithm based optimization model, a temperature field calculation model, a phase fraction calculation model and experimentally measured kinetic data.

Approach

The procedure used to estimate the three unknown JMA parameters involved a combination of numerical heat transfer and fluid flow calculations, JMA equation for nucleation and growth for non-isothermal systems, and a genetic algorithm based optimization tool that utilized a limited volume of experimental kinetic data. The experimental data consisted of phase fraction of γ -austenite measured at several monitoring locations in the heat affected zone (HAZ) of a gas tungsten arc (GTA) weld in 1005 steel. These data were obtained by an in-situ spatially resolved x-ray diffraction (SRXRD) technique using synchrotron radiation during welding. The thermal cycles necessary for the calculations were determined for each monitoring location from a well tested three-dimensional heat transfer and fluid flow model. A parent centric recombination (PCX) based generalized generation gap (G3) genetic algorithm (GA) was used to obtain the optimized values of the JMA parameters.

Results/Discussion

The temperature field in the weldment was calculated by using a well tested three dimensional numerical heat transfer and fluid flow model. The computed shape and size of the fusion zone agreed well with the corresponding experimentally determined values. Thus, the temperature field was thought to be reliable and was used in the phase transformation calculations from the non-isothermal JMA equation.

Genetic algorithm (GA) approach is a population based search technique where a population consists of many individuals. Here each individual represents a set of randomly chosen values of the three JMA parameters. To start the calculations, the initial values of these parameters were assigned as their values reported in the literature. Initially a small set of experimental data were used to check if GA can estimate all three JMA parameters from a limited volume of experimental data. The optimized values of JMA parameters estimated by GA were found to lie in the respective range of values reported in the literature. The optimized values of the three JMA parameters were not affected by the choice of the starting values of the parameters. The austenite phase fractions computed by using the optimized JMA parameters agreed well with the

corresponding experimental results showing the appropriateness of the optimized values.

The quality of the JMA parameters obtained by GA depends on the volume and accuracy of high temperature kinetic data. When the three JMA parameters were determined using all the available experimental data sets, the parameter values were found to be as follows: Q equal to 99.91 kJ/mol, n equal to 1.12, and $\ln(k_0)$ equal to 11.06. These parameters gave lower average error in austenite phase fractions than that computed from any other set of JMA parameters obtained to date, and hence these values are recommended for phase fraction calculations during transformation of α -ferrite to γ -austenite during heating of 1005 steel.

Conclusions

A genetic algorithm (GA) based model was used to estimate the parameters of the non-isothermal Johnson-Mehl-Avrami (JMA) equation, i.e., the activation energy (Q), pre-exponential term (k_0) and exponent (n) for the transformation of α -ferrite to γ -austenite during heating from a limited volume of experimental kinetic data. The austenite phase fractions calculated by using the recommended JMA parameters, i.e., Q equal to 99.91 kJ/mol, n equal to 1.12, and $\ln(k_0)$ equal to 11.06, show better fit with the experimental data than the JMA parameters reported previously on the basis of a graphical technique for estimating the values of n and k_0 assuming a fixed value of Q . Determination of all three JMA parameters by GA provides better results than those previously achieved by the graphical calculation of two of the three JMA parameters.