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Prediction of Dendritic Parameters and Macro Hardness Variation in Permanent Mould Casting of Al-12%Si Alloys Using Artificial Neural Networks

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Abstract: Aluminium-Silicon alloys are in high demand as an engineering material for automotive, aerospace and other engineering applications. Mechanical properties of Al-Si alloys depend not only on chemical composition but also more importantly on micro structural features such as dendritic alpha-aluminium phase and eutectic silicon particles. As an additive to Al-Si alloys, sodium improves mechanical properties by forming finer and fewer needles like microstructures. Thus, prediction of the macro and microstructures obtained at the end of the solidification is of great interest for the manufacturer of aluminium alloys. Neural networks are sophisticated non-linear regression routines that, when properly "trained", allow for the identification of complex relationships between a series of inputs and one or more outputs. In this paper, an approach using artificial neural networks for predicting alpha- aluminium dendritic parameters (fraction and secondary dendritic arm spacing) and macro hardness variation (Brinell hardness number) of permanent mould casting of Al-12%Si alloy is described. This approach has the advantage that complex interactions among cooling rate, solidification velocity and chill position on the amount of dendritic alpha Aluminium phase within a fixed modifier content alloy can easily be taken into account.

keyword: Dendritic parameters, BHN, Permanent Mold Casting, ANN.

1 Introduction

Aluminium-Silicon alloys are in high demand as an engineering material for automotive, aerospace and other engineering applications. Mechanical properties of Al-Si alloys depend not only on chemical composition but also more importantly on micro structural features such as dendritic alpha-aluminium phase and eutectic silicon particles. As an additive to Al-Si alloys, modifiers like strontium and sodium improve mechanical properties by forming finer and fewer needles like microstructures. Microstructures are the strategic link between materials processing and materials behavior. Microstructure control is therefore essential for any processing activity. Thus, prediction of the macro and microstructures obtained at the end of the solidification is of great interest for the manufacturer of aluminium alloys.

During the last 40 years, major advances have been made towards an increased understanding of the effects of heat and mass transfer on the microstructure evolution. Recent mathematical and computational advances for the analysis of fluid flow and heat transfer during the casting process have fashioned a number of researches focusing on several aspects of modeling and simulation of solidification microstructures. Hence, deterministic and stochastic approaches are available for predicting cast microstructure and thus to estimate mechanical properties of the cast component. The deterministic approach takes nucleation and growth into account while solving energy and solute conservation equations in the casting-mold domain. These macro-micro models usually yield information on grain size and dendrite arm spacings at different locations within the casting. These models use a variety of computer modeling strategies like Finite Element Method (FEM), Boundary Element Method (BEM), Finite Difference Method (FDM), Control Volume Method (CVM) and their coupled algorithms to determine the desired combination of thermal parameters (a quality of index or criteria functions).

With the advent of powerful computers, with the increased knowledge gained from experimental observations, with the advent of new numerical techniques (phase field, cellular automata, granular methods, etc.) and with the development of new approaches (hot tearing, two phase method, etc.), modeling of solidification processes at the macroscopic scale has become a standard practice in industry, in particular in continuous casting processes. Indeed, commercial software packages are available for the modeling of heat and fluid flow, as well

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as for stress-strain calculations and to deal with common defects like macro segregation. Modeling of macro segregation is still a critical issue as it can have different origins: convection, solidification shrinkage, grain movement/sedimentation, deformation of the mushy zone. Recently, significant studies have been made in modeling microstructure & microporosity formation [Rappaz (2004)] and to find the impact of different convective effects like inlet flow, thermal and solutal buoyancy flow on the formation of macro segregations [Ludwig et al. (2005)]. As an example, Ludwig et al. (2005) have stated that a higher permeability increases the possibility of fluid movement in the mushy zone which goes hand in hand with more pronounced macrosegregations in the casting.

Along these lines, the reader may also consider the recent review by Lappa (2005) where a variety of convective effects potential affecting the microstructure of an alloy were considered together with a critical discussion of possible related numerical approaches. In general, the mechanical behaviors of castings are dependent on various factors such as the grain size, secondary dendritic arm spacing, alloy composition, which in turn depend on aspect ratio, solidification rate, cooling rate, volume to surface area ratio (V/A) etc. From solidification analyses carried out using advanced commercial codes like FLUENT, ProCAST CalcoSOFT and MagmaSoft, it has been understood that velocity, pressure and temperature fields across casting and mould domain can critically influence the structure formation, grain orientation and grain size (usually quantified in terms of dendritic arm spacings).

Unfortunately, the aforementioned mathematical approaches and models are often limited in their ability to account for the effects of these variables because of the restrictive and at times incorrect assumptions.

Since, as illustrated before, the effect of heat and mass transfer on the formation of dendritic arm spacing is very a complex phenomenon and existing numerical techniques are often inadequate, this study introduces a new simulation strategy (artificial neural networks (ANN)) largely based on experimental data.

Artificial Neural networks are sophisticated non-linear regression routines that, when properly "trained", allow for the identification of complex relationships between a series of inputs and one or more outputs. Because of this ability to learn and generalize interactions among many variables, ANN technology has potential in modeling the material behavior and especially for nonlinear modeling applications. In this work, an approach using artificial neural networks for predicting properties of dendritic alpha-Aluminium (fraction and secondary dendritic arm spacing) and macro hardness variation (Brinell hardness number) of permanent mould casting of Al-12%Si alloy is described. This approach has the advantage that complex interactions among cooling rate, solidification velocity and chill position on the amount of dendritic alpha aluminium phase within a fixed modifier content alloy can easily be taken into account. In order to obtain training pairs for ANN simulation studies, experiments were conducted.

2 Experimental studies

Aluminium alloys with silicon as a major alloying element, represent a class of alloys, which provides the most significant part of all shaped castings manufactured. This is mainly due to the outstanding effect of silicon in the improvement of casting characteristics. An optimum range of silicon content can be assigned to casting processes. For slow cooling rate processes (sand, plaster, investment) the range is 5–7 wt.%, for permanent moulds 7–11.5 wt.% and for die-castings more than 12 wt.% [Peres, Asiqueira and Goncia (2004)]. The columnar growth was observed to prevail throughout the casting for cooling rates higher than a critical value, which is dependent on the alloy system. It is well established that under most conditions of solidification, the dendritic morphology is the dominant characteristic of the microstructure of off-eutectic alloys. Fine dendritic microstructures in castings, characterized by the dendrite arm spacing, are recognized to yield superior mechanical properties to coarser ones, particularly when considering the tensile strength and ductility. The improvement in mechanical properties are generally attributed through the variations of the morphology and size of the eutectic silicon phase particles .It is worth noting, however, that at the same time when eutectic silicon particles changes from acicular to fiber, the amount, morphology and size of dendritic α-Al phase are varying too. The contribution of these to the improvement of the mechanical properties has not been paid more attention.

Much research has been devoted to the definition of the factors affecting microstructures and the fineness of the dendritic structures [Chen and Wu (2003), Ai and Xu (2003)]. It is well known that grain refining is beneficial to mechanical properties. However, no final conclusion has yet been reached on whether the transition of dendritic α-Al phase from longer column morphology to a fine equated one results in improved mechanical properties in near eutectic Aluminium silicon alloy. From the point of view of microstructure control, it is necessary to investigate the correlation between mechanical properties and dendritic α in near eutectic Al-Si alloy. The main theme of present study is to evaluate the effect of cooling rate, solidification velocity, size and shape of sodium modified aluminium silicon alloy on secondary dendritic arm spacing, dendritic fraction and Brinell hardness value and to simulate these variables using neural networks. Methodology for present investigation is explained with a flow process diagram shown in Fig. 1.

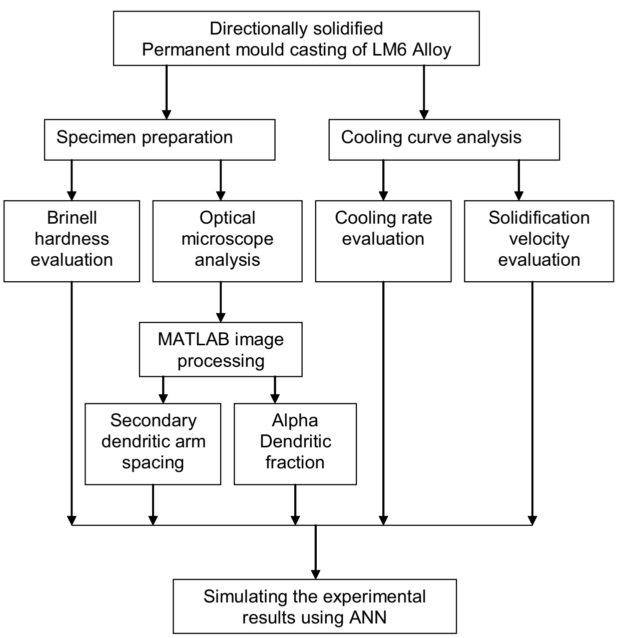


Figure 1 : Flow process diagram for experimental and simulation studies.

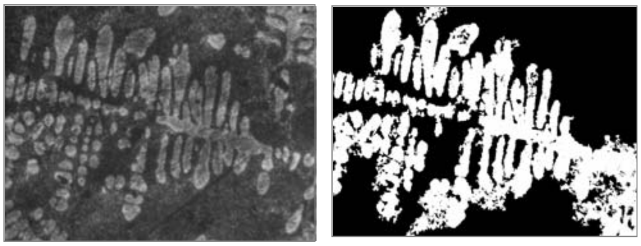
Directional solidification of commercially available LM6 (Al-12%Si) alloy modified with 0.015 % sodium is performed with cylindrical dies. The cooling direction is made opposite to the direction of gravitational force by using an appropriate die with insulated lateral surfaces and water circulating jacket at its bottom face. Temperature history for a fixed time interval is recorded using a data acquisition system (Agilent Bench Link Data Logger) with thermocouples (K-type) placed at different locations in the die. Cooling curves thus obtained are used to evaluate cooling rate and growth rate. Metallurgical specimens for different locations of solidified casting are prepared and micrographs are obtained using scanning electron microscope. Micrographs obtained from optical microscopic studies are processed using MATLAB to find out fraction of α-Al phase solidified. Data obtained from the above analysis are used to train a feed forward back propagation artificial neural network in which training input variables are cooling rate, solidification velocity & position from chill and output values are dendritic alpha-aluminium fraction, secondary dendritic arm spacing & Brinell hardness number.

2.1 Generation and Collection of Experimental Data

The results of experimental thermal analysis have been used to determine the velocity of the liquidus isotherm and the cooling rate. The dendritic morphology is dependent on solidification thermal parameters such as the liquidus isotherm velocity and cooling rate, all of which vary with time and position during solidification. It would be difficult to measure accurately these parameters at each desired positions using thermocouples. In order to determine parameters more accurately, the raw data are fitted numerically in order to provide interpolations that are more accurate. The thermocouples readings have been used to generate a plot of position from the solid liquid metal interface as a function of time corresponding to the liquidus front passing by each thermocouple. A curve fitting technique on these experimental points has generated a power function of positions a function of time. The derivative of this function with respect to time has yielded values for tip growth rate or solidification velocity. The cooling rate was determined by considering the thermal data recorded immediately after the passing of the liquidus front by each thermocouple.

The dendrite arm spacings were sufficiently distinct to make reasonably accurate measurements along the casting length. Fig.2. shows RGB image and binary image of micrographs used to find out alpha dendritic aluminium fraction and secondary dendritic arm spacing with MATLAB image processing technique.

The RGB Micrograph is converted to grey scale and after adjusting the intensity uniformly, a binary image is created from grey scale image. Now binary matrix can be obtained and secondary dendritic arm spacing is evaluated using Euclidian distance method by considering the



(a) (b)

Figure 2 : (a) Micrograph (RGB image) obtained using optical microscope. (b) Binary image of micrograph after image processing.

pixels of known coordinates, at the centers of a dendritic arms. Counting the number of ones (f) in the binary image matrix and total number of ones and zeros (μ) the matrix, the dendritic fraction is given by f/μ. After the microscopic studies, metallurgical specimens of different locations in solidified casting were used for macro hardness (BHN) evaluation. Data collected from a set of experimental studies for ANN simulation studies is shown in Appendix -A.

3 ANN simulation studies

Over the last few decades, important advances have been made in our fundamental understanding of artificial neural networks and its application in various fields of science and engineering [Zurada (1997), Kartalopoulos (2000), Uhrig (2003), and Haykin (2004)]. Artificial neural networks (ANN) have been widely used for many areas, such as control, data compression, forecasting, optimization, pattern recognition, classification, speech, vision, etc. The use of the ANN for modeling and prediction purposes is increasingly becoming popular in the last decades [Victorbabu, Joseph and Sudarsan (2005), Zupan (1994), Cherian, Smith and Midha (2000)]. ANN has been trained to overcome the limitations of the conventional approaches to solve complex problems that are difficult to model analytically.

3.1 The ANN Model

The following matters are important in the design and training of neural networks: (i) architecture of the neural network; (ii) training algorithm; and (iii) transfer function. The term "architecture of the neural network" refers to the number of the layers in the neural network and the number of the neurons in each layer [Chester (1990), Villiers and Barnard (1992)]. The structure of ANN model used for the present work is shown in Fig. 3.This multi layer feed forward network consist of four layers. One input layer two hidden layers and one output layer. Input layer has three neurons and the two successive hidden layers have three and eight neurons respectively. Output from the networks is given by three neurons each give secondary dendritic arm spacing, dendritic fraction and Brinell hardness values respectively. Considering the input neurons as inactive, active layers of neurons are named as input layer, hidden layer and output layer. The input layer and the output layer are determined by the numbers of input and output parameters respectively. In order to find the optimal architecture, the number of neurons and hidden layers are selected on the basis of trial and error method.

There are many different training algorithms. In order to achieve the best result, different training algorithms were developed by various researchers [Math Works Inc. (2002)], which includes Batch Gradient Descent, Batch Gradient Descent with Momentum, One-step-secant, Scaled Conjugate Gradient, Resilient Back propagation, Polak-Ribiere Conjugate Gradient, Fletcher-Powell Conjugate Gradient, Powell-Beale Conjugate Gradient, Variable Learning Rate and Levenberg–Marquardt. From which the Levenberg–Marquardt training algorithm is used in this study. The transfer function transforms the neuron input value into the output value. For this simulation studies, neural network linear transfer function was used in the output layers. In the input layer and hidden layer tangent sigmoidal transfer function was employed. Network configuration for training Levenberg-Marquardt algorithm is furnished in Tab.1.

3.2 Levenberg Marquardt Algorithm

There are essentially two types of ANN learning models-supervised learning and unsupervised learning. With supervised one, input is presented to the network along with the desired output and the weights are adjusted so that the network attempts to produce the desired output. The weights, after training, contain meaningful information whereas before training they are random and have no meaning. Neural networks that do not rely on the use of target data are trained using unsupervised learning. As mentioned earlier, there are different learning algorithms. A popular algorithm is the back-propagation algorithm,

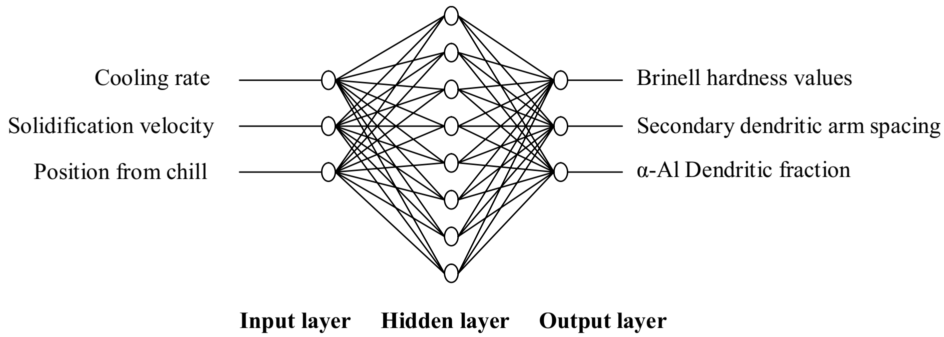


Figure 3 : Architecture of the artificial neural network model used in the present study.

1	Type of architecture	Multi layer feed forward
2	No of hidden layers	2
3	No of Neurons	17 (*3*-3-8-*3*)
4	Training Function	Levenberg Marquardt
5	Activation Function	Tan -sigmoidal and linear
6	No of training sets	10
7	No of Testing sets	5
8	Maximum Epochs	1395
9	Error Goal	0.0000001

Table 1 : Network configuration for training Levenberg-Marquardt Algorithm.

which have different variants. Back-propagation training algorithms gradient descent and gradient descent with momentum are often too slow for practical problems because they require small learning rates for stable learning. In addition, success in the algorithms depends on the user dependent parameters such as learning rate and momentum. Several high performance algorithms that can converge from ten to one hundred times faster than above algorithms were developed. These algorithms use heuristic or standard numerical optimization techniques. Faster algorithms such as conjugate gradient, quasi-Newton, and Levenberg–Marquardt use standard numerical optimization techniques.

A mathematical description of the LM neural network-training algorithm was presented by Hagan and Menhaj [Hagan and Menhaj (1994)]. The LM algorithm was originally designed and to serve as an intermediate optimization algorithm between the Gauss–Newton (GN) method and gradient descent algorithm, and address the limitations of each of those techniques. The GN algorithm has quadratic convergence properties that make it very fast. However, the convergence of this method depends, highly, on the choice of the initial weight values. Since, in real-world problems, the prediction of an appropriate set of initial values is not always possible, the GN method is impractical for many applications. Unlike the GN algorithm, the performance of the gradient descent algorithm is less dependent on the initial choice of weights. However, since the gradient-descent an algorithm approach the minimum in a linear manner, its speed of convergence is normally low and, thus, does not always possess adequate convergence properties.

The LM algorithm, which combines the positive attributes of GN and gradient descent algorithms, is suitable for many real-world applications [Bulsari and Saxen (1992)]. The LM algorithm possesses quadratic convergence (approximates the GN method) when it is in the vicinity of (but not too close to) a minimum. LM uses gradient descent to improve on an initial guess for its parameters and transforms to the GN method as it approaches the minimum value of the cost function. Once it approaches the minimum, it transforms back to the gradient descent algorithm to improve the accuracy. Since its creation, researchers have used the LM algorithm for curve fitting. Due to its desirable convergence capabilities, in many optimization applications, the LM method is usually preferred over many other optimization techniques.

4 Results and Discussions

Temperature history for a fixed time interval of 0.01 seconds is recorded using a data acquisition system (Agilent

Bench Link Data Logger) with K-type thermocouples (measuring range of 300-1000 degree centigrade) placed at 10 different locations in the die. Cooling curves thus obtained at these locations are used to evaluate cooling rate and growth rate. Logarithmic relationship was established between cooling rate (dT/dt) and position (x) as well as between position (x) and time (t) as shown in equation (1) and (2). Metallurgical specimens for different locations of solidified casting are prepared and micrographs are obtained using scanning electron microscope. Micrographs obtained from optical microscopic studies are processed using MATLAB to find out fraction of α-Al phase solidified and secondary dendritic arm spacings (SDAS). The average value of dendritic fraction and SDAS obtained are 0.31 and 0.139 respectively. For each specimen Brinell Hardness Number (BHN) was evaluated. BHN ranging from 29 to 42 varied according to the solidification velocity along the vertical axis of castings. Data obtained from image processing analysis are used to train a feed forward back propagation artificial neural network in which training input variables are cooling rate, solidification velocity & position from chill and output values are dendritic alpha-aluminium fraction, secondary dendritic arm spacing & Brinell hardness number.

$$log(dT/dt) = -0.26 log(x) + 0.65 \tag{1}$$

$$log(x) = 2.2 log(t) - 0.33 \tag{2}$$

Multi layer feed forward neural network with Levenberg Marquardt learning algorithm was developed for predicting α-Al dendritic parameters and macro hardness variations in casting. Neural network toolbox available in MATLAB was used to construct afore mentioned model. A MATLAB script was written which loaded the data file, trained and validated the networks and saved the model architecture and performance in a file ready for use in Microsoft Excel. A major portion of the data set obtained through experimentation was used for training the network and the rest was utilized for validation of the model. From the fifteen data set shown in table 1, five were selected randomly for test purpose. The neural network model was tested by: (i) linear regression between NN predictions and new experimental data; (ii) statistical analysis of the error of NN predictions; and (iii) direct comparison of NN predicted and experimental data.

Learning or training involves modifying the connection weights until the network is capable of reproducing the target output within some specified error margin. The connection weights are adjusted such that a mean squared error is minimized. This is done by continually changing the values of the weights in the direction of the steepest descent with respect to the error. Training takes place in an iterative fashion. Each iteration cycle involves a forward step followed by a back-propagation step to update the connection weights. Bias values, which controls the activation function while learning process and helps neurons to be flexible and adaptable. Hence final bias plots for three layers are shown in Fig. 4.

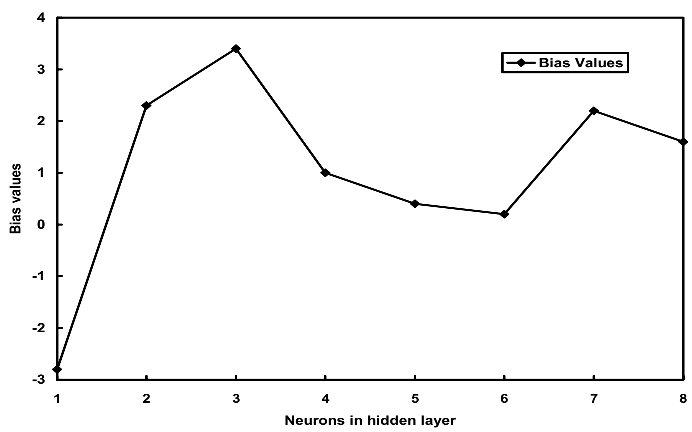
Fig. 5 & Fig. 6 show the comparison between experimental and ANN predicted results with present network model. From the above comparative study, overlapping of data points indicated a very good performance of the model used. Also, it can be observed that Brinell hardness number has a direct relation with solidification velocity and secondary dendritic arm spacing has an inverse relation with solidification velocity. Inference can be made that, Brinell hardness values have an inverse relation with secondary dendritic arm spacing and direct relation with dendritic fraction.

Absolute error v/s sample number (Fig. 7.) also indicates the efficiency of the model, which can be used for further simulations and predictions of different correlations and phenomena during Aluminium –Silicon alloy casting process.

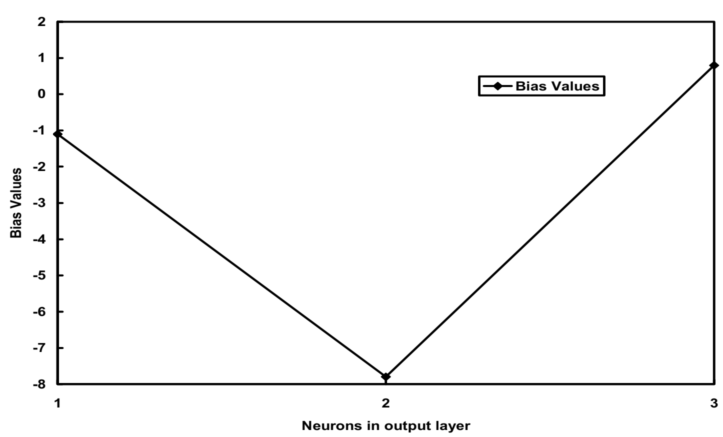
5 Conclusions

From neural networks simulation studies using experimental data, it was observed that secondary dendritic arm spacing has inverse relation with cooling rate and solidification velocity. Also, Brinell hardness values indicated an inverse relation with secondary dendritic arm spacing and direct relation with dendritic fraction. ANN predicted results were found to be in good agreement with experimental data. Hence, the ANN approach used in this study is appropriate to predict the α-Al dendritic parameters and Brinell hardness variation across the casting length with available input data like solidification velocity, cooling rate and position from the chill. Thus, ANN can be used as a good tool for microstructure and mechanical property simulation, which can be employed successfully by using the MATLAB Neural Network Toolbox. In this work, one-dimensional solidification

(a)



(b)



(c)

Figure 4 : Bias plot of ANN model: (a) Input layer (b) Hidden Layer (c) Output Layer.

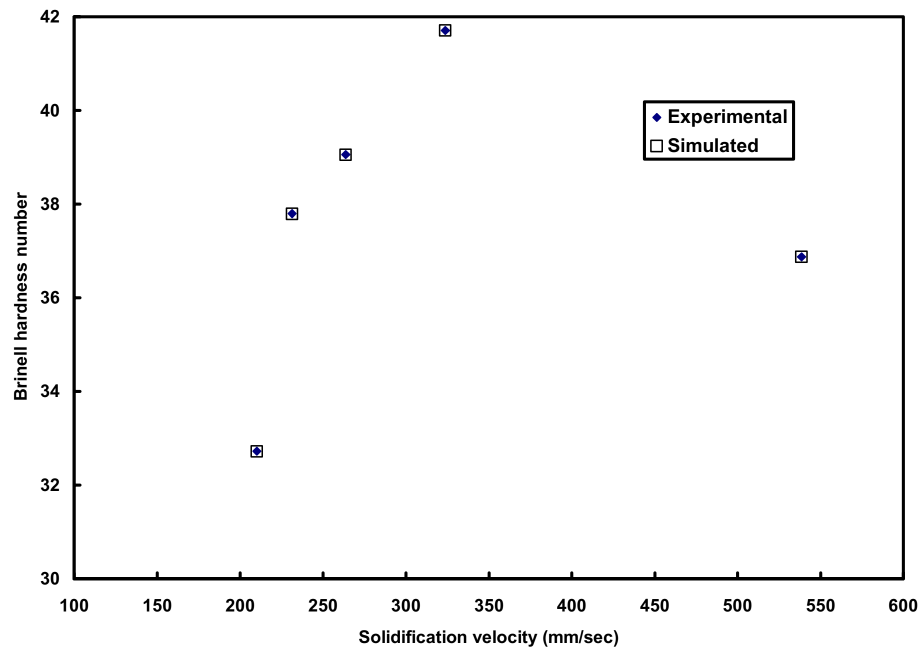


Figure 5 : Variation of Brinell hardness number with solidification velocity for experimental and ANN simulation study.

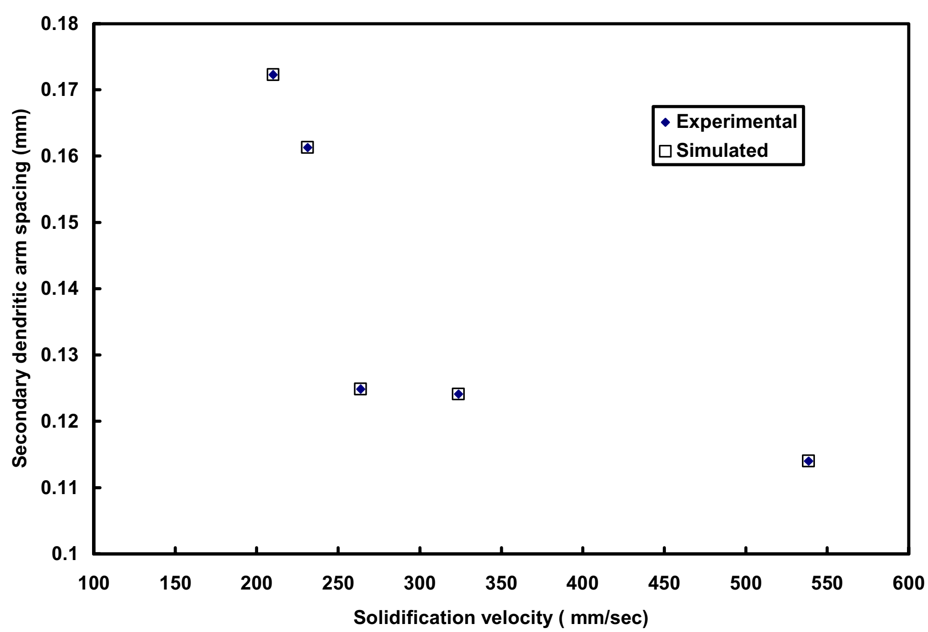


Figure 6 : Variation of secondary dendritic arm spacing with solidification velocity for experimental and ANN simulation study.

with, only a few parameters affecting the microstructure were considered. Thus, simulation studies may be extended to predict the influence of other parameters such as composition, casting modulus (V/A ratios) and other thermo-mechanical properties.

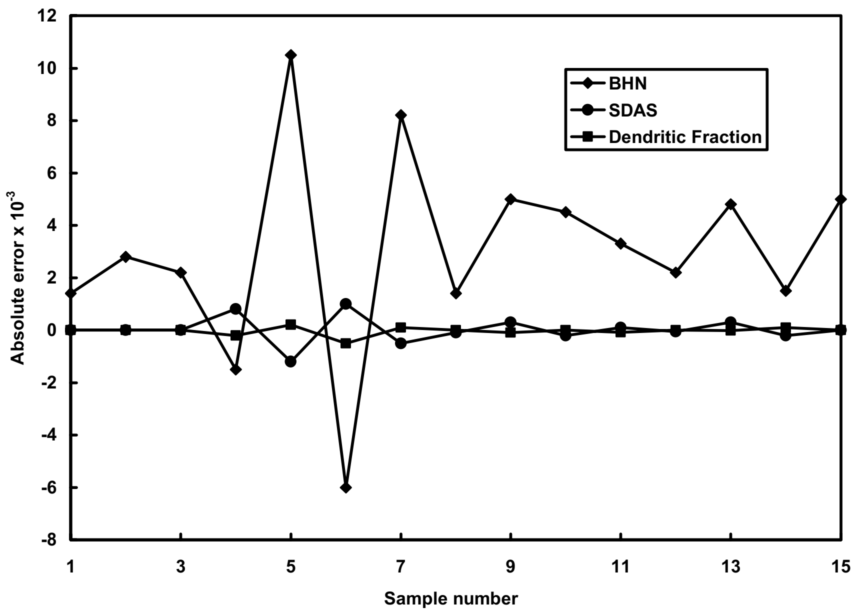


Figure 7 : Absolute error of output variables versus sample number of training set.

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Appendix A: A set of Training Data Obtained From Experimental Studies.

Sl.No.	Position cm	Solidification velocity (cm/sec)	Cooling rate (cm/sec)	Dendritic fraction	Dendritic arm spacing (mm)	Brinell hardness (250kg Ball)
1	1.3000	53.8564	4.1099	0.2890	0.1140	36.8748
2	2.6000	41.7599	3.4321	0.3050	0.1088	40.9078
3	3.9000	35.9860	3.0887	0.3160	0.1255	39.5230
4	5.2000	32.3803	2.8661	0.3200	0.1241	41.7037
5	6.5000	29.8343	2.7046	0.3170	0.1081	38.6967
6	7.8000	27.9033	2.5793	0.2970	0.1100	37.6293
7	9.1000	26.3686	2.4780	0.3010	0.1249	39.0576
8	10.4000	25.1075	2.3934	0.3140	0.1180	37.1085
9	11.7000	24.0453	2.3213	0.3450	0.1384	35.3389
10	13.0000	23.1333	2.2585	0.3390	0.1613	37.7947
11	14.3000	22.3381	2.2033	0.3220	0.1365	38.4227
12	15.6000	21.6360	2.1540	0.3030	0.1384	29.9594
13	16.9000	21.0097	2.1096	0.3090	0.1723	32.7234
14	18.2000	20.4460	2.0694	0.3270	0.1724	31.1962
15	19.5000	19.9348	2.0326	0.3370	0.1557	32.6801