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A new modeling of electrical resistivity properties of ZnFe alloys using genetic programming

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The electrical resistivity of electrodeposited $Zn_{1-x}Fe_x$ alloys has been formulated as a function of temperature between the 10 and 330 K for an iron concentration x from 4 to 39 using Genetic Programming (GP) as a new tool. There are no well established formulations for predicting electrical resistivity properties of electrodeposited alloys related to film composition, electrodeposition bath composition and corrosion potential. Therefore, the objective of this paper is to develop robust formulations based on the experimental data and to verify the use of GP for generating the formulations for electrical resistivity of electrodeposited ZnFe alloys. To generate databases for the electrical resistivity formulations, training and testing sets in total of 260 samples were selected at different temperatures and ratios of components. The training and testing sets consisted of randomly selected 208 and 52 for the electrical resistivity. The paper showed that the GP based formulation appeared to be in line with the experimental data and was found to be quite reliable.

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1. Introduction

Zinc and zinc alloys are widely used to electroplate steel to provide corrosion resistance, mainly in the automobile industry. The corrosion resistance of a pure zinc coating on steel is not satisfactory and unacceptable under severe atmospheric conditions [1]. A possibility to enhance corrosive strength is alloying. It has been observed that when alloyed with irongroup metals, zinc shows better corrosion resistance than the pure metal [2-5]. However, there has been much interest in the use of electrodeposited zinc alloys for similar purposes. In particular, zinc–iron coatings have attracted considerable attention in the automotive industry because they combine high corrosion resistance with excellent mechanical performance and improved capability for organic coatings [6-8]. Zinc deposits offer decorative appeal at low cost, too. Zinc alloys also offer an important eco-friendly alternative to toxic cadmium coatings.

Different techniques have been used to produce heterogeneous alloys although the structure and therefore properties depend closely on the preparation techniques [9-12]. Electrodeposition, which is a relatively cheap technique, is an alternative method to other complex and sophisticated ones such as evaporation, sputtering, Molecular Beam Epitaxy and it is also suitable for producing multilayer and immiscible metal combinations by control of the electrodeposition variables. We previously reported an experimental study on the crystal structure and electrical conduction properties of $Zn_{1-x}Fe_x$ (x=4, 22, 31, 39) alloy films produced by electrodeposition and the effect of Fe addition on the electrical resistivity and corrosion properties [6].

Influence of additional element on electrical resistivity properties is well known in the literature. However, there exist no explicit formulations for estimating the electrical resistivity properties of electrodeposited alloys related to magnetic component like iron. For this purpose, empirical formulations were proposed by applying the genetic programming for prediction of electrical resistivity of ZnFe alloys.

2. Experimental details

The electrodeposition solutions were prepared using distilled water and laboratory reagent-grade chemicals. The bath solution was prepared as described elsewhere. [6]. The resistivity measurements were done using the traditional four-point probe method. The thermal voltage effect was eliminated by taking the average of voltage readings with two reverse currents at each temperature. Each sample was measured several times to make sure the obtained data was reliable. A closed-cycle helium cryostat (Leybold RW2) was used to control the sample temperature with a sensitivity of ±0.2 K. Sample dimensions for the resistivity measurements were 1 mm · 4 mm · 4 · 10–4 mm.

3. Genetic programming

Genetic programming was proposed by Koza [13] to automatically extract intelligible relationships in a system and has been used in many applications such as symbolic regression [14, 15] and classification [16, 17]. A schematically overview of genetic programming is given in Fig. 1.

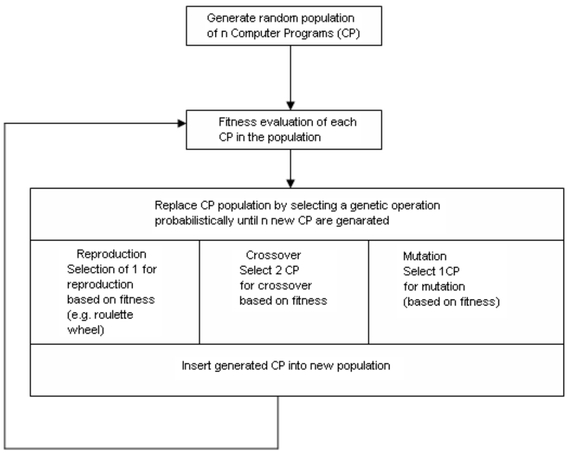


Fig. 1. Schematically overview of GP [18].

Koza [13] explains the flowchart of GP in four main steps:

1. Generate an initial population of random compositions of the functions and terminals of the problem (computer programs)
2. Execute each program in the population and assign it a fitness value according to how well it solves the problem.
3. Create a new population of computer programs.
   - Copy the best existing programs (reproduction)
   - Create new computer programs by mutation
   - Create new computer programs by crossover (sexual reproduction)
   - Select an architecture-altering operation from the program stored so far.
4. The best computer program that appeared in any generation, the best solution so far, is designated as the genetic result of genetic programming.

The GP creates a population of computer programs with a tree structure. In this study, empirical models are used for prediction of electrical resistivity properties of electrochemically deposited ZnFe alloys. Randomly generated programs are general and hierarchical, varying in size and structure. GP's main goal is to solve a problem by searching through highly fit computer programs (in the space of) for all possible solutions. This aspect is the key for finding near global optimum solutions by keeping many solutions that may potentially be close to minima (local or global). The creation of initial population is a blind random search of the space defined by the problem. The output of the GP is a program rather than a quantity [19].

3.1 Brief overview of gene expression programming

Gene-Expression Programming (GEP) is a natural development of GP and it was invented by Ferriera [20]. GEP evolves computer programs of different sizes and shapes encoded in linear chromosomes of fixed length. GEP algorithm begins with the random generation of the fixed-length chromosomes of each individual for the initial population. Chromosomes and expression trees (ETs) are the two main parameters of GEP. The process of information decoding (from the chromosomes of the ETs) is called translation, which is based on a set of rules. The genetic code is very simple where there exist a one-to-one relationship between the symbols of the chromosome and the function or terminal they represent. GEP program utilizes two different languages: the language of genes and the languages of ETs. A noteworthy advantage of this is that it permits the user to infer exactly the phenotype, when given the sequence of a gene and vice versa. This is called Karva notation [21]. A typical program representing the expression $(((d3+d5)+d4)/d_2)*(d_2-d_1)$ is shown in Fig. 2. Fig. 3 shows tree structure for electrical resistivity of ZnFe alloys.

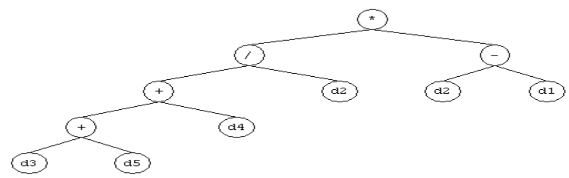


Fig. 2. A typical tree structure for $(((d3+d5)+d4)/d_2)*(d_2-d_1)$.

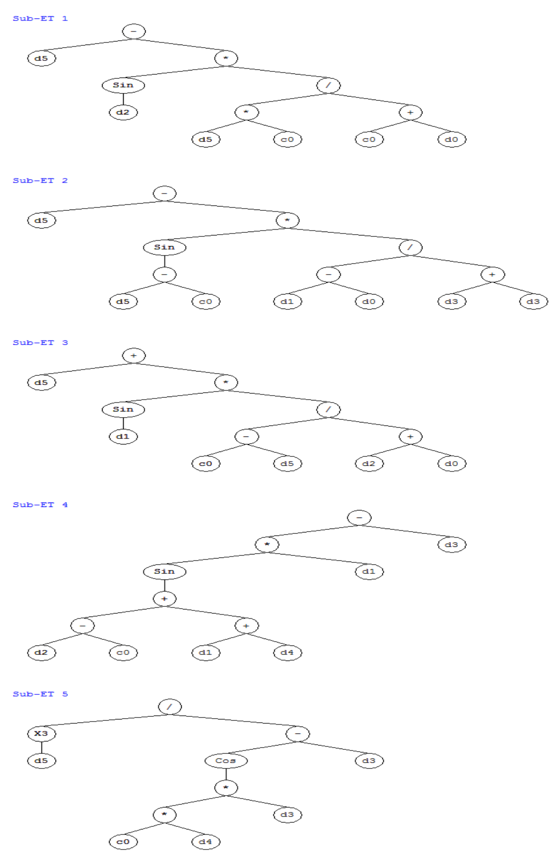


Fig. 3. Tree structure for electrical resistivity of ZnFe alloys.

4. Application of genetic programming (GEP)

The database built in the experimental part was used for the modeling of the electrical resistivity properties of ZnFe alloys. The major task herein is to define the hidden function connecting the input variables (X1, X2, X3, X4, X5 and X6) and output Y1. The expected empirical models may be written in the form of following equation

$$Y_1 = f(X1, X2, X3, X4, X5, X6) \tag{1}$$

The functions obtained by GEP will be used for estimating the relationship between film components and electrical resistivity characteristic of ZnFe alloys. The variables used in the GEP models were presented in Table 1.

Table 1. The variables used in model constructions.

Code	Input variable	Output
X1	Temperature (T) (as Kelvin)	Y1 Electrical resistivity (ρ_0) ($\mu\Omega$cm)
X2	% Zn content in the electrolyte ($E_{zn\%}$)	
X3	% Fe content in the electrolyte ($E_{Fe\%}$)	
X4	% Zn content in the film ($F_{Zn\%}$)	
X5	% Fe content in the film ($F_{Fe\%}$)	
X6	Corrosion Voltage (V_{Cor})	

In order to construct empirical models and show the generalization capability of GEP, the database produced in the experimental part is subdivided into two sets, namely training and test, respectively. The empirical formulations were developed based on the former while the latter was employed to test the proposed models so as to measure their generalization capabilities [21]. Of all 260 alloys, the training and testing sets consisted of randomly selected 208 and 52 mixtures, respectively. It must be kept in mind that the proposed empirical equations are valid for the ranges of training set given in Table 2. The parameters used within the proposed empirical models were given in Table 3. Even though there might be various combinations of GEP parameters, running the GEP algorithm for all of them requires very long computational time. Therefore, the GEP parameters were selected intuitively to investigate the performance of GEP models so as to predict the electrical resistivity of ZnFe alloys.

Table 2. Ranges of experimental database used in the proposed GEP models.

Code	Parameter	Min	Max
X1	Temperature (K)	10	330
X2	% Zn content in the electrolyte ($E_{Zn\%}$)	50	80
X3	% Fe content in the electrolyte ($E_{Fe\%}$)	20	50
X4	% Zn content in the film ($F_{Zn\%}$)	61	96
X5	% Fe content in the film ($F_{Fe\%}$)	4	39
X6	Corrosion Voltage (V_{Cor})	-1,14	-1,054
Y1	Resistivity (ρ_0)	0,77	6,085

Table 3. GEP parameters used for proposed models.

p1	Number of generation	46190
p2	Function set	+,-,*,/,$\sqrt{}$, Power, Exp,x^2, x^3, $\sqrt[3]{x}$, Sin(x), Cos(x)
p3	Number of Chromosomes	70
p4	Head size	8
p5	Number of genes	5
p6	Linking function	Multiplication
p7	Mutation rate	0.044
p8	Inversion rate	0.1
p9	One-point recombination rate	0.3
p10	Two-point recombination rate	0.3
p11	Gene recombination rate	0.1
p12	Gene transposition rate	0.1

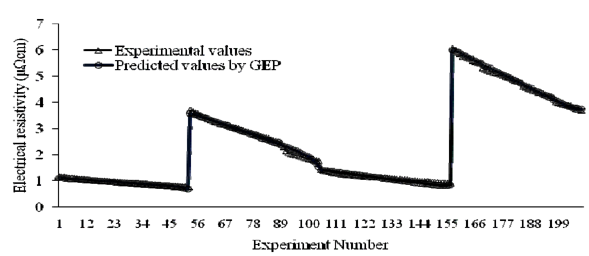
The functions generated for the best solutions by GEP algorithm to estimate the electrical resistivity predictions of electrodeposited alloys were presented in Equation 2.

$$\rho_0 = \left(V_{Cor} - SinE_{Fe\%} * \left(\frac{2T}{(2+T)}\right)\right) * \left(V_{Cor} - \left(Sin(V_{Cor} - 8) * \left(\frac{E_{Zn\%} - T}{2F_{Zn\%}}\right)\right)\right) * \left(V_{Cor} + SinE_{Zn\%} * \left(\frac{3 - V_{Cor}}{E_{Fe\%} + T}\right)\right) * \left(Sin((E_{Fe\%} - 9) + (E_{Zn\%} + F_{Fe\%})) * E_{Zn\%} - F_{Zn\%}\right) * \frac{V_{Cor}^3}{Cos(9 * F_{Fe\%} * F_{Zn\%}) - F_{Zn\%}} \tag{2}$$

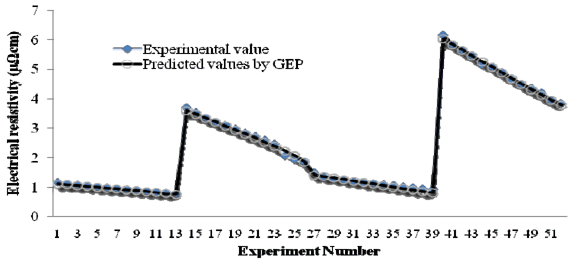
5. Performance of empirical models

Predicted values achieved through the proposed GEP formulations are compared with the experimental results for the electrical resistivity in Fig. 4. It was observed in Fig. 4 that the proposed GEP formulation for electrical resistivity of ZnFe alloys is able to follow closely the trend seen in the experimental data within both train and test sets.

It was observed in Fig. 4 that the proposed model for the electrical resistivity provided consistent predictions for both data sets.



(a)



(b)

Fig. 4. Evaluation of experimental and predicted electrical resistivity (a) Train set; (b) Test set.

The figures showed clearly that there was a clear distinction between the predicted and the actual values when the model was applied to the test set. However, this model conformed well to the experimental values in the train set.

Statistical parameters of test and training sets of GEP formulations are given in the Table 4, where R corresponds to the coefficient of correlation; MSE is the mean square error, RMSE is the root mean square error; MAE is the mean absolute error. As can be seen in Table 4, correlation coefficient of the test set of empirical model is higher than correlation coefficient of the training set.

Table 4. Statistical parameters of GEP formulations.

Properties	Set	MSE	RMSE	MAE	Correlation coefficient (*R*)
Electrical resistivity	Train	0.003583	0.059864	0.045165	0,999388
	Test	0.003602	0.060018	0.044653	0,999412

6. Conclusions

This paper presents a new and efficient approach for developing empirical formulations of electrical resistivity properties of electrodeposited ZnFe ternary alloys. The presented genetic programming approach for modeling the electrical resistivity properties of ZnFe alloys strongly differs from the conventional methods, since it does not use strict mathematical rules and does not derive equations in a rational human way of thinking.

The proposed empirical formulations are based on a comprehensive experimental study.

Because of the high precision of the models developed by the GEP approach leads to reduction of the costs of product development. The proposed GEP formulations suggested acceptable agreement with the experimental results. To the knowledge of the authors, there exists no explicit formulations for predicting the electrical resistivity properties of electrodeposited ZnFe alloys in the literature. Therefore, the proposed explicit formulations may be employed in the prediction of the electrical resistivity properties considered in this study.

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