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Research Paper

Modelling Dependency of the Steady-State Grain Size on the Stacking Fault Energy in Severely Plastic Deformed Materials

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ABSTRACT

In the present work, a computer-based method is proposed to investigate the relationship between the steady-state grain size (ds) and stacking fault energy (SFE) in severely plastic deformed (SPDed) materials. The stacking fault energy, γ, plays an important role in determining the mechanical properties of face-centered cubic (fcc) metals. A number of models have been proposed to show this role. These models have several shortcomings, including complex computational variables, data constraints and small computational range constraints. The present model compatible with experimental results does not employ hard calculable variables. Besides, it is applicable not only for pure metals but also for alloys. The squared regression (R^2) and error sum of squares (SSE) for the training and testing data of the presented model are 0.93, 0.0006 and 0.98, 0.00018, respectively, which indicates the high accuracy of the proposed model. The slope of the $\log\frac{\gamma}{Gb}$ versus $\log\frac{d_s}{b}$ is about 0.6453 which is comparable to all the models offered in this field.

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1. Introduction

Severe plastic deformation (SPD) is a method to produce ultrafine bulk materials for industrial applications. In various systems such as Cu-Al, Cu-Zn, and Pd-Ag, it has been demonstrated that *d*s or dmin (minimum grain size) is dependent on stacking fault energy (SFE) [1]. Many models have been proposed to confirm this dependence [2-9].This dependence is represented by a parameter called *q* (the average parameter *q* is approximately 0.65.), which is essentially the slope of the $\log\frac{\gamma}{Gb}$ versus $\log\frac{d_s}{b}$, where *b* is the Burgers vector and *G* is the shear modulus. The proposed models are based on limited data and do not have a high computational theory. On the other hand, they cannot be used in alloys and are used only for pure metals, which confirms the lack of high potential in these models. In the present work, Gene Expression Programming (GEP) as one of the most important branches of artificial intelligence (AI) has been used for simulating the SPD process and providing a relation between the γ and d_s. According to the obtained results, the presented model overcomes the mentioned shortcomings (in other models) and then assesses its reliability and accuracy by experimental results.

2. The model

The exact functionality of this model has been explained in our previous work [10]. It is worth mentioning that prior to introducing the data to the model, they are divided into two groups, namely the training and the testing datasets. Testing data are randomly selected from all data and entered into the model to test the training data (see Table 1 and Table 2). This guarantees that the model output for the training data will not be false. Genetic programming (GP), one of the newest paradigms of evolutionary computations, can automatically learn the introduced problem by mimicking the Darwinian evolution process [10]. Gene expression programming (GEP) as an extension of GP, is used in this paper to develop the model. GEP method includes individuals referred to linear strings with fixed-size called genome or non-linear entities containing various sizes and shapes called expression trees (ETs). Generally, any individual contains one chromosome having one or more genes, divided into head and tail parts [10]. Moreover, there are two languages in GEP: the language of the genes and the language of ETs. A simple chromosome as a linear string with two genes is encoded, as shown in Fig. 1 as an example for ET language. Its ET and the corresponding mathematical formula are also shown in the same figure**.**

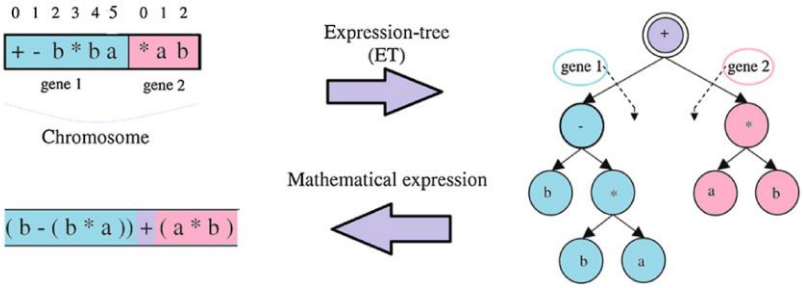


Fig. 1. A simple chromosome as a linear string with two genes

3. Results and discussion

Seven input parameters comprised of *b*, *D*, *G*, *H*, γ, *Q* and *T* were inserted to the GEP model as input layers, while the output layer was set on d_s. Fig. 2 shows an expression tree for the steady-state grain size values (d_s or d_{min}) of the SPDed materials as output layer in this research. It should be noted that the variables of d0, d1, d2, d3, d4, d5 and d6 are the values for the abovementioned input layers, which are b, *D*, *G*, *H*,γ, *Q* and *T*, respectively.

Table 1. Modeling database for various metals and alloys in training mode [6]

Materials used in SPD process	***T* (K)**	***G* (GPa)**	***b* (nm)**	**D (m^2s^{-1})**	***Q* (kJ/mol)**	**γ (mJm^{-2})**	***H*(GPa)**	**d_s(nm)**
Mg	922	17	0.3197	1.75	138	125	0.34	1000
Fe	1809	82	0.2482	1.9	240	180	3.02	200
Co	1768	82	0.2497	0.55	298	31	3.28	100
Ni	1728	75	0.2492	1.77	285	125	3.02	170
Pd	1825	46	0.2751	20.5	266	180	2.13	240
Ag	1234	27	0.2889	27.8	182	16	0.94	220
Al-Mg	906	26	0.2881	4.4	140	27	1.98	190
Al-Ag	928	26	0.2864	0.33	125	175	0.59	500
Al-Ag	920	26	0.2864	1.5	136	190	0.74	500
Al-Cu	923	26	0.2858	0.18	126	166	2.01	207
Cu-Al	1350	47	0.2565	0.287	188	37	2.1	65
Cu-Al	1335	46	0.2578	1.293	191	8	2.51	118
Cu-Zn	1283	41	0.2593	0.36	170	18	2.4	108
Cu-Zn	1223	37	0.261	1.7	172	14	2.49	74
Pd-Ag	1733	42	0.2779	17.6	126	125	2.92	150
Ni-Fe	1713	78	0.2537	41.5	316	79	3.92	120
Ni-Co	1733	76	0.2493	0.725	273	120	3.58	197
Ni-Co	1738	78	0.2497	0.166	258	90	4.06	115

Table 2. Modeling database for various metals and alloys in testing mode [6]

Materials used in SPD process	***T* (K)**	***G* (GPa)**	***b* (nm)**	**D (m^2s^{-1})**	***Q* (kJ/mol)**	**γ (mJm^{-2})**	***H*(GPa)**	**d_s(nm)**
Al	933	26	0.2864	17.6	126	166	0.31	1500
Cu	1357	48	0.2556	35	204	45	1.3	400
Al-Mg	930	26	0.2867	0.49	124	87	1.25	330
Al-Mg	916	26	0.2874	0.32	122	54	1.8	230
Al-Ag	906	26	0.2864	11	155	210	1.11	500
Cu-Zn	1330	45	0.2575	0.13	170	35	2.23	110
Pd-Ag	1774	44	0.2758	1.75	138	165	2.61	206
Pd-Ag	1648	38	0.28	1.9	240	119	3	144

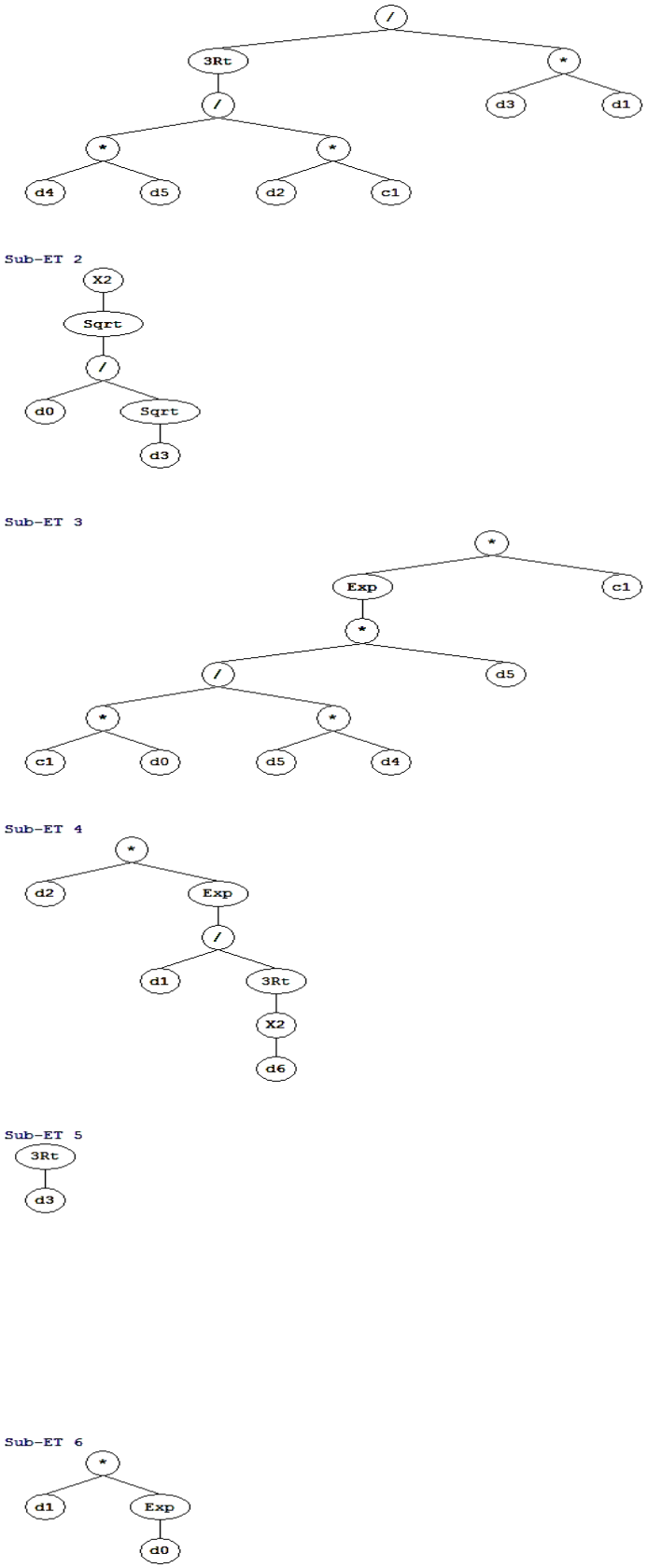


Fig. 2. The expression tree with 6 genes for predicting d_s

Table 1 and Table 2 show the experimental sets collected from the literature for the modelling process [5]. There are two sets of data in any simulating/modelling process, including training and testing which used for learning and generalizing model, upheaval buckling predictive models (for additional details, please refer to our previous work [10]). In this research 18 data were randomly chosen as the training and remained 8 data were used as testing. The model containing the best-predicted

values of d_s in both of the training and testing data sets is adopted as the best model for simulating SPD process. The formula derived from the ETs presented in Fig. 2, with the procedure shown in Fig. 1, is in accordance with the following equation:

$$d_s = \left(\left(\frac{\gamma Q}{8.7\,\mathrm{G}}\right)^{1/3} / HD\right)\left(\frac{b}{H^{1/2}}\right)\left(7.3\exp\left(\frac{7.3b}{\gamma}\right)\right)\left(\mathrm{G}\exp\left(\frac{D}{T_m^{2/3}}\right)\right)(H)^{1/3}\left(D\exp(b)\right) \quad (1)$$

Or

$$\frac{d_s}{b} = 3.5\left(\frac{\gamma}{Gb}\right)^{1/3}\left(\frac{G\left(HbQ\right)^{1/3}}{H^{3/2}}\right)\exp\left(\frac{7.3b}{\gamma}+\frac{D}{T_m^{2/3}}+b\right) \quad (2)$$

Two points are extracted from Eq.2:

1- The Burgers vector, the frequency factor for pipe diffusion and the melting temperature play an exponential role, indicating they have a more important effect than the other mentioned parameters.

2- There is a linear relationship between $\frac{\gamma}{Gb}$ and $\frac{d_s}{b}$ or between $\log\frac{\gamma}{Gb}$ and $\log\frac{d_s}{b}$.

The latter has been also reported in previous works. To illustrate, Qu et al. [1] analyzed the dependency of the normalized steady-state grain size on the normalized SFE for SPDed materials. They reported a simple linear relationship between $\frac{\gamma}{Gb}$ and $\frac{d_s}{b}$.

Moreover, Mohamed et al. [2] presented a model in which $\log\frac{\gamma}{Gb}$ and $\log\frac{d_s}{b}$ have a linear connection as follows:

$$\frac{d_s}{b} = A\exp\left(\frac{-\beta Q}{4RT}\right)\left(\frac{DGb^2}{vkT}\right)^{1/4}\left(\frac{\gamma}{Gb}\right)^{1/2}\left(\frac{G}{H}\right)^{5/4} \quad (3)$$

where, A is a constant, β= 0.04, Q is the activation energy for self-diffusion, R is the gas constant, T is the absolute temperature, D is the frequency factor for pipe diffusion, v is the initial dislocation velocity, k is Boltzmann's constant, γ is the stacking fault energy, and H is the steady-state hardness.

Another model which has been expressed by using thermodynamic relations and almost confirms the results of our model is Kazeminezhad model [3], which is expressed as follows:

$$\frac{d_s}{b} = A\exp\left(\frac{-\alpha Q}{3RT}\right)\left(\frac{DGb^2}{vkT}\right)^{1/3}\left(\frac{\gamma}{Gb}\right)^{2/3} \quad (4)$$

where $\alpha = 0.037$.

In addition, there are many experimental works reporting a power-law relationship for the dependency of ds to SFE [2-9]. These models have great potential for simulating SFE. However, several major flaws are common to all of them:

a) The initial speed of dislocation to which these relations have referred is almost hardly calculable and, as a consequence, it reduces the precision of the models.

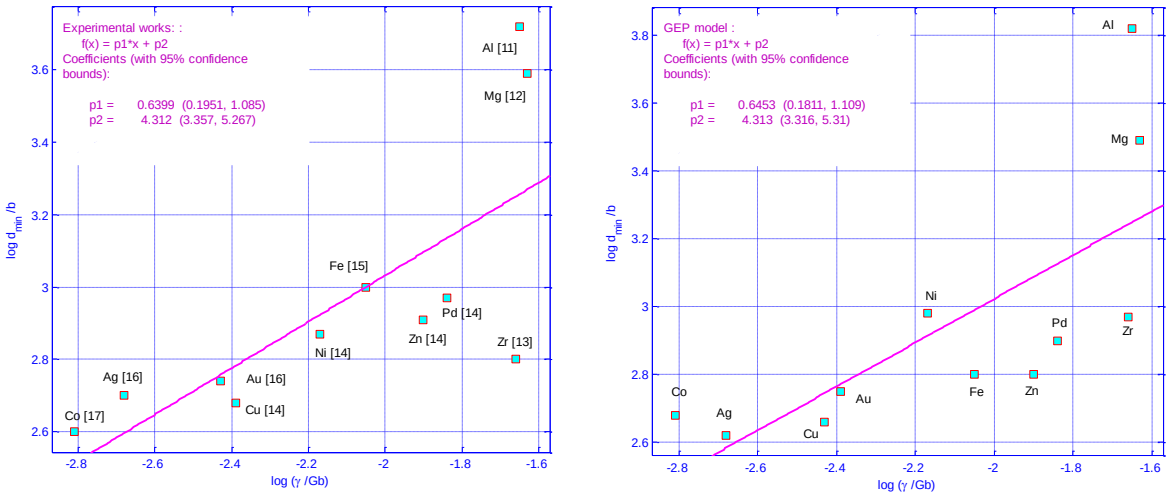
b) The amounts of α and β can only be measured by experimental data and no mathematical theory supports them. This also results in obscurity and the reduction of the precision of the models.

c) The number of experimental data for making a linear relationship is too small.

d) They are applicable only for pure metals but not for alloys

Our presented model (Eq.1) covers all the above flaws. Firstly, it does not need to calculate ambiguous variables (such as α or β); secondly, it covers a wide range of alloys and pure metals, and thirdly, it is very accurate.

In order to assess the precision of the presented model, we have to compare the slope of the straight line in Fig. 3a (which the slope of the $\log\frac{\gamma}{Gb}$ versus $\log\frac{d_s}{b}$) with that of the diagram obtained from the presented model (Fig. 3b). If we consider Fig.4a which has been drawn on the basis of experimental data [11-17], it can be observed that the slope of the straight line (q) is 0.63 (plotting the logarithm of the normalized steady-state grain size against the normalized stacking fault energy, gives a straight line), which is in agreement with the results obtained by previous studies [2-9]. In the latter diagram, which has been drawn based on the predicted d_s, it can be seen that the slope is q=0.6453. Mohammed et al. [2], and Kazeminejard et al. [3] reported a value of 0.65 and 0.66 for q, respectively. Other studies in this field have reported almost the same results for the value of q as 0.65 [7], 0.69 [8], 0.63 [9], 0.64 [19].



(a) (b)

Fig. 3. Normalized steady-state grain size (d_s / b) vs. the normalized stacking fault energy (γ/Gb) for a: experimental and b) modelling results

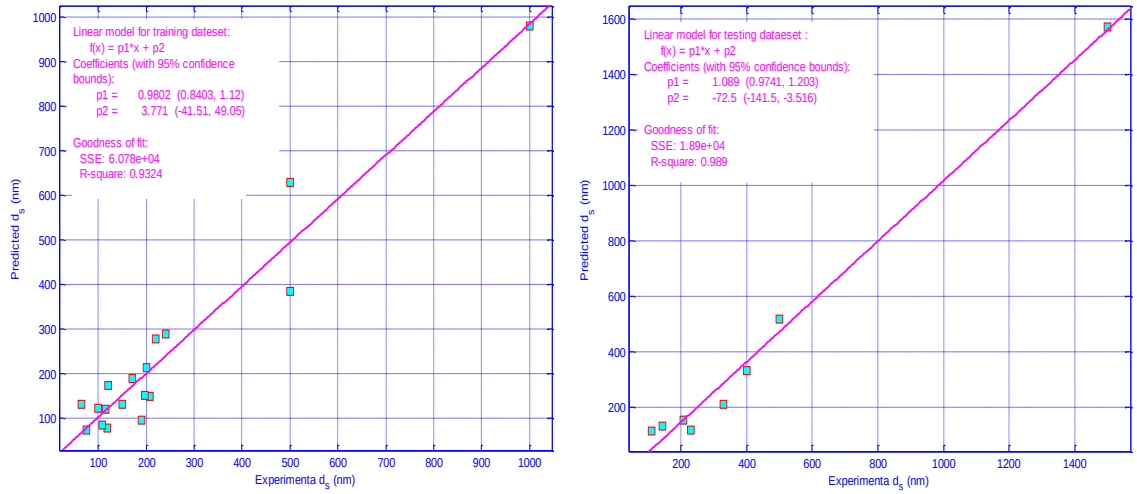
One of the significant advantages of this model over the other mentioned models is its rich database (Table 1 and Table 2). As can be seen in these Tables, the materials selected for modelling process are not only pure metals but also a variety of different alloys. This makes the model applicable for both pure metals and alloys.

To assess the ability of the GEP-based formulation (Eq. 1), the developed regression-based formulation R-square (R^2) was used as the measurements index between the experimental and predicted d_s values according to the following equation [18]:

$$R^2 = \frac{\left(n\sum t_i o_i - \sum t_i \sum o_i\right)^2}{\left(n\sum t_i^2 - \left(\sum t_i\right)^2\right)\left(\left(n\sum o_i^2 - \left(\sum o_i\right)^2\right)\right)} \qquad (5)$$

where ‘‘t’’ is the experimental value, ‘‘o’’ is the predicted value, and ‘‘n’’ is total number of data.

Figure 4 shows the comparison between the experimental values of *d*s and the predicted ones obtained from the training and testing results of the GEP model. As can be seen, the R^2 and error sum of squares (SSE) values are shown in this figure for the training (Fig. 4a) and testing (Fig. 4b) datasets. There is no need to explain that the high amount of R^2 ensures that the values obtained for the training and testing datasets in the GEP model are very close to the experimental results. The R^2 values in the training and testing sets show that the proposed GEP is suitable and can predict *d*s very close to the experimental values.



(a) (b)

Fig. 4. The correlation of the measured and predicted d_s in (a) the training and (b) the testing phase

4. Conclusion

In this study, a computer-based model was introduced for dependent of the steady-state grain size to stacking fault energy. The evaluation of model using experimental data showed that there is a perfect match between the current and previous models. However, there are several advantages to this model. First, it is applicable not only for pure metals but also for alloys, second, it does not employ hardly calculable variables and third, it is more accurate and more diverse. The slope of the $\log\frac{\gamma}{Gb}$ versus $\log\frac{d_s}{b}$ is about 0.6453 which is comparable to all the models offered in this field. In this research, 18 sets were randomly chosen as the training and remained 8 sets were used as testing. R^2 values for training and testing datasets of the proposed model are 0.93 and 0.98, respectively, which confirms the high accuracy of the model.

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