Application of Abductive Network and FEM to Predict the Stress-Strain Curve with strain hardening effect of Bulk Metals by Nanoindentation test

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ABSTRACT

The purpose of the present work was to investigate the nanoindentation process by FEM of bulk materials such as pure copper, titanium, iron and so on, considering strain hardening effect of material. In order to verify the FEM simulation results of the mechanical parameters such as Young's modulus, yield stress and tangent modulus, the experimental data are compared with the results of the current simulation. The abductive network was then applied to synthesize the data sets obtained from the numerical simulation. The predicted results of the mechanical properties from the prediction model are consistent with the results obtained from experiment. After employing the predictive model can provide valuable references in prediction of the mechanical parameters after nanoindentation tests.

Keywords: finite element method, abductive network, nanoindentation, stress-strain curve

1 INDROTUCTION

Finite element method (FEM) has been widely used for numerical simulation of indentation tests on bulk material in order to analyze its deformation response and investigate the influence of indenter geometry, friction and material elastic and plastic properties. Pelletier et. al [1] have investigated the influence of material bilinear elastic-plastic behaviour model for numerical simulation of nanoindentation testing of various bulk metals. They employed an axisymmetric rigid cone and equal volume to the Berkovich pyramid indenter to simulate the test. The indenter and the specimen were treated as a revolution body in order to have three-dimensional situation. The numerical simulation results of loads verse displacement compare reasonable well to experimental results of nanoindentation tests of pure metals as Fe, Ni, Ti and Cu. In order to determine dimensionless functions correlating rheological factors with parameters extracted from loading and unloading curves, Pelletier [2] used a comprehensive parametric study of 48 cases was conducted; elastic modulus ranges from 70 to 430 GPa, yield stress from 100 to 600 MPa and the tangent modulus from 3 to 40 GPa. They defined two dimensionless equations which link the parameters extracted from the experimental load–displacement curve with material parameters, such as Young's modulus, yield stress and tangent modulus. The equations have been tested with success first on load–displacement curves simulated with FEM and then on experimental curves obtained by nanoindentation testing using a Berkovich tip. Lin [3] predicts the rolling force and deformation in three-dimensional cold rolling by using the FEM and neural network. Lin and Lin [4] used the finite element method in conjunction with abductive network to investigate the geometrical shape of the deformation profile and its related fold defect during forging-extrusion process. The prediction models are established for radius ratio estimation of the barrels and fold occurrence situation judgment under various combinations of process variables.

In order to verify the FEM simulation results of the mechanical parameters such as Young's modulus, yield stress and tangent modulus, the experimental data are compared with the results of the current simulation. The abductive network was then applied to synthesize the data sets obtained from the numerical simulation. After employing the predictive model can provide valuable references in prediction of the mechanical parameters after nanoindentation tests.

2 BASIC THEORY

2.1 Finite Element Modeling

A commercial FE code DEFORM-2D [5] is adopted to analyze the plastic deformation of the nanoindentation process. For the nanoindentation process of a elastic-plastic deformation problem, the governing equations for the solution of the mechanics in plastic deformation for materials involve equilibrium equations, yield criterion, constitutive equations and compatibility conditions. The duality of the boundary value problem and the variation problem can be seen clearly by considering the construction of the functional [6]:

$$\pi = \int_v \bar{\sigma}\,\dot{\bar{\varepsilon}}\,dv - \int_s F_i u_i\,ds \qquad (1)$$

where $\bar{\sigma}$ is the effective stress, $\dot{\bar{\varepsilon}}$ is the effective strain-rate, F_i represents the surface tractions and, u_i is the velocity components. The variational form for finite-element discretization is given by:

$$\delta\pi = \int_v \bar{\sigma}\delta\dot{\bar{\varepsilon}}\, dv + k\int_v \dot{\varepsilon}_v \delta\dot{\varepsilon}_v\, dv - \int_s F_i \delta u_i\, ds = 0 \qquad (2)$$

where $\dot{\varepsilon}_V = \dot{\varepsilon}_{ii}$ is the volumetric strain rate, π is functional of the total energy and work, and k, a penalty constant, is a very large positive constant. $\delta\dot{\bar{\varepsilon}}$ and $\delta\dot{\varepsilon}_v$ are the variations in effective strain rate and volumetric strain rate. Eq. (1) and Eq. (2) are the basic equation for the finite element formulation.

2.2 Abductive Network Synthesis

In the abductive network, a complex system can be decomposed into smaller, simpler subsystems grouped into several layers using polynomial functional nodes. The polynomial network proposed by Ivakhnenko [7] is a group method of data handing (GMDH) techniques. Theses nodes evaluate the limited number of inputs by a polynomial function and generate an output to serve as an input to subsequent nodes of the next layer. It consists of sigma (summation) units in the hidden layer and pi (product) units in the output layer. Output of a sigma unit is a weighted sum of its inputs, and output of a pi unit is a product of its input. Let the k^{th} input pattern to the network be specified by $X_k = [x_{0k}, x_{1k}, x_{2k}, \ldots, x_{nk}]$, and let the weight associated with connection from input unit i to hidden unit j be w_{ij}. Then, the output z_{jk} of the j^{th} sigma unit is given by

$$z_{jk} = \sum_{i=0}^{n} w_{ij} x_{ik} \qquad (3)$$

and output y_k of the network is given by

$$y_k = \prod_{j=1}^{h} z_{jk} \qquad (4)$$

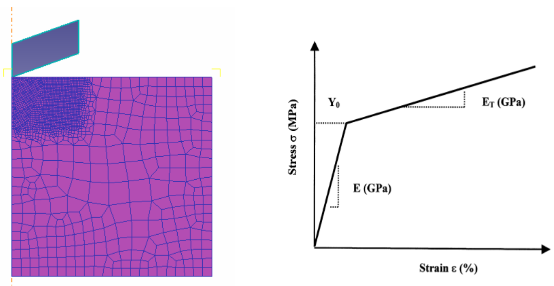
where h is the number of hidden units in the network. Cobinining Eqs. (3) and (4), the general polynomial function in a polynomial functional node can be expressed as:

$$y_k = c_0 + \sum_{i=1}^{n} c_i x_i + \sum_{i=1}^{n}\sum_{j=1}^{n} c_{ij} x_i x_j + \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n} c_{ijk} x_i x_j x_k + \cdots \qquad (5)$$

where x_i, x_j, x_k are the inputs, y_k is the output and c_i, c_{ij}, c_{ijk} are the coefficients of the polynomial functional nodes. In the present study, several types of polynomial nodes are used in polynomial network for predicting the limiting drawing ratio under a suitable range of process parameters. For more detailed explanation of these polynomial functional nodes, please refer to the paper of Ivakhnenko [7].

3 RESULTS AND DISCUSSION

FEM has been widely used to simulate the nanoindentation process. The schematic diagram of the nanoindentation process and the stress-strain relationship of the elastic-linear work-hardening materials used in DEFORM-2D software are shown in Fig. 1. An axisymmetric cone with half-included angle of 70.3° in which the conical indenter has the same area function as a Berkovich tip was used in this study. The contact region of both tip and bulk material were finely meshed for good simulation accuracy. In order to confirm the feasibility of the finite element method, the results published by Pelletier et. al [1] is used to compare with the present numerical results by DEFORM-2D software. The experimental data of Pelletier et. al [1] is compared with the results of the current simulation. Figures 2, 3 and 4 show the comparison between the current simulation and the results of Pelletier et. al [1]. The loading and unloading curve predicted by current simulation show good agreement with the experimental results of Pelletier et. al [1]. Therefore, the simulation by DEFORM-2D for nanoindentation process is reasonable accurate.



(a) (b)

Fig. 1(a) The finite element mesh of the indentation process by current simulation (DEFORM -2D)
(b) a schematic representation of the bilinear constitutive law used in current simulation

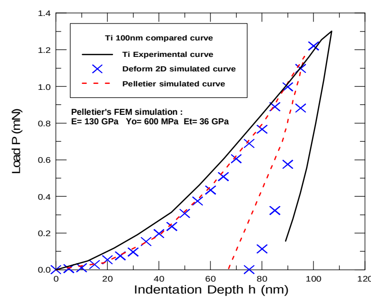


Fig. 2 Comparison between the current simulation and the results of Pelletier et. al [1] for loading and unloading curve (bulk material Ti and indentation depth = 100 nm)

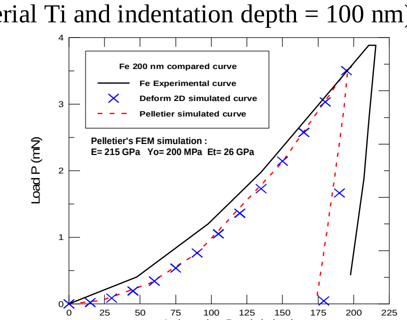


Fig. 3 Comparison between the current simulation and the results of Pelletier et. al [1] for loading and unloading curve (bulk material Fe and indentation depth = 200 nm)

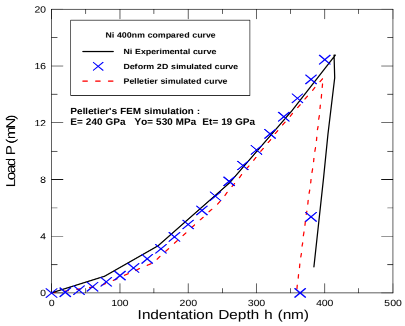


Fig. 4 Comparison between the current simulation and the results of Pelletier et. al [1] for loading and unloading curve (bulk material Ni and indentation depth = 400 nm)

3.1 Database Training

The yielding stress is varied between 100-600 MPa, whereas the other material's properties were selected by varying the Young's modulus, the tangent modulus and the indentation depth in the ranges of 72-430 GPa, 3.6-40 GPa and 100-400 *nm*, respectively. There are four variables of material properties, each of which was set at three levels. Therefore, 81 (3*3*3*3) combinations of parameters of material's property are constituted totally, and theses are shown in Table 1. The load–displacement curves obtained with FEM have been analyzed with the same method as the experimental load–indentation depth curves, as shown in Fig. 5. The curves corresponding to the loading part have been fitted using a polynomial law, $P=Ah^2+Bh$; and the unloading part can be mathematically described with a polynomial law, $P=Ch^2+Dh+F$. The loading and unloading curve can be obtained by the FEM simulation of indentation process for the different parameters such as E, Y_0, E_t and h. The coefficient of polynomial law such as A, B, C, D, F can be obtained from the curve fitting skill. Base on the training database regarding the parameters of material's property and coefficient of polynomial law such as Y_0, E, E_t, A, B, C, D, F, P and *h*, as shown in Table 1, the abductive networks with a criterion of minimum square error can be developed for predicting the E, Y_0 and E_t under a suitable range of parameters such as A, B, C, D, F, P and *h*. Five-layer networks shown in Fig. 6 is built for prediction of the tangent modulus. The prediction of networks for the Young's modulus and yielding stress are similar to Fig. 6.

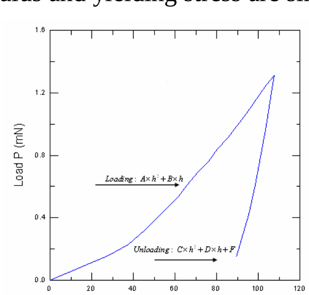


Fig. 5 The curves corresponding to the loading and unloading curves are fitted using a polynomial law $P=Ah^2+Bh$ and $P=Ch^2+Dh+F$, respectively.

Table 1 The training database of Y_0, E, E_t, A, B, C, D, F and *h*

E	Et	Yo	h	P	A	B	C	D	F
72	3.6	100	100	2.32E-01	2.32E-05	-7.47E-07	0.002224	-0.39522	17.5145
			250	1.35E+00	2.06E-05	0.000414	0.003307	-1.51464	173.344
			400	2.90E+00	1.34E-05	0.002208	0.004192	-3.12631	582.777
72	21.8	100	100	5.65E-01	5.67E-05	-3.37E-05	0.000643	-0.08865	3.01036
			250	3.37E+00	5.15E-05	0.00074	0.000718	-0.25584	22.5259
			400	8.66E+00	5.31E-05	0.000226	0.000846	-0.49875	72.9722
72	40	100	100	7.48E-01	7.53E-05	-5.44E-05	0.000456	-0.0533	1.5297
			250	4.62E+00	7.28E-05	0.000295	0.000481	-0.14333	10.4188
			400	1.22E+01	7.86E-05	-0.00127	0.000559	-0.27782	33.9831
72	3.6	350	100	4.07E-01	4.10E-05	-3.49E-05	0.001497	-0.24585	10.0282
			250	2.50E+00	3.93E-05	0.000221	0.00188	-0.79318	83.3299
			400	5.66E+00	3.11E-05	0.002437	0.002179	-1.50131	257.656
72	21.8	350	100	7.06E-01	7.16E-05	-6.94E-05	0.000531	-0.06491	1.89046
			250	4.41E+00	7.03E-05	0.000189	0.000647	-0.2113	16.8396
			400	1.06E+01	6.15E-05	0.002467	0.000777	-0.43239	59.3783
72	40	350	100	8.75E-01	8.84E-05	-0.00012	0.000403	-0.0416	1.01157
			250	5.48E+00	8.77E-05	7.47E-05	0.000463	-0.12769	8.51444
			400	1.38E+01	8.36E-05	0.00107	0.00053	-0.24806	28.3655
72	3.6	600	100	5.36E-01	5.40E-05	-6.35E-05	0.000985	-0.14521	5.21164
			250	3.31E+00	5.24E-05	0.000154	0.001286	-0.4995	47.8391
			400	7.80E+00	4.57E-05	0.002004	0.001505	-0.96326	152.36
72	21.8	600	100	8.04E-01	8.13E-05	-9.31E-05	0.000487	-0.05513	1.45451
			250	5.09E+00	8.22E-05	-0.00016	0.000589	-0.17935	13.1459
			400	1.24E+01	7.38E-05	0.002094	0.000686	-0.35476	44.6874
72	40	600	100	9.52E-01	9.65E-05	-0.00016	0.000386	-0.03741	0.841522
			250	6.07E+00	9.88E-05	-0.00042	0.000433	-0.11053	6.67013
			400	1.52E+01	9.29E-05	0.001121	0.000513	-0.22897	24.8792
256	3.6	100	100	2.69E-01	2.69E-05	-1.31E-06	0.035478	-6.89493	334.986
			250	1.47E+00	2.08E-05	0.000994	0.041326	-20.1489	2455.88
			400	3.08E+00	1.27E-05	0.002939	0.0556	-43.6467	8565.73
256	21.8	100	100	7.62E-01	7.63E-05	9.82E-06	0.005151	-0.88758	38.0143
			250	4.32E+00	6.26E-05	0.00183	0.007113	-3.17862	354.49
			400	1.10E+01	6.65E-05	0.000748	0.007428	-5.31027	946.794

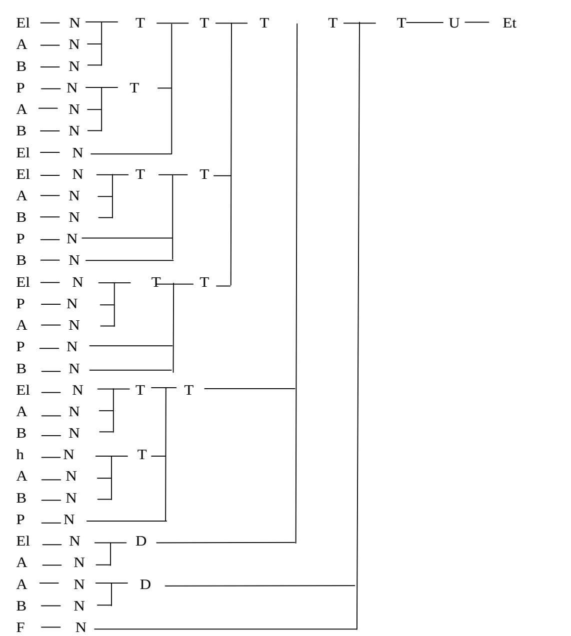


Fig. 6 The prediction model of tangent modulus E_t

3.2 Validating the Accuracy of the Prediction Model

In order to validate the accuracy of the prediction model, the experimental results of Figs. 2 and 3 are tested for the predictions of the Young's modulus, the yielding stress and the tangent modulus. Tables 2 and 3 show a comparison of the values of E, Y_0 and E_t between the abductive network prediction, the FEM simulation and the experimental data under various combinations of the values of A, B, C, D, F, P and *h*, which are around the threshold of the suitable range. The predicted results of the E, Y_0 and E_t are in good agreement with those obtained from the FEM simulations. Therefore, the developed networks have a reasonable accuracy for predicting the value of E, Y_0 and E_t.

Table 2 Prediction of E, Y_0 and E_t between FEM [1] and abductive network for Fig. 2 (bulk material Ti and indentation depth = 100 nm) (Experiment: A=80.4853, B=3.8613, C=0.001469, D=0.03750, F=0.000389)

	E(GPa)	Y_0 (MPa)	E_t (GPa)
FEM [1]	130	600	36
abductive network	139	569	38

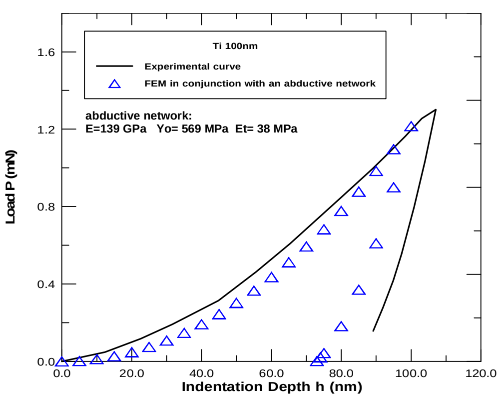


Fig. 7 Comparison between the Pelletier's experimental results [1] and DEFORM-2D in conjunction with an abductive network.(E=139GPa, Y_0 =569 MPa, E_t = 38GPa)

Table 3 Prediction of E, Y_0 and E_t between FEM [1] and abductive network for Fig. 3 (bulk material Fe and indentation depth = 200 nm) (Experiment: A=49.91503, B=7.7529, C=0.004083, D=0.12378, F=-0.005434)

	E(GPa)	Y_0 (MPa)	E_t (GPa)
FEM [1]	215	200	26
abductive network	201	178	25

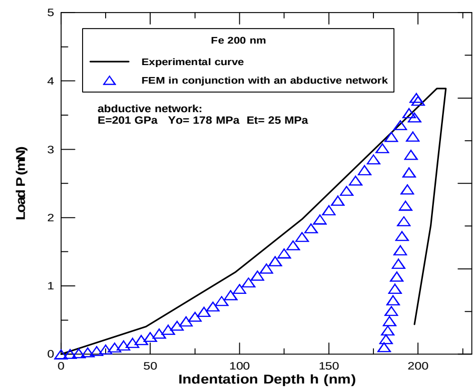


Fig. 8 Comparison between the Pelletier's experimental results [1] and DEFORM-2D in conjunction with an abductive network. .(E=201GPa, Y_0 =178 MPa, E_t = 25GPa)

4 CONCLUSION

In this paper, a prediction model has been established for the E, Y_0 and E_t by using the finite element method in conjunction with an abductive network. The predicted results are consistent with the results obtained from experiment. After employing the predictive model can provide valuable references in prediction of the mechanical parameters such as E, Y_0 and E_t after nanoindentation tests.

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