MATERIAL CHARACTERIZATION VIA NEURAL NETWORKS

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ABSTRACT

Essential mechanical properties of materials can be assessed via the reverse analysis based on load-displacement curves of dual indenters of different geometries. Two models namely the artificial neural networks (ANN) involving empirical risk minimization and the least squares support vector machines (LS-SVM) of the structural risk optimization group are constructed to determine the material properties via the load-indentation curves. The mapping of the load-indentation parameters to the material properties is formed and calibrated using function approximation procedure. Extensive large strain-large deformation finite element analyses were carried out to simulate the indentation of elasto-plastic materials obeying power law-strain hardening using both Berkovich and conical indenters. The study covers the material properties of a wide practical range with 680 datasets for each indenter. The results are displayed as surfaces describing the variations of load-indentation parameters and employed as inputs to the proposed neural network models. Both networks are robust and directly relate the the load-indentation parameters to the elasto-plastic material properties without involving iterative procedure. The method has wide potential applications on material characterization in semi-conductor and thin film industries including MEMS and NEMS.

KEY WORDS

computing, finite element simulation, indentation, material characterization, neural networks.

INTRODUCTION

The instrumented indentation test can be adopted to extract essential mechanical properties of materials. The advent of the high precision instrumented indentation equipment and the need to characterize small volume of materials at micron and sub-micron levels inspired many researchers to carry out their work in the past decade (Oliver and Pharr. 1992). Forward and reverse analyses based on finite element results were proposed by Dao et al. (2001). The approach was extended to results based on dual indenters by Bucaille et al.

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(2003), and Swaddiwudhipong et al. (2005c). Tho et al. (2004) demonstrated that the latter is necessary for uniqueness of reverse analysis.

Neural network models (Huber et al, 2002 and Suykens et al, 2002) formulated based on statistical learning theory are adopted to relate the characteristics of load-indentation curves with the mechanical properties of materials. Both traditional artificial neural networks (ANN) based on empirical risk minimization and the support vector machines (SVM) of the structural risk minimization group are employed to extract the material properties from the characteristics of the load-displacement response of dual indenters of different geometries. The sets of information used for training and verification of the neural network models are obtained from extensive large strain-large deformation finite element analyses simulating the indentation of elasto-plastic materials obeying power law-strain hardening using both Berkovich and conical indenters. The extent of material properties included in the study covers the wide practical range of this class of materials. The tuned models will be shown to be able to predict the properties of a new set of materials reasonably accurately. Both proposed models are able to relate the characteristics of the load-indentation curves to the elasto-plastic material properties without resorting to any iterative procedure.

SIMULATED INDENTATION TESTS

Berkovich indentation is simulated by 3-D finite element analyses using ABAQUS (2002). Only one-sixth of the target materials have to be modeled as the Berkovich indenter possesses a three-fold symmetry. The indenter is idealized as a rigid body while the target material as deformable solids. A series of solid elements, C3D20-C3D27, is adopted to model the target materials with finer mesh in the vicinity of the contact region where high stress gradient is expected and gradually further away from the region. Convergence studies and the insensitivity to the far-field effect from boundary conditions have earlier been carried out by Swaddiwudhipong (2005a, 2006). For indentation depth of up to 5 microns, Tho (2005) has shown that both can be satisfied if 5338 second-order solid elements are employed for the domain size of 115.5, 200 and 150 micron for length AH, HI and AJ indicated in figure 1 respectively. Conical indentation tests have also been simulated via ABAQUS (2002). To satisfy the above 2 requirements at the same indentation depth of 5 µm, the target bulk materials of 200x200 μm^2 are modelled as 28900 four-node, bilinear axisymmetric quadrilateral elements.

Materials considered in this study are those obeying power law strain-hardening with the uniaxial true stress-true strain relationship expressed in Eq.(1).

$$\sigma = E\varepsilon \quad \text{for } \sigma \le Y \tag{1a}$$

$$\sigma = R\varepsilon^n \quad \text{for } \sigma \ge Y \tag{1b}$$

$$R = Y\left(\frac{E}{Y}\right)^n \tag{1c}$$

Dao et al (2001) reported that the effect of indenter elasticity can be considered by replacing the Young's modulus, E, of the target materials by a reduced value, E^*, expressed in Eq.(2).

$$E^* = \left[\frac{1-v^2}{E} + \frac{1-v_i^2}{E_i}\right]^{-1} \tag{2}$$

Y is the yield stress, n the strain-hardening power and v the Poisson's ratio of the target materials while subscript $(\ )_i$ implies those of the indenter. A Poisson's ratio of 0.33 which is common for the class of material considered is adopted. Smooth contact is assumed in this study as the effect of friction for indenters with half-angle larger than 60° can be ignored (Bucaille et al. 2003).

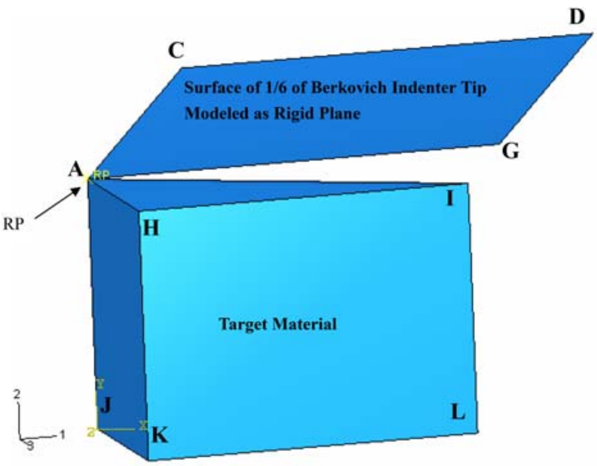


Figure 1: Berkovich indentation model.

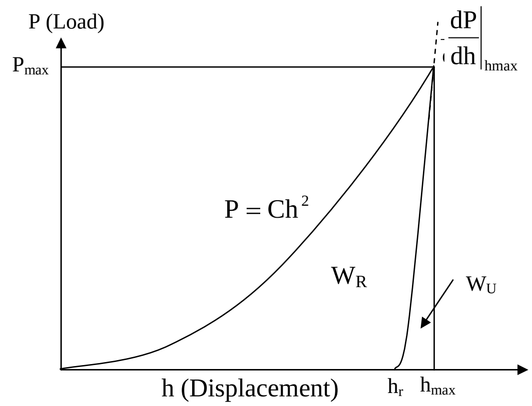


Figure 2: Load-Indentation Relation

Swaddiwudhipong et al (2005c) showed via the relationship derived by Luk et al (1991) and Cheng and Cheng (1998) for results obtained from Berkovich and conical indentations respectively that

$$\frac{C_B}{Y} = f_{1B}(\frac{E^*}{Y}, n) \qquad \frac{C_C}{Y} = f_{1C}(\frac{E^*}{Y}, n) \tag{3}$$

$$\left[\frac{W_T - W_U}{W_T}\right]_B = \left[\frac{W_R}{W_T}\right]_B = f_{2B}(\frac{E^*}{Y}, n) \qquad \left[\frac{W_T - W_U}{W_T}\right]_C = \left[\frac{W_R}{W_T}\right]_C = f_{2C}(\frac{E^*}{Y}, n) \tag{4}$$

C represents the constant curvature of the loading protion, W_T and W_U are the areas under the loading and unloading curves respectively.as shown in figure 2 and the subscripts $(\ )_B$ and $(\ )_C$ indicate the types of indenters used. Based on the results obtained from dual indenters, i.e. (i) Berkovich and (ii) conical of 60° half angle,

$$\frac{C_B}{C_C} = \frac{f_{1B}(\frac{E^*}{Y}, n)}{f_{1C}(\frac{E^*}{Y}, n)} = f_3(\frac{E^*}{Y}, n) \tag{5}$$

The functions $f_{1B}(E^*/Y,\ n)$, $f_{2B}(E^*/Y,\ n)$, $f_{1C}(E^*/Y,\ n)$, $f_{2C}(E^*/Y,\ n)$ and $f_3(E^*/Y,\ n)$ are established based on the finite element results and the surfaces describing these functions are depicted in figures 3 to 5 respectively. Each small circle in the figures represent a numerical data point. Swaddiwudhipong et al (2005a) and Tho et al (2004a) demonstrated that the reverse analysis based on dual indenters leads to unique solutions of E^*/Y and n and hence a one-to-one mapping of $(C_B)/(C_C)$, $(W_R/W_T)_B$ and $(W_R/W_T)_C$ to E^*/Y and n.

NEURAL NETWORK MODELS

The reverse analysis to extract material mechanical properties is usually carried out through an iterative process. Analytical closed form solutions, if possible, are difficult to establish due to the complexity of the highly nonlinear problem involved in the reverse analyses. A viable alternative is to establish analytically the functions relating the load-indentation parameters to the material characteristics and then calibrate them numerically through function approximation procedure. The latter can be conveniently handled through artificial neural network (ANN) approach as adopted by Huber et al. (2000, 2002) for material characterization of thin film on substrate based on results from a single indenter. The method was later extended to characterize elasto-plastic materials with power-law strain hardening using the results obtained from dual indenters by Tho et al. (2004a). The latter requires the construction of 2 artificial neural networks (ANN1 and ANN2) as 2 stages of mapping have to be performed. The flow chart for the reverse analysis via ANNs is depicted in figure 6. Each ANN model created by Neural Network Toolbox (Matlab V6.5) comprises 3 layers, namely, (i) an input, (ii) a hidden and (iii) an output layers. The tangent sigmoid transfer function is employed in the hidden layer while the output layer adopts the linear transfer function. The numbers of input and output parameters dictate the numbers of neurons used in the corresponding layer. The number of neurons in the hidden layer is calibrated based on the training and validation processes.

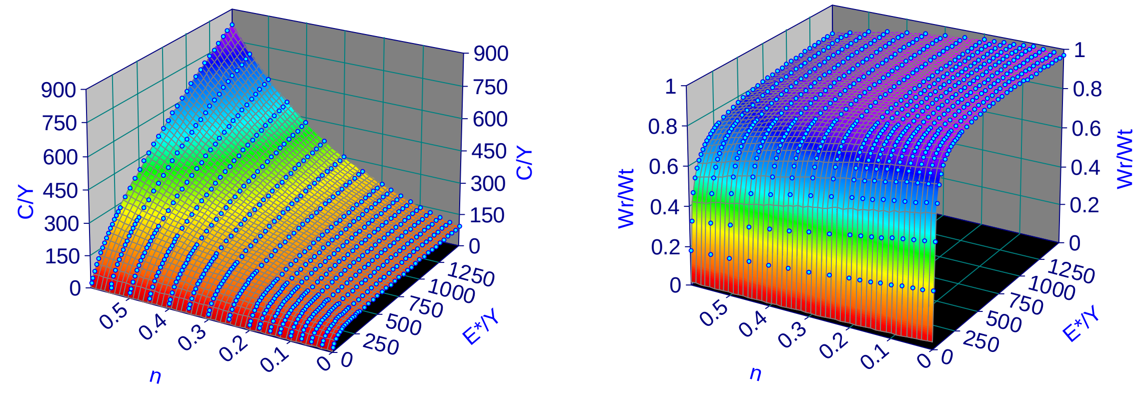
The information used for training and verification of the neural network models may be obtained from either actual or simulated dual indentation tests based on a large number of data covering the wide practical range of material properties. In the present study, numerical results from 1360 (680 for each indenter) finite element analyses covering a domain of E^*/Y from 10 to 1500 and n varying from 0.0 to 0.6 are adopted for the training and validation of the neural network models. The ranges of the values cover most metallic materials obeying power law strain-hardening. About 550 training inputs are randomly selected from the 680 datasets of finite element results while the remaining 130 data points which were concealed during the training of the models are adopted for validation purpose.

Training methods for traditional neural network architectures occasionally suffer from the existence of local minima and the number of neurons required for a given task has to be tuned carefully to ensure neither over-fitting nor under-fitting. In support vector machines, a unique solution is obtained and the number of weights follows automatically from a convex program. However, kernel functions and parameters have to be selected carefully such that a bound is minimized. The least-squares support vector machines (LS-SVM) established by Suykens et al (2002) are proposed for material characterization based on simulated load-displacement response of dual indenters of different geometries (Swaddiwudhipong et al. 2005b). The approach is a class of learning algorithms motivated by results from statistical learning theory (Vapnik, 1995). The method is an efficient and robust tool for multi-dimensional function approximation. The primary advantage of the latter approach is its insusceptibility to over-fitting which could occur in the case of an artificial neural network model.

Four least-squares support vector machines LS-SVM are constructed for the interpretation of the instrumented indentation results. The solution algorithm is depicted in figure 7. They are created using LS-SVMlab1.5 toolbox implemented in MatlabV6.5 package (Pelckmans et al, 2002). In order to conduct a LS-SVM model effectively, the appropriate values of the two control parameters, γ and σ^2, have to be evaluated using the *tunelssvm* function in the toolbox for a minimum associated cost function and the values reported in Table 2. The former, γ, is the regularization parameter determining the trade-off between the fitting error minimization and smoothness while σ^2 is the bandwidth for the radial basis function (RBF) kernel. Once again, the data adopted are results from extensive finite element analyses carried out to investigate the response of elasto-plastic materials obeying power law strain-hardening during indentation of two indenters of different geometries. A similar number of randomly re-selected datasets used earlier for the training and validation of the artificial neural networks (ANNs) is employed in the same operations involving the proposed least-squares support vector machines. Both proposed models (ANNs and LS-SVMs) are robust and directly relate the characteristics of the indentation load-displacement curve to the elasto-plastic material properties without resorting to any iterative procedure.

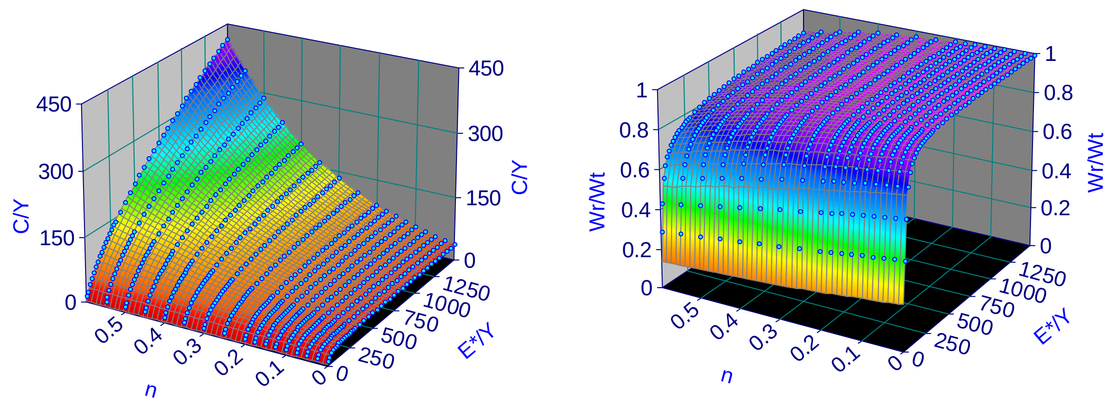
COMPARISON OF RESULTS

The characteristics of the load-indentation curves obtained from the simulated indentation tests using a Berkovich indenter and a conical indenter of 60.0° half-angle on Al6061, Al7075, steel and iron based on the material properties reported earlier by Chollacoop et al. (2003) and Bucaille et al. (2003) respectively are given in Table 3. These values are adopted as inputs for the reverse analyses using the proposed ANN and LS-SVM models. The predictions from both models are compared with those obtained by the uni-axial compression tests and via the Oliver and Pharr method as reported by Dao et al. (2001) for the first 2 materials and the values provided by Bucaille et al. (2003) for the remaining two. They show a more favorable agreement for the values of E^* (reduced Young's modulus) for the former (both Aluminium allloys), with less than 8% deviations as compared to 17-21% obtained by the Oliver and Pharr method. Both proposed neural network models generate reasonably accurate values of Y (yield strength) for all 4 materials adopted in the present study. The prediction of the values of the strain hardening power, n, is less accurate than those of E^* and



(a) (b)

Figure 3. Variation of (a) C/Y and (b) W_R/W_T based on Berkovich indenter (f_{1B} & f_{2B}).



(a) (b)

Figure 4. Variation of (a) C/Y and (b) W_R/W_T based on conical indenter of 60° half angle (f_{1C} & f_{2C}).

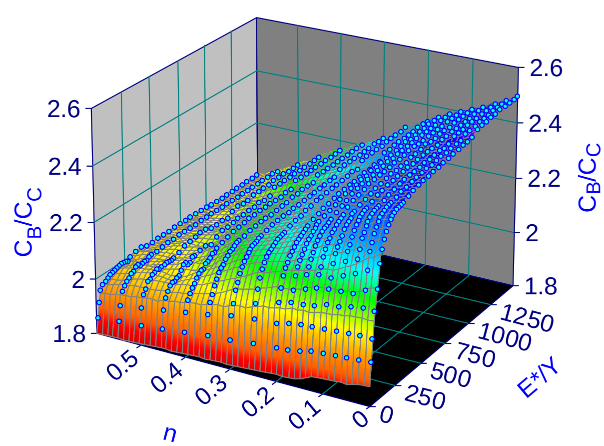


Figure 5. Variation of C_B/C_C (f_3).

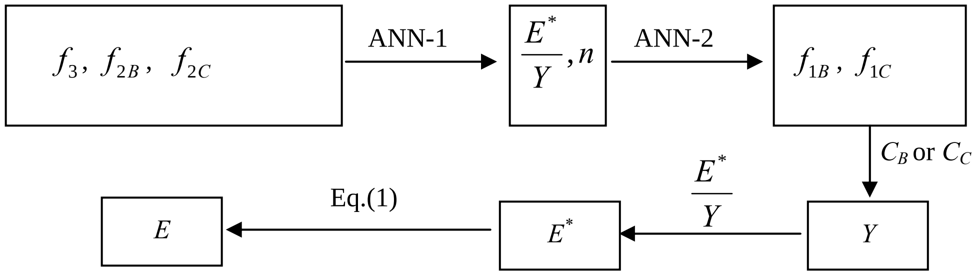


Figure 6: Flow Chart of Reverse Analysis via ANNs.

Table 1: Characteristics of ANNs

	Range of outputs	Number of neurons in the hidden layer	Mean Square Error	
			Training	Validation
ANN-1	0 – 1.5	31	5.76E-05	1.29E-04
ANN-2	10-850	40	1.09E-02	2.48E-02

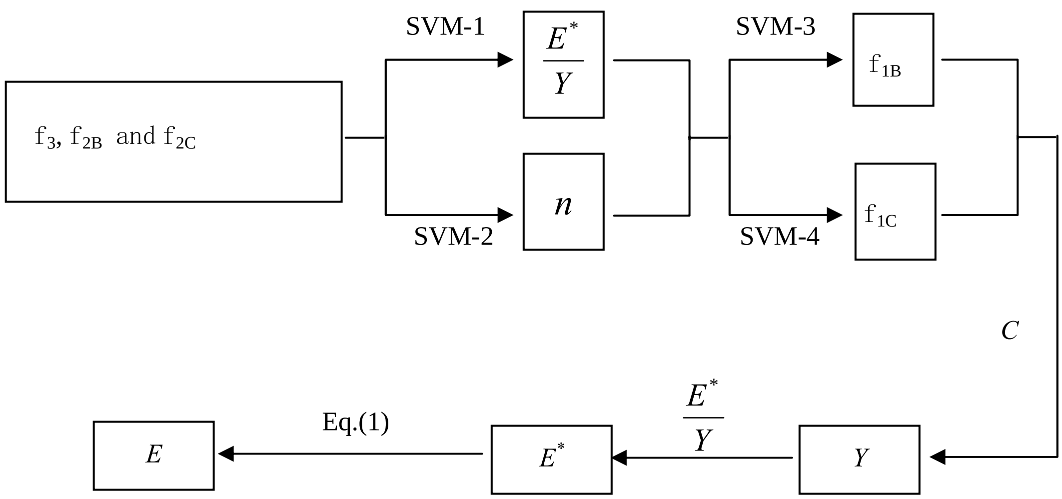


Figure 7: Material Characterization via SVMs.

Table 2: Characteristics of LS-SVMs

	Range of output	Regularization parameter, γ	RBF kernel bandwidth, σ^2
SVM-1	10-1500	10589	0.7778
SVM-2	0-0.6	25134	2.8432
SVM-3	10-420	41406	0.3767
SVM-4	20-850	68161	0.4677

Table 3: Load-Indentation Characteristics of Al6061, Al7075, Steel and Iron

Material	Berkovich Indenter		Conical Indenter	
	C_B (GPa)	$(W_R/W_T)_B$	C_C (GPa)	$(W_R/W_T)_C$
Al6061	28.1	0.915	11.87	0.944
Al7075	46.6	0.858	20.35	0.903
Steel	56.9	0.938	23.907	0.96
Iron	55.9	0.927	24.598	0.949

Table 4: Comparison of Results

	Al6061	Al7075	Steel	Iron
E^* [GPa]				
Actual	70.2	73.4	194.3	170.8
ANN[% deviation]	65.1[-7.2]	77.5[+5.6]	192.5[-0.9]	169.0[-1.1]
SVM [% deviation]	70.9 [+1.1]	71.3[-2.9]	195.7[+0.7]	172.3[+0.9]
Oliver and Pharr Method (Dao et al 2001) [%Deviation]	85.0[+21.1]	86.2[+17.4]	-	-
Y [MPa]				
Actual	284.0	500.0	500.0	300.0
ANN[% deviation]	321.3[+13.2]	572.8[+14.6]	548.4[+9.7]	336.7[+12.2]
SVM [% deviation]	316.8[+11.6]	586.8 [+17.4]	558.2[+11.6]	340.1 [+13.6]
n				
Actual	0.080	0.122	0.1	0.25
ANN[% deviation]	0.043[-46.1]	0.059[-52.0]	0.072[-27.7]	0.225[-10.0]
SVM [% deviation]	0.043 [-45.8]	0.058 [-52.6]	0.068 [-31.9]	0.217 [-13.1]

Y as the values of n of all materials are low ranging from 0.0 to 0.6. It is also not surprising that higher values of deviation for Al6061, Al7075 and steel are observed as compared to that of iron as the values of n for the first 3 types of materials are significantly smaller (0.1 or less) as compared to the higher value of 0.25 for iron.

CONCLUSIONS

Extensive finite element analyses simulating both Berkovich indentatin and conical indentation tests covering wide practical ranges of materials obeying strain hardening power law have been carried out. Characteristics of load-indentation curves have been extracted and depicted as surfaces spanning the wide range of key material properties. Reverse analyses based on dual-indenter approach have been carried out via both traditional artificial neural network model and lease-square support vector machines. The approach alleviates any iteration process as direct mapping between the characteristic values of load-indentation curves and material properties is adopted. Comparison of the predicted results by the proposed models agree reasonably well with reported experimental data. The approach has great potential for material characterization of thin film, MEMS and NEMS.

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