International Journal of Solids and Structures 81 (2016) 151–159

Contents lists available at ScienceDirect

International Journal of Solids and Structures

journal homepage: www.elsevier.com/locate/ijsolstr

Identification of material properties using nanoindentation and surrogate modeling

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ARTICLE INFO

Article history:
Received 28 July 2015
Revised 4 November 2015
Available online 4 December 2015

Keywords:
Nanoindentation
Material properties
Die cast aluminum alloy
Surrogate model
Finite-element analysis
Optimization
Neural networks
Infill sampling criteria
Differential evolution

ABSTRACT

In theory, identification of material properties of microscopic materials, such as thin film or single crystal, could be carried out with physical experimentation followed by simulation and optimization to fit the simulation result to the experimental data. However, the optimization with a number of finite element simulations tends to be computationally expensive. This paper proposes an identification methodology based on nanoindentation that aims at achieving a small number of finite element simulations. The methodology is based on the construction of a surrogate model using artificial neural-networks. A sampling scheme is proposed to improve the quality of the surrogate model. In addition, the differential evolution algorithm is applied to identify the material parameters that match the surrogate model with the experimental data. The proposed methodology is demonstrated with the nanoindentation of an aluminum matrix in a die cast aluminum alloy. The result indicates that the methodology has good computational efficiency and accuracy.

1. Introduction

Contrasting to the conventional material development process, the ongoing project *Reverse 4D Materials Engineering* aims at rapid development of high-performance materials (Toda et al., 2014). The objective of the project is to develop methods and tools that generate the optimum microstructure structure with a minimum computational effort. Such a challenge requires addressing reverse engineering problems and this paper is a first step towards that direction.

Determining material properties is crucial in the design of materials that are resistant to fatigue, wear, and other behaviors. Unfortunately, conventional mechanical methods are often destructive and complex. As an alternative, nanoidentation is a widely recognized technique that is relatively non-destructive and can be applied to small specimens for use in the measurement of mechanical properties of both bulk materials and thin coatings (Haggag et al., 1996).

Much research has been done on methods that extract mechanical properties of materials from indentation tests. For example, Oliver and Pharr proposed an analytical method to nanoindentation-data to estimate hardness and elastic modulus (Oliver and Pharr, 1992). Dao et al. (2001) proposed a reverse algorithm based on explicit equations that enables the extraction of elasto-plastic properties. In the same vein, Cao and Lu (2004) extended the work of Dao et al. to spherical indentation. However, such methods are limited to certain parameters and materials.

Several authors have developed inverse algorithms based on finite element (FE) simulations to extract material properties. Some of these algorithms rely on methods that reduce the number of unknowns. For example, Cheng and Zheng (2004), Ma et al. (2012) and Heinrich et al. (2009) use dimensional analysis for this purpose.

Surrogate modeling has been used as an approach to predict FE simulations. For example, Heinrich et al. (2009) proposed the method of Kriging to predict material properties from nanoindentation curves as an approach of curve fitting between experimental and numerical data. Other researchers used Artificial Neural Networks (ANNs) in which the inputs to the network are defined by the load–displacement response data and the desired outputs are the material

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http://dx.doi.org/10.1016/j.ijsolstr.2015.11.022
0020-7683/

parameters (Huber et al., 2000; Huber and Tsakmakis, 1999; Huber and Tsakmakis, 2004). In their work, response curves are generated by finite element simulations for various parameter combinations in an attempt to match experimental data. However, these methods rely heavily on the finite element simulations which are expensive in terms of computation time. Furthermore, it becomes impractical when the number of parameters increases, since a large dimensional problem require a large number of simulations.

In general, surrogate models are constructed using data drawn from rigourous models (e.g. high-fidelity models), and provide a fast approximation of the original model, making optimization studies more efficient. Surrogate models have been successfully used in the design of aerospace devices (Queipo et al., 2005), heat transfer devices (Qian et al., 2006), chemical process optimization (Caballero and Grossmann, 2008), and combustion engine design (Jakobsson et al., 2010).

In the field of material science and engineering, Jin et al. (2012) used surrogate models combined with sharp indentation, dimensional analysis, and an energy method for calculating residual stress. The surrogate model was constructed as an Artificial Neural Network (ANN) that was trained with 240 finite element simulations, which were validated with other 40 simulations chosen randomly.

Haj-Ali et al. (2008) developed ANN models trained with FE simulations for reproducing nanoindentation curves. However, only the loading part of the curve was used to generate the ANN models.

Theoretically, the application of an optimization technique directly to FE simulations can identify the material parameters. However, a typical optimization would require thousands of function evaluations, which would make this approach impractical. The problem is also complex because the nonlinearity from plasticity and large deformation adds non-convexity to the optimization problem. To cope with these issues, this paper proposes a combination of a sampling scheme, surrogate modeling, and a global optimization approach.

The rest of this paper is organized as follows. Section 2 describes problem statement. The proposed methodology is presented in Section 3. Then, Section 4 discusses a case study to evaluate the proposed approach. Finally, Section 5 provides discussion and conclusions.

2. Problem statement

The proposed approach employs surrogate modeling and a sampling method as the means to reduce the number of FE simulations. Specifically, we focus on the estimation of elastic and plastic parameters from load–displacement curves obtained from nanoindentation experiments. Therefore, the problem is formulated as the minimization of the objective function given in Eq. (1), which is composed of two parts:

1. the error between the experimental load–displacement curve and the curve estimated by the surrogate model (first term in Eq. (1)); and
2. the difference between the areas under the experimental and estimated curves (second term in Eq. (1)).

$$\text{Minimize } \gamma_1 I_{\tilde{f}}(\tilde{\boldsymbol{p}}) + \gamma_2 \left| \int_{x_0}^{x_{final}} f(x, \boldsymbol{p})dx - \int_{x_0}^{x_{final}} \tilde{f}(x, \tilde{\boldsymbol{p}})dx \right| \tag{1}$$

Subject to:

$$g(x, \tilde{\boldsymbol{p}}) = 0 \tag{2}$$

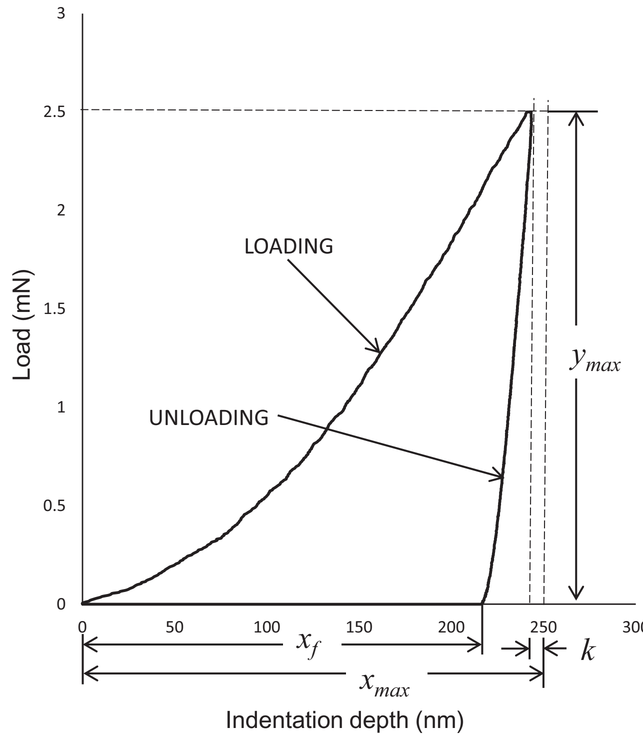

Fig. 1. Indentation load–displacement curve

where $\tilde{\boldsymbol{p}}$ is the decision variable which represents a vector of parameters whose values are known a priori; $\boldsymbol{p}$ is a vector of mechanical parameters which are intrinsically present in the material but whose range and values are initially unknown; $f(x_j, \boldsymbol{p})$ is the experimental indentation-load evaluated at depth (displacement) x_j; $\tilde{f}(x_j, \boldsymbol{p})$ is the indentation-load calculated by the surrogate model at depth x_j; x is the depth of the indenter in the material (the known independent variable); x_0 is the initial value of x, and x_{final} is its last value; $I_{\tilde{f}}(\tilde{\boldsymbol{p}})$ is the root mean square error between the experimental curve and the curve estimated by the surrogate model, as calculated by Eq. (11); and γ_1 and γ_2 are weight parameters. Finally, the constraint $g(x, \boldsymbol{p})$ guarantees that the experimental and predicted responses overlap.

To convert the above constrained-problem into an unconstrained optimization problem, Eq. (2) is added as a penalty function to Eq. (1), resulting in:

$$\text{Minimize } \gamma_1 I_{\tilde{f}}(\tilde{\boldsymbol{p}}) + \gamma_2 \left| \int_{x_0}^{x_{final}} f(x, \boldsymbol{p})dx - \int_{x_0}^{x_{final}} \tilde{f}(x, \tilde{\boldsymbol{p}})dx \right| + \gamma_3\, h(g(x, \boldsymbol{p})) \tag{3}$$

where γ_3 is an additional weight parameter and $h(g(x, \boldsymbol{p}))$ is the penalty function.

If $g(x, \boldsymbol{p})$ represents the requirement to make the curves coincide at the point of maximum depth then $h(g(x, \boldsymbol{p}))$ can be expressed as:

$$h(g(x, \boldsymbol{p})) = |f(x, \boldsymbol{p})|_{x=x_{max}} - |\tilde{f}(x, \tilde{p})|_{x=x_{max}} \tag{4}$$

where x_{max} is the maximum depth of the indenter.

The problem of inferring the parameter vector $\boldsymbol{p}$ from the load–displacement response curves is ill-posed because of the existence of a large number of solutions. To solve this, a global optimization algorithm is applied.

In order to facilitate the quantification of the differences between the experimental data and the simulation, the experimental data is processed by decomposing the original data set into its loading and unloading segments (Fig. 1). Then, in order to obtain continuous and