# DATA-LED MECHANICAL AND THERMAL ANALYSIS OF LAYERED STRUCTURES BASED ON PARAMETRIC FINITE ELEMENT ANALYSIS AND NEURAL NETWORK

# T. KAID<sup>\*</sup>, E. ELMSHAWET<sup>\*</sup>, V. HERENCIA<sup>\*</sup>, X. QING<sup>\*</sup>, L. WANG<sup>†</sup> AND J. REN<sup>\*</sup>

\*School of Engineering, Faculty of Engineering and Technology, Liverpool John Moores University, Liverpool, UK;

e-mail: T.Kaid@2016.ljmu.ac.uk; http://www.ljmu.ac.uk

<sup>†</sup> School of Engineering and Materials Science, Queen Mary University of London, London UK

**Key words:** Layered Structure, Numerical Modelling, Data system, ANN, Synergy in Mechanical-thermal properties

**Abstract.** The mechanical and thermal behaviours of layered structures is of great importance for many advanced material systems and loading conditions. The responses of layered structures are controlled by the constitutive properties of each layer as well as the thicknesses. A comprehensive data-based approach is essential for both material analysis and design in direct or inverse problems. In this work parametric numerical modelling and Artificial Neural Network (ANN) are jointly used to develop data for layered structures. Mechanical and thermal finite element (FE) models are used to produce data for different material property and thickness domains. The use of ANN program is established and evaluated for different loading conditions. Using indentation as a typical case for mechanical loading and localized heating as typical example for thermal loading, ANN program was used to predict the behaviour of layered structures with different properties and layer thicknesses. Use of the data system in establishing dominating factors, synergetic effect on mechanical-thermal performance in advanced materials design is discussed.

# **1 INTRODUCTION**

Layered materials are widely used in different groups, including metals, plastics, rubbers, foams and composites<sup>[1][2][3][4][5]</sup>. Many processing techniques could be used to manufacture layered structures for example, welding, brazing, adhesive bonding, co-injection, compression, etc. In some cases, materials need to satisfy a combination of design requirements, including combination of mechanical and physical properties. In the material design process, it is relatively straight forward to design or estimate the material properties when the material is under uniform/uniaxial loading conditions, either along the in-plane or out-of-plane directions, usually, following a mixture of rules for laminating perfectly bonded structures<sup>[6]</sup>. For localised loading conditions, such as indentation<sup>[7][8]</sup>, the stress strain state is complicated and the constitutive properties of each layer and the thickness. It is even more challenging for complex interface profiles. In addition, for thermal properties, the through-thickness heat conduction under uniform heating can follow a simple rule for perfect contact conditions, but the in-plane

behaviour is difficult to be represented by a normalised conductivity value when the material for each layer has significantly different thermal conductivities. This may cause difficulties in the design, materials selection and analysis processes, more comprehensive data is required for different conditions and applications.

Neural network has been increasingly used to study materials of complex systems for which a robust closed-form analytical solution is not attainable <sup>[9][10][11][12]</sup>. This process is able to predict material behaviours from known properties/structures or inversely used to predict the material properties or geometrical variables. It is particularly useful when multiple variables have to be considered. In many cases it is combined with numerical modelling for situation with complex stress strain conditions or materials such as indentation, in which the stress strain field around the indenter is not uniform even for homogenous materials. For layered systems, a fully trained ANN could be used as a powerful tool in the selection of materials or determine the optimal layers number, sequency and/or layer thickness without the requirement of rerunning multiple FE models. ANN-FE combination can also be used to produce large scale off-line data for design optimisations and analysis, which could be particularly useful for application-specific layered material design.

In this work, a comprehensive data-based approach is explored. Parametric numerical modelling and Artificial Neural Network (ANN) are jointly used to develop data for layered structures under indentation loading and thermal loading. Different types of data are produced from the FE models then trained with different programs including the Levenberg-Marquardt and Bayesian Regularization. The use of ANN program for predicting different types of data is presented associated with varying layer properties or thickness. The work highlighted some key dominating factors for layered system and key issues for mechanical-thermal performance design and analysis is discussed

#### 2 FE MODELS AND DATA DEVELOPMENT

#### 2.1 FE indentation models

Figures 1&2 show typical indentation and thermal models of a layered system. A parametric program is produced with the key parameters of the .inp file, which allows altering sample size, number of layers, layer thickness, etc. Other tunable parameters also include material properties for each layer with both linear and nonlinear models. The interface profiles between each layer can also be changed to include curved interfaces. The work in this paper is focused on presenting some typical data with straight layer interfaces. A python program with loop function is used for the purpose of extracting the key data (such as P-h curves, temperature profiles) from multiple models. The program automatically open ABAQUS .odb files from the parametric studies, extract the data, and save them as data file, which can be used as input/target in the ANN program.

For the indentation model (Figure 1), the indenter shape/size, indentation depth can all be parameterized. The contact condition, frictional coefficient can be varied when dealing with different materials. A range of data such as indentation force-displacement data (a typical data is shown in Figure 1(b)) and other key deformation data (the stress between each layer, the sinking-in and pile up) can also be used as the target data.



(a) Typical FE model of indentation process (b) Typical force-indentation depth data. with a rigid spherical indenter.

**Figure 1** FE model of spherical indentation of layered systems and typical force-indentation depth data.

#### 2.2 Thermal model o layered systems

Two typical types of thermal models are shown in Figure 2. Figure (a) is for a situation in which the heat is applied uniformly for through-thickness heat transfer, Figure (b) shows a situation where the heat is applied over a finite length (localized heat flux). For a layered system with straight interfaces, the temperature could be effectively transfer through the layers represented by the effective thermal conductivity for case of the through-thickness conduction. Under uniform heat transfer (Figure a), the normalized effective thermal conductivity is not significantly affected by how many layers rather than the overall volume fraction under a perfect contact condition/assumption. However, it could be influenced by the interfacial heat transfer coefficient and profiles as well as contact conditions (imperfect contacts), which can be considered in the FE model through parametric studies. The localized/finite heating area model reflects a case in which the heat conduction is affected by the through-thickness and in-plane configuration in particular the layer stacking sequence. In the model, the heat can be applied either across the surface or localized areas through parametric studies. These features allow a comprehensive data set to be produced reflecting different loading and boundary conditions to study the effects of variables with different level of significance.





(a) FE model of through-thickness (b) FE model of localized heating model. (Steady state)
Figure 2 Typical thermal models of layered systems and typical data.

#### 2.3 ANN

ANN has been developed into a generalized tool, which can be used for both, direct or inverse modelling processes. The direct approach is useful for materials and thickness selection in design while inverse modelling can be used for predicting the properties and other parameters which cannot be measured directly. The nature of the data input is critical to the performance of an ANN program. The FE parametric modelling allows production of data for ANN in an effective way. It also allows a systematic assessment of ANN's performance rather than an assessment based on limited amount of data. Figure 3 shows the general structure of the proposed ANN's network. The program used a back-propagation learning method, which is applicable to a multilayer network that uses differentiable activation functions and supervised training. As illustrated in figure 3, the forward connections are used for both the learning and operational phases, while the backward linkages are used only for the learning phase. Each training pattern is propagated forward, layer by layer until an output pattern is computed. The computed output is then compared to a desired/target output and an error value is determined.

The errors are then used as inputs to feedback connections from which adjustments are made to the synaptic weights layer by layer in a backward direction. Different optimisation algorithms were evaluated including the Levenberg-Marquardt, Bayesian Regularization and Scaled Conjugate Gradient. As the work is focused on practical application of ANN, the evaluation has been focused on key issues such as their accuracy, time to converge for acceptable accuracy, sensitivity to number of training, testing and validation data. It was also tested based on its sensitive to data perturbation and bias on data continuity, which will enhance the practical application function of the program. For ANN, a large number of data will be required. Both data input and image-based approaches have been developed. This work is to focus on data input approach. For example, different approaches have been proposed to represent the P-h curves. One is using trendline method, the other is to use force at different depth. The optimisation of the ANN has been focused on selection of transformation function, use of early stopping, number of neurons, etc. In the thermal modelling with the localized heating, the temperature can be represented by the temperature profiles at key location such as the horizontal line on the surface away from the heating zone and the vertical line underneath the heating zone.



Figure 3 Proposed feed-forward neural network with back propagation algorithms.

## **3 TYPICAL DATA AND ANALYSIS**

#### 3.1 Typical indentations data of different material systems

The force-displacement data for a layered material is affected by many factors such as layer thickness, properties and interface properties. One typical case is the properties of each layer. Figure 4 shows a typical training process of ANN based on material properties of a two layers system: the stiffness of the two layers E1 and E2 are varied, the thickness of the two layers are fixed and supported by a stiffer base. The stiffness is ranged between 1-5MPa for the two layers. This is part of a research in developing conductive rubbers for corrosion control in welded metal systems, for which the conductivity needs to be increased in the meantime maintaining the softness/flexibility of the materials. Different training algorithm has been explored including The Levenberg-Marquardt (LM), Bayesian Regularization (BR) and Scaled Conjugate Gradient (SCG). As shown in the figures, both the LM approach and the BR approach are able to converge quickly, and the Mean Squared Error (MSE) and the R squared error shows that the system is able to achieve a high level of fitting of the indentation depth-forces data.



(a) ANN fitting process: MSE. (LM)



(c) ANN fitting process: MSE (BR)



(b) R squared error for training, testing and validation. (LM)



(d) R squared error for training, testing and validation. (BR)

**Figure 4** Typical ANN traing with the Levenberg-Marquardt (LM) and Bayesian Regularization (BR) approach.

#### T. KAID, V. E. ELMSHAWET, V. ZEVALLOS HERENCIA, X. QING, L. WANG AND J. REN

Figure 5 shows typical error when predicting indentation data using the LM algorithms and Bayesian Regularization. Figure 5(a) is the prediction accuracy of the data used in the training, while Figure 5(b) is the prediction accuracy/error range for data that have not been used in the training. Many different sets of data have been tested and these are some typical results reflecting the range of error. In both cases the error range is relatively low. The error for the untrained data is slightly higher in some data set than that of the trained data but both are within a reasonable range for materials design. The error of predicted data based on the Bayesian Regularization is better than LM, but no major difference on the design margins.





Figure 6 shows a typical fitting process of thermal model with localized heat flux over a finite area. In the model, the thermal properties of the materials are fixed and the thickness for the two layers are varied. Figures 6 (a&b) is the fitting data for temperature distribution along the vertical line underneath the heating zone with Levenberg–Marquardt algorithm and Bayesian regularization. Figure 6(c&d) is the fitting process for the temperature profile along the horizontal line away from the heating area. In both cases, low MSE has been reached showing that ANN is effective in predict the temperature distribution.



(a) Mean squared error in ANN training for fitting temperature distribution underneath the heating zone (Levenberg–Marquardt algorithm).



(b) Mean squared error in ANN training for fitting temperature distribution underneath the heating zone (Bayesian regularization).



- (c) Mean squared error in ANN training for fitting temperature distribution along the horizontal line away from the heating zone. (Levenberg– Marquardt algorithm)
- (d) Mean squared error in ANN training for fitting temperature distribution along the horizontal line away from the heating zone. (Bayesian regularization)

Figure 6 Typical ANN training data for the temperature distribution along the vertical line underneath the heating zone and the horizontal line away from the heating zone.

Figure 7(a) shows typical prediction accuracy/error range for thickness data that has not been used in the training (LM approach). An average error value is used to represent the difference between the predicted temperature profile and the target values of the temperature along the horizontal lines. Many different sets of data have been tested and these are some typical results representing the range of error. The error for the untrained data is within 5%. The error for the trained data is much better (not shown). This suggests that the ANN is effective in predicting the temperature profile along the horizontal lines away from the center of the heating area predicted by the ANN. The data near the heating zone shows no major difference between different layer thickness combination, but there is a clear difference away from the thermal behavior of a layered system.



(a) Average error of the ANN predicted temperature using untrained data



(b) ANN predicted temperature profile for different combination of layer thicknesses (in mm).

**Figure 7** Typical ANN fitting data and predicted data of the temperature distribution alon the horizontal line away from the heating zone.

# **4 DISCUSSION**

Layered structures offer the freedom in design properties balancing the mechanical and functional properties. For indentation resistance the contribution of each layer is dependent on the properties and the thickness of the layer as well as the indentation depth. For homogeneous materials, the elastic behavior can be represented by the analytical solution at lower strain levels. But for layered system the force-displacement is complicated and difficult to be represented by simple model. This becomes even more complicated with nonlinear properties in different material property domains (elastic-plastic, hyperelastic and hyperfoam models). For example, the post yielding behaviors of an elastic plastic make it more difficult to predict the indentation force as the factor of significance varies with the strain levels<sup>[13]</sup>. Similarly, hyperelastic or hyperfoam behavior also make it more difficult to predict once the material reaches the plateau stage or the densification stage<sup>[14]</sup>. ANN program offers the flexibility in the number and forms of input and the data type of output. The Bayesian regulation also offers the capacity to deal with limited numbers. The output offers more flexibility, including data, curves or even images. For example, the force-displacement data can be represented by either the coefficients of the curve or directly by the force data. This is essential for developing practical applications of data for applications with outcome relevant to different service requirements. As illustrated by FE and ANN data, the thermal conductivity process combined with thickness and in-plane directions of layered systems, could be complicated, particularly for localised heating. In many cases, the properties of material could not be represented by a single effective or normalised values. The ANN approach offers a way to predict complex temperature distributions. As shown in Figure 7, the temperature at specific locations can be predicted for different layer thicknesses. This is applicable to many material systems such as metal, rubber, and foams. For composites materials, the filler could significantly affect the thermal properties of matrix such as rubber. In foam materials, the thermal properties can be modified by controlling the porous structures, the length and thickness of the cell wall or beams. The recent development in advanced joining (such as hybrid welding) has also opened new

opportunities, which can joint materials with different properties and interfacial profiles. For example, stainless steel (either single phase or duplex stainless steels (DSS)) are increasingly being bonded with other steels, aluminum and coppers to balance the corrosion, toughness and thermal properties. These metals have significant difference in thermal conductivities. The thermal conductivity of stainless steel is much lower than that of aluminum and coppers. The large range of thermal properties could offer more freedom on the design optimization process. The approach also offers data relevant to some manufacturing process such as welding. For example, in electrical resistance welding of layered structures, the heat is generated over a local area, predictive data within a certain range for the heat transfer over the layered (both throughthickness and in-plane) is useful for the welding process design. In additional, the development of 3D printing and additive manufacturing also offer the capacity to produce gradient or layered systems with controlled properties. All these examples are clearly indicating that there is an opportunity to tune both the mechanical and thermal process by combining FE and ANN, offering an effective alternative to pure experimentally based approached. Future work would include developing FE-ANN models to modulate synergy of mechanical, thermal, and other properties by tuning multiple materials and geometrical parameters.

### **5 SUMMARY**

In this work, a comprehensive data-based approach is explored for both layered material analysis and design. Parametric numerical modelling and artificial neural network are jointly used to develop a data system for layered structures. Different types of data are produced from the FE models then used in training, testing and validation of ANN with different programs including the Levenberg-Marquardt and Bayesian Regularization. The data for some typical cases of mechanical loading (indentation with a spherical indenter) and thermal loading (localised heating) is presented. The use of ANN program for predicting different types of data is presented associated with varying layer properties or thickness. The work highlighted some key factors for layered system, relevant application cases in materials and manufacturing. The key issues for mechanical-thermal performance design and analysis are also discussed.

#### **6** ACKNOWLEDGEMENT

The fundamental study and framework development is supported by the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie grant agreement (No 823786).

#### REFERENCES

- [1] Kuteneva S.V., Gladkovsky S.V., Vichuzhanin D.I., Nedzvetsky P.D., Microstructure and properties of layered metal/rubber composites subjected to cyclic and impact loading, *Composite Structures* (2022), 285(1), 1150781.
- [2] Xiang X., Zou S., Ha N.S., Lu G.X., Kong I. Energy absorption of bio-inspired multilayered graded foam-filled structures under axial crushing, *Composites Part B: Engineering* (2020), 198(1), 108216.

- [3] McCoy J.H, Kumara A.S., Stubbins J.F., Deformation and fracture of Cu alloy-stainless steel layered structures under dynamic loading, *Journal of Nuclear Materials*(1998), 258– 263, 1033-1039.
- [4] Alizadeh-Sh M., Marashi S.P.H., Resistance spot welding of dissimilar austenitic/duplex stainless steels: Microstructural evolution and failure mode analysis, *Journal of Manufacturing Processes* (2017), 28(1),186-196.
- [5] Jiang J., Liang Y., and Song G., Detection of interfacial debonding in a rubber- steellayered structure using active sensing enabled by embedded piezoceramic transducers, *Sensors (Basel)* (2017), 7(9).
- [6] Öchsner A., Foundations of Classical Laminate Theory, Advanced Structured Materials, *STRUCTMAT*, 163.
- [7] Dossa B.L., Eliato K.R., Lin K. and Ros R., Quantitative mechanical analysis of indentations on layered, soft elastic materials, *Soft Matter* (2019),15, 1776-1784.
- [8] Sachan D., Sharma I., Muthukumar T., Indentation of a periodically layered, planar, elastic half-space, *Journal of Elasticity* (2020), 141, 1–30.
- [9] Sha W., Edwards K.L., The use of artificial neural networks in materials science based research, *Materials & Design* (2007), 28(6) 1747-1752.
- [10] Hellström M. and Behler J., Neural Network Potentials in Materials Modeling, *Handbook* of Materials Modeling(2018), 1–20.
- [11] Bhadeshia H. K. D. H., Dimitriu R. C., Forsik S., Pak J. H. & Ryu J. H., Performance of neural networks in materials science, *Materials Science and Technology* (2009), 25(4).
- [12] Thankachan T., Prakash K.S. and Jothi S. Artificial neural network modeling to evaluate and predict the mechanical strength of duplex stainless steel during casting, *Sādhanā* (2021), 46, 197.
- [13] Kang B. S.J, Yao Z. and Barbero J. E., Post-yielding stress-strain determination using spherical indentation, *Mechanics of Advanced Materials and Structures* (2006), 13, 129-138.
- [14] Li B., Gu Y.D., English R., Rothwell G., Ren X.J., Characterisation of nonlinear material parameters of foams based on indentation tests, *Materials and Design* (2009), 30:2708-2714.