A MACHINE LEARNING-BASED DESIGN APPROACH FOR OPTIMISING IMPEDANCE-GRADED MULTI-METALLIC SYSTEMS SUBJECTED TO SHOCK WAVE PROPAGATION

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DECLARATION

I declare that this is my own work and this thesis/dissertation does not incorporate without acknowledgement any material previously submitted for a degree or diploma in any other university or institute of higher learning and to the best of my knowledge and belief it does not contain any material previously published or written by another person except where the acknowledgement is made in the text. I retain the right to use this content in whole or part in future works (such as articles or books).

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The above candidate has carried out research for the PhD/MPhil/Masters thesis/dissertation under my supervision. I confirm that the declaration made above by the student is true and correct.

Name of Supervisor: Dr P.L.N. Fernando

Signature of the Supervisor: Date:06.02.2026

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ABSTRACT

Understanding and predicting shock wave propagation in functionally graded multi-material systems is critical for advancing impact-resistant materials. As such, impedance-graded multi-metallic (IGMM) systems, where the materials are arranged in their reducing order of impedance, have shown to offer superior performance over monolithic materials by effectively mitigating the effects of shock wave transmission. Due to complex relationships among variables that influence performance of IGMM systems (e.g. individual metal layer thicknesses, total thickness, and impact velocity or stress), using numerical modelling techniques to study each parameter can be time-consuming. In contrast, machine learning (ML) models, once trained, have the potential to provide quick responses with minimal user input. Therefore, this study introduces an ML-based approach to predict stress-time history, velocity-time history, and maximum tensile stress at the final layer in IGMM systems consisting of steel, titanium, and aluminium, subjected to high-velocity impacts generating shock waves in materials. A total of 370 impact events were simulated using LS-DYNA, changing the input variables, to generate datasets for training and testing three tree-based ML models; Decision Tree, Random Forest, and Extreme Gradient Boost (XGB). Experimental results from a previously conducted single-stage gas gun test were used in the numerical model validation. XGB outperformed other models, achieving testing coefficient of determination (R^2) values of 0.98 and 0.99 for stress and velocity-time history predictions, and 0.92 for maximum tensile stress predictions. Shapley Additive Explanations (SHAP), which is an explainable machine learning technique, were used to interpret how material and system parameters influence predictions, ensuring alignment with fundamental shock wave physics. Finally, an inverse prediction framework was developed to identify optimal thickness combinations of steel, titanium, and aluminium that meet predefined mechanical performance criteria. This study acts as an interpretable, data-driven alternative to numerical modelling which offers a feasible approach to optimising IGMM systems under shock wave propagation.

Keywords: Impedance-graded multi-metallic systems; Machine learning; Shapley Additive Explanations; Shock wave propagation; Optimal thickness combinations

TABLE OF CONTENTS

DECLARATION i
ACKNOWLEDGEMENT ii
ABSTRACT iii
TABLE OF CONTENTS iv
LIST OF FIGURES vi
LIST OF TABLES viii
LIST OF ABBREVIATIONS ix
LIST OF APPENDICES xi
CHAPTER 1 1
1 INTRODUCTION 1
1.1 Background 1
1.2 Research Problem 3
1.3 Scope of the Study 3
1.4 Aim 4
1.5 Objectives 4
1.6 Significance of the Research 5
1.7 Outline of the Thesis 5
CHAPTER 2 6
2 LITERATURE REVIEW 6
2.1 Introduction 6
2.2 Impedance-Graded Multi-Metallic (IGMM) Systems 6
2.3 Shock Wave Propagation 10
2.4 Machine Learning (ML) in Structural Response Predictions 11
2.5 Identified Research Gap 13
CHAPTER 3 15
3 METHODOLOGY 15
3.1 Introduction 15
3.2 Experimental Program 16
3.3 Analytical Study 18

3.4 Numerical Modelling 19
3.4.1 Numerical modelling methodology 20
3.4.2 Mesh sensitivity analysis 21
3.4.3 Validating numerical models 22
3.4.4 Generation of the datasets 23
3.5 Machine Learning (ML) 27
3.5.1 Data preprocessing 27
3.5.2 Algorithms for modelling 30
3.5.3 Explainable machine learning (XML) 33
3.5.4 Software environment and Python libraries 35
CHAPTER 4 36
4 RESULTS AND DISCUSSIONS 36
4.1 Introduction 36
4.2 ML Model Training and Hyperparameter Optimisation 36
4.3 ML Model Performance Evaluation 38
4.4 Explainable Machine Learning (XML) Analysis for Impact Loading Responses 44
4.4.1 Stress-time history prediction 44
4.4.2 Velocity-time history prediction 45
4.4.3 Maximum tensile stress prediction 47
4.4.4 SHAP-based optimisation 48
4.5 Inverse Prediction 49
CHAPTER 5 53
5 CONCLUSIONS 53
REFERENCES 55

LIST OF FIGURES

Fig. 2.1: Stress waves propagation through an IGMM system. Adapted from Fernando et al., 2019 [15] 7

Fig. 2.2: Numerical model geometries used for simulating (a) 1D and (b) 2D wave propagation in IGMM systems. Adapted from Fernando et al., 2019 [15] 8

Fig. 2.3: Protective application of monolithic and IGMM systems in a concrete structure. Adapted from Fernando, 2019 [16] 9

Fig. 2.4: Setup utilised in ballistic performance study of multi-metal systems. Adapted from Ranaweera et al., 2020 [18] 10

Fig. 2.5: Typical shock wave profile (a) for a homogeneous medium and (b) for a heterogeneous/layered medium. Adapted from Shah et al., 2025 [28] 11

Fig. 3.1: Proposed methodology of this study 15

Fig. 3.2: (a) Overall experimental setup and (b) main chamber. Adapted from Fernando et al., 2020 [20] 16

Fig. 3.3: (a) Mono-metallic – C1, (b) bi-metallic – C2, and (c) tri-metallic – C3 target configurations. Adapted from Fernando et al., 2020 [20] 16

Fig. 3.4: (a) Flyer assembly with the sabot and (b) target assembly with the ring. Adapted from Fernando et al., 2020 [20] 17

Fig. 3.5: Development of the two-dimensional numerical model based on the axisymmetric representation of the three-dimensional model 20

Fig. 3.6: (a) Stress vs mesh size variation from mesh sensitivity study and (b) zoomed-in region of interest 22

Fig. 3.7: Comparison of free surface velocity history from experiment and back face velocity history from numerical model 23

Fig. 3.8: Data extraction locations on the aluminium target 24

Fig. 3.9: (a) Stress-time history at the centre of the aluminium and (b) Velocity-time history at the back face of the aluminium for Models a, b, c, and d 26

Fig. 3.10: Distribution of the dependent variables (a) Y-Stress, (b) Y-Velocity, and (c) Maximum tensile stress 28

Fig. 3.11: Pairwise correlation plot 30

Fig. 4.1: Comparison of overall predictions and numerical results: Stress-time history 40

Fig. 4.2: Comparison of overall predictions and numerical results: Velocity-time history 40

Fig. 4.3: Comparison of overall predictions and numerical results: Maximum tensile stress 41

Fig. 4.4: Comparison of R^2 of optimised tree-based model predictions 42
Fig. 4.5: Comparison of predicted and numerical responses for ‘Model a’ – (a) stress-time history and (b) velocity-time history 43
Fig. 4.6: SHAP global explanation for stress-time history prediction 44
Fig. 4.7: SHAP global explanation for velocity-time history prediction 46
Fig. 4.8: SHAP global explanation for maximum tensile stress prediction 47
Fig. 4.9: Workflow of inverse prediction process 50
Fig. B.1: Numerical simulation results of (a) Stress-time history and (b) Velocity-time history for all 370 impact events 64
Fig. B.2: Numerical simulation results of (a) Stress-time history and (b) Velocity-time history for selected impact events in Table B.1 65
Fig. B.3: Numerical simulation results of (a) Stress-time history and (b) Velocity-time history for selected impact events in Table B.2 66
Fig. C.1: Pairwise scatter plot matrix of input and output features 67
Fig. D.1: Comparison of numerical and ML-predicted stress-time histories for selected impact events 69
Fig. D.2: Comparison of numerical and ML-predicted velocity-time histories for selected impact events 70

LIST OF TABLES

Table 3.1: Material properties of metals. Adapted from Fernando et al., 2020 [20] 18

Table 3.2: Material parameters used for numerical models 21

Table 3.3: Overview of LS-DYNA models utilised for dataset generation 25

Table 3.4: Model combinations with varying target thickness and initial stress for impact analysis 26

Table 3.5: Data description for training ML models 27

Table 3.6: Descriptive statistics of the independent and dependent variables 28

Table 4.1: Hyperparameter configurations tested during optimisation and corresponding optimal results from random search method 37

Table 4.2: Estimated computational requirements for simulation and model training 38

Table 4.3: Performance indices for optimised tree-based models 42

Table 4.4: Effect of target features on the reduction of stress-time history, velocity-time history, and maximum tensile stress predictions 48

Table 4.5: Numerical model results for configurations with 30 mm total thickness at 12 GPa initial stress level 49

Table 4.6: Optimal thickness configurations satisfying both Y-Stress and Y-Velocity criteria 51

Table A.1: IGMM target combinations used in the study 62

Table B.1: IGMM system combinations with total thickness of 30 mm under 12 GPa impact stress 65

Table B.2: IGMM system combinations of varying thicknesses subjected to all initial stress levels 66

Table D.1: Selected impact events for comparative evaluation of numerical and ML-predicted responses 68

LIST OF ABBREVIATIONS

ANN	Artificial Neural Network
BPNN	Back-Propagation Neural Network
C_0	Bulk Sound Velocity
DT	Decision Tree
e	Internal Energy
FEM	Finite Element Method
FGM	Functionally Graded Materials
GBM	Gradient Boosting Machine Learning
g_x	Expected Value for SHAP Function
h	Explanation Model
HEL	Hugoniot Elastic Limit
IGMM	Impedance-Graded Multi-Metallic
K	Input Feature Subset
KNN	K-Nearest Neighbors
LIME	Local Interpretable Model-agnostic Explanation
M	Complete Input Set
MAE	Mean Absolute Error
ML	Machine Learning
N	Maximum Coalition Size
nMAE	Normalised Mean Absolute Error
nRMSE	Normalised Root Mean Squared Error
P	Pressure
R	Pearson Correlation Coefficient
R^2	Coefficient of Determination
RC	Reinforced Concrete
RF	Random Forest
RMSE	Root Mean Squared Error
s	Dimensionless Parameter in Hugoniots
SSE	Sum of Squared Errors
SHAP	Shapley Additive Explanations

SVC	Support Vector Classifier
SVR	Support Vector Regression
U_s	Shock Velocity
u_{HEL}	Particle Velocity at HEL
u_p	Particle Velocity
v	Poisson's Ratio
VEcv	Variance Explained by Cross-Validation
VI	Variable Importance
XGB	Extreme Gradient Boost
XML	Explainable Machine Learning
Y_d	Dynamic Yield Stress
Z	Impedance
$\acute{z}$	Fundamental Features
ρ	Density
$\emptyset$	Feature Attribution

LIST OF APPENDICES

Appendix A: Impedance-Graded Multi-Metallic (IGMM) Target Combinations..... 62

Appendix B: Numerical Simulation Results of Responses under Varying Impact Conditions 64

Appendix C: Pairwise Scatter Plot Matrix of Input and Output Features.................. 67

Appendix D: Comparison of Numerical Simulation Results and Predicted Results of Responses 68