Predicting Stress-Strain Curves of Irradiated Eurofer 97 from Indentation Curves using Deep Learning

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ABSTRACT

In the field of materials science, understanding the mechanical behavior of irradiated materials is crucial for the design and development of advanced nuclear systems. Eurofer 97, a reduced-activation ferritic/martensitic steel, is a widely used structural material in such systems. However, accurately predicting the stress-strain curves of irradiated Eurofer 97 presents a significant challenge due to the complex interaction of various factors.

In this study, we propose a novel approach to predict stress-strain curves of irradiated Eurofer 97 using deep learning techniques. Specifically, we employ an LSTM-based (Long Short-Term Memory) model, a recurrent neural network well-suited for sequence prediction tasks. The input data for our model consists of indentation curves, which are commonly used to extract material properties such as hardness and elastic modulus.

By training the LSTM model on a dataset comprising indentation curves and corresponding stress-strain curves of Eurofer 97, we aim to capture the underlying relationships between indentation and mechanical behavior. The model learns to recognize patterns in the indentation data and subsequently generates predictions of stress-strain curves for irradiated Eurofer 97.

Introduction

Micro-indentation and nano-indentation are experimental techniques used to characterize the mechanical properties of materials at small scales. In micro-indentation, a small indenter tip is pressed into the material surface, creating a controlled indentation. Important material properties such as hardness and elastic modulus can be determined by measuring the depth and load during indentation. Nano-indentation is a similar technique but performed at a smaller scale, allowing for more precise measurements.

On the other hand, stress-strain curves provide valuable information about a material’s mechanical behavior under applied stress. They depict the relationship between stress (force per unit area) and strain (deformation) experienced by a material. Stress-strain curves exhibit various regions, including elastic deformation, plastic deformation, and failure. These curves offer insights into a material’s stiffness, yield strength, and ability to resist deformation. Understanding micro-indentation, nano-indentation, and stress-strain behavior is crucial for material characterization, design, and analysis in fields such as materials science, engineering, and biomechanics.

Obtaining stress-strain data is generally more challenging than micro-indentation data due to the complexity and sophistication of the experimental setup involved. Stress-strain data requires subjecting a material to controlled and gradually increasing stress levels while simultaneously measuring the resulting strain. This typically requires specialized equipment, such as a mechanical testing machine capable of applying precise loads and capturing accurate strain measurements. Additionally, the testing procedure for stress-strain analysis often involves sample preparation and careful alignment, ensuring consistent and reliable results. In contrast, micro-indentation data can be obtained relatively easily by performing localized indentations on the material’s surface, requiring less complex instrumentation and setup.

In this study, our objective is to extract macro-scale properties, such as Young’s modulus and stiffness, using readily available micro/nano-indentation data. To achieve this, we propose utilizing a Long Short-Term Memory (LSTM) based model, a type of recurrent neural network, which allows us to process the indentation data as an input sequence to obtain the desired macro-scale properties. LSTM, or Long Short-Term Memory, is a type of recurrent neural network architecture that excels at capturing long-term dependencies in sequential data. In our problem of predicting stress-strain curves from indentation data, LSTM is employed to effectively model the sequential relationships and patterns within the indentation sequence.
Additionally, we aim to establish the reliability and generalizability of the proposed LSTM model by evaluating its performance on previously unseen data samples. By demonstrating its effectiveness in predicting macro-scale properties from micro/nano-indentation data, we seek to validate the applicability and utility of this model for efficient material characterization and analysis.

1 Data Pre-processing

The micro-indentation dataset has a few peculiarities that make it difficult to work with. A series of essential data pre-processing steps were implemented to address these challenges. Firstly, a smoothing procedure was applied to reduce noise and irregularities. The micro-indentation dataset was then uniformly sampled to ensure a consistent length across all samples. This is demonstrated in Fig. 1.

Similarly, the stress-strain curve necessitated data pre-processing procedures. Initially, the data were appropriately shifted so as to start at zero stress and strain. After that, the data is smoothened. This can be seen in Figure 2.

![Figure 1. Preprocessing: Micro-indentation](image)

Methodology

1.1 Pipeline

Our study presents a well-defined pipeline for predicting stress-strain curves from indentation data. The pipeline comprises several crucial steps. Initially, the input indentation data and the corresponding output stress-strain data undergo thorough preprocessing and cleaning procedures to ensure the data’s quality and consistency. Subsequently, the cleaned input indentation data is augmented with additional features generated in parallel. This augmented input is then used to train the model.

Once the model is trained, it can be employed to predict stress-strain curves for unseen configurations of the same material but at different temperatures. By providing the appropriate inputs for the unseen temperature, the model utilizes its learned knowledge to generate accurate predictions of the stress-strain curve for the given configuration. This enables the assessment of the material’s mechanical behavior at various temperature conditions, aiding in the understanding and optimizing its performance in different operating conditions without requiring explicit tensile analysis.

1.2 Model Architecture

The proposed model architecture for predicting stress-strain curves from indentation data consists of several interconnected layers. The indentation data is initially provided as a sequence input to the LSTM cell, which allows the model to capture sequential dependencies and patterns within the data. The output from the LSTM cell is then connected to a fully connected layer.
**Figure 2.** Preprocessing: Stress-strain

**LEARNING PIPELINE**

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<th>DBTT (°C)</th>
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P-h curves except 400°C and Stress Strain curves except 400°C

P-h curve for 400°C and Predicted Stress Strain curve for 400°C

**Figure 3.** Workflow: The indentation and stress-strain data are cleaned, augmented with additional features, and fed to the model. The model is used to predict macro-scale properties at unseen configurations.
Simultaneously, other relevant features are processed through a parallel, fully connected layer, enabling the model to incorporate additional information alongside the indentation data. The output from the LSTM and feature sides are concatenated to combine their respective representations.

**MODEL**

![Diagram](image)

**Figure 4.** Model: architecture

The concatenated output is subsequently passed through a fully connected layer, followed by a rectified linear unit (ReLU) activation layer, which introduces non-linearity and enhances the model’s expressive capabilities. Finally, the output is passed through another fully connected layer to obtain the regression output, representing the predicted stress-strain curve.

This model architecture effectively integrates both the temporal information from the indentation data through the LSTM cell and the additional features through the parallel fully connected layer, enabling comprehensive and accurate predictions of stress-strain curves.

**Results**

**Using Extra features**
This is our standard pipeline; the indentation input is appended using additional features, and then the model gives us the predictions. As we see from the figure, the model is powerful enough to learn good mappings from P-h curves to Stress Strain (SS) curves using very few data points.

**Without using Extra features**
In this case, we do not use additional features, i.e., the indentation input is used as is, and then the model gives us the predictions. As we see from the figure, the model cannot generate accurate mappings from P-h curves to Stress Strain (SS) curves.

**Discussion**

- Sequence to Sequence models, like the LSTM model, are able to learn accurate mappings from P-h (indentation) curves to Stress Strain (SS) curves, even with limited data points.

- Incorporating extra features alongside the indentation data is critical in enhancing the learning process and achieving good mappings. These additional features provide supplementary information that enriches the model’s understanding of the underlying relationships between P-h curves and SS curves.
Figure 5. Force-Extension prediction with linear Features

Figure 6. Force-Extension prediction without Features
• The absence or inability to provide extra features alongside the indentation data has detrimental effects on the accuracy of the learned mappings and overall results.

• Having more relevant data, a better feature set leads to better learning outcomes.