**Machine Learning Modelling of Potential Energy Based on Thermal Parameters of CuNi alloy**

**Abstract**

In this study, we develop a predictive model to estimate the potential energy (PE) of CuNi alloys using molecular dynamics (MD) simulation data. The model leverages a simple linear regression approach, using temperature and volume as input features to predict PE, demonstrating an interpretable and computationally efficient alternative to more complex methods. MD simulations were performed to generate a dataset capturing a range of thermodynamic states, which was then normalized and split into training and testing sets for model development. The linear regression model successfully captures the relationship between the structural variables and potential energy, achieving robust predictive performance while maintaining simplicity. This approach provides an effective framework for rapid estimation of PE in CuNi systems, offering valuable insights for materials modelling and enabling efficient exploration of thermomechanical behaviour without extensive computational cost.

**Keywords:** CuNi alloy, Molecular dynamics, Potential energy prediction, Linear regression, Temperature, Volume, Materials modelling.

**Introduction**

Copper-nickel (CuNi) alloys are renowned for their exceptional mechanical properties, including high strength, corrosion resistance, and excellent thermal and electrical conductivity. These attributes make them ideal candidates for a wide range of applications, such as in marine engineering, heat exchangers, and electronic components. While significant research has been dedicated to understanding the bulk properties of CuNi alloys, a comprehensive understanding of their atomistic-level behaviors remains limited. Accurate prediction of potential energy (PE) is crucial for elucidating structural stability, phase transformations, and mechanical responses under varying conditions.

Molecular dynamics (MD) simulations serve as a powerful tool for probing atomic-level properties in metallic alloys. Classical MD (CMD) simulations, utilizing predefined empirical interatomic potentials (EIPs), are commonly employed for CuNi systems due to their computational efficiency. These simulations provide valuable insights into energy and force distributions across various thermodynamic states. However, EIP-based CMD simulations are limited by the accuracy of the empirical potential and may fail to capture subtle energy fluctuations or the influence of temperature and volume variations outside the calibrated range.

Conversely, ab initio MD (AIMD) simulations, based on density functional theory (DFT), offer high accuracy in predicting atomic interactions but are computationally intensive and impractical for large-scale simulations or extensive parameter sweeps. The computational cost and time constraints associated with AIMD simulations hinder their applicability in studying complex systems and exploring a wide range of thermodynamic conditions.

To address these challenges, data-driven approaches have emerged as effective alternatives for predicting PE with reduced computational overhead. Machine learning (ML) techniques, particularly linear regression models, offer a promising avenue for constructing predictive models that can estimate PE based on easily accessible thermodynamic variables such as temperature and volume. By training a linear regression model on data generated from CMD simulations, it is possible to develop a predictive framework that balances computational efficiency with predictive accuracy.

In this study, we employ a linear regression model to predict the potential energy of CuNi alloys. The model utilizes temperature and volume as input features, providing an interpretable and efficient framework to estimate PE across a range of thermodynamic conditions. The training data, generated from CMD simulations, are normalized and split into training and testing sets to ensure robust evaluation. The linear regression model allows rapid predictions while maintaining reasonable accuracy, offering a practical compromise between computational efficiency and predictive reliability.

The primary objective of this research is to develop and validate a predictive model for the potential energy of CuNi alloys using linear regression. We aim to assess the model's performance on unseen datasets, evaluate its robustness, and compare its predictive capabilities with those of existing methods. By establishing a reliable and efficient model, this study contributes to the advancement of computational materials science, enabling more accessible and rapid assessments of alloy properties.

Furthermore, this approach provides a foundation for future studies exploring the application of machine learning techniques in materials science. The insights gained from this work have the potential to inform the design and optimization of CuNi alloys for various applications, promoting innovation and efficiency in materials engineering. The integration of machine learning models with traditional simulation methods can enhance the understanding of complex material behaviors and facilitate the development of advanced materials with tailored properties.

In conclusion, the development of a linear regression-based predictive model for the potential energy of CuNi alloys represents a significant step towards bridging the gap between computational efficiency and predictive accuracy. By leveraging the simplicity and interpretability of linear regression, this study offers a practical framework for estimating PE across a range of thermodynamic conditions. The findings have implications for the design and optimization of CuNi alloys and pave the way for the integration of machine learning techniques in materials science research.