Heat Treated Steel Hardness Predictor

An Approach to Accelerate Alloy Design Through Computational Metallurgy

Department of Metallurgical and Materials Engineering

भारतीय प्रौद्योगिकी संस्थान पटना
Indian Institute of Technology Patna

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Dr. G. Mohan Muralikrishna

Importance of Steel & its Hardness

Why Steel Matters

- Backbone material of construction, infrastructure, automotive, aerospace, tooling
- Used where strength, toughness, durability, and cost-efficiency are required
- Modern manufacturing depends heavily on predictable mechanical performance

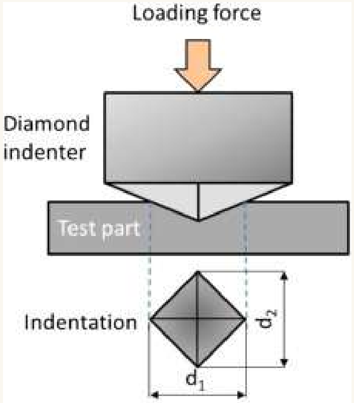
Why Hardness Matters

- Directly relates to:

1. Wear resistance
2. Strength and fatigue performance
3. Hardenability of the steel

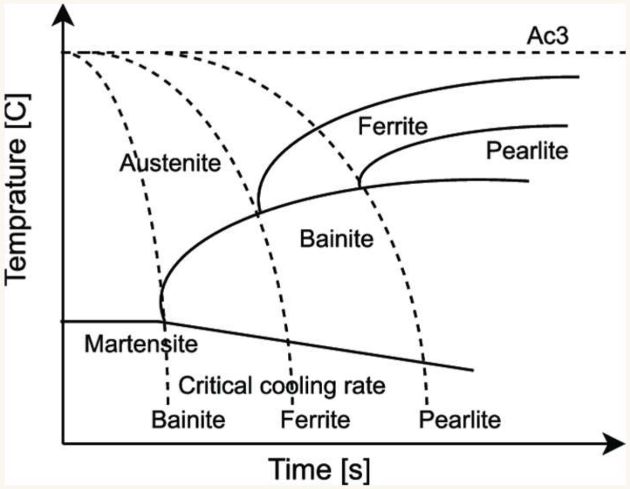
- Hardness also reflects microstructure:
    - Ferrite (soft)
    - Pearlite (moderate)
    - Bainite (hard)
    - Martensite (very hard)

Traditional Hardness Prediction Methods



How Hardness is Traditionally Determined

1. Generate a CCT Diagram
   - Heat to austenite → controlled cooling → metallography
2. Analyze Microstructure
   - Identify ferrite, pearlite, bainite, martensite fractions
3. Perform Hardness Tests
   - Vickers, Rockwell, or Brinell indentation
4. Multiple experimental trials to map composition → hardness relationship



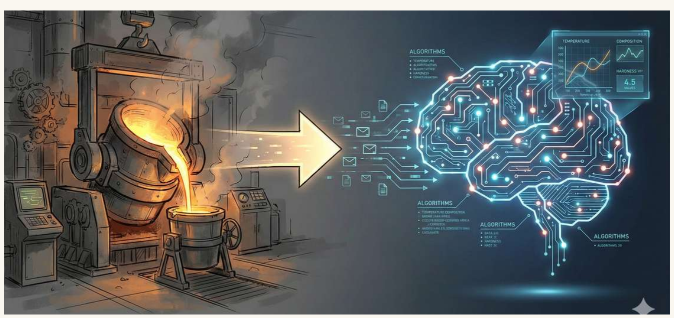
Limitations

- Time-consuming (each CCT diagram takes days)
- Expensive (furnaces, polishing, microscopy)
- Labor-intensive
- Not scalable to explore new alloy compositions quickly

Challenges & Motivation for Computational Approach

Challenges with Traditional Methods

- Require controlled heat treatment, quenching, and metallographic work
- Hard to experimentally generate CCT diagrams for many compositions
- Limited data availability makes alloy design slow
- Industry needs rapid, predictive tools for hardness estimation



Motivation

- Shift from costly lab experiments → computational metallurgy
- Use ML to learn from historical transformation/hardness data
- Predict properties using composition + cooling rate
- Enable faster alloy optimization with minimal experiments
- Support decision-making in steel design & processing

Proposed Solution: ML-Based Hardness & CCT Type Prediction

Our Solution

A two-stage machine learning pipeline that predicts:

1. CCT Diagram Type (classification)
2. Final Hardness (HV) (regression)

Inputs for training ML model

- Chemical composition
- Starting transformation time(Cp,Cf,Cz)
- Composition to CCT diagram type
- Cooling time to hardness values

Why This Works

- Captures phase-transformation behavior using CCT knowledge
- Uses ML to compute hardness from measurable inputs
- Eliminates need for full-scale experiments for each alloy

Benefits

- Fast property prediction
- Reduces cost and experiment load
- Scalable to thousands of compositions
- A tool for modern computational alloy design

Chemical composition
Cooling TIme

CCT classifier classifies it into one CCT Type

Hardness Predictor takes CCT type and other inputs

Predicting the steel hardness(HV)

Sources: Liu et al., "Machine Learning for Predicting Mechanical Properties of Steels," Materials & Design, 2019.

Continuous Cooling Transformation (CCT) diagram

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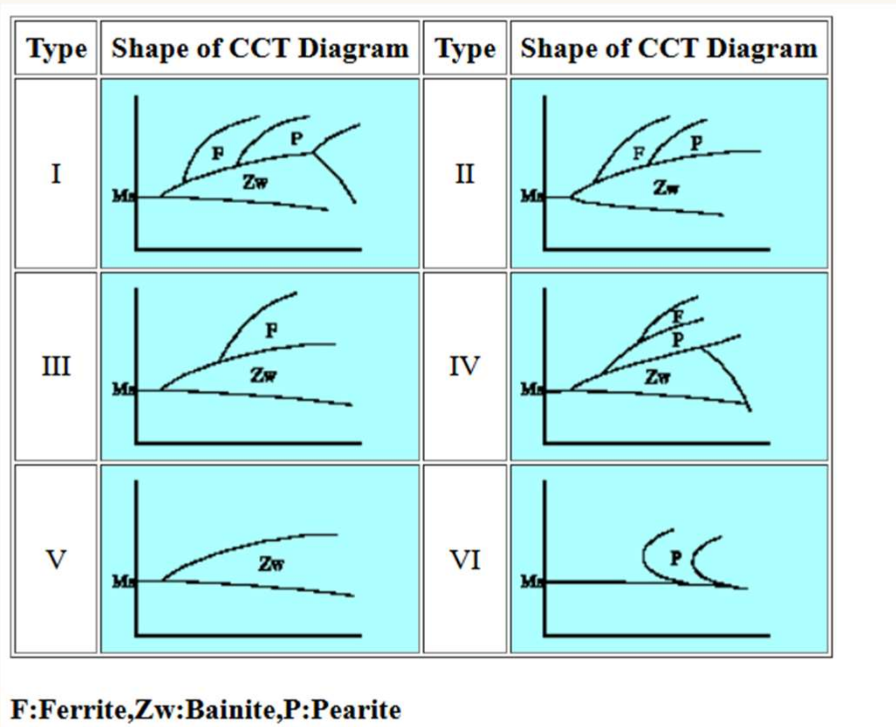

Type	Transformation Characteristics
Type I	**F + P + Bainite (Zw); all curves present**
Type II	Similar to Type I but shifted due to alloying
Type III	F + Bainite; Pearlite suppressed
Type IV	P + Bainite; Ferrite suppressed
Type V	Only Bainite (Zw); very high hardenability
Type VI	Only Pearlite; occurs at very slow transformations

Sources: CCT Diagram Database (CCTD): https://weldcct.nims.go.jp/Weld/search/en/diag_e.html
National Institute for Materials Science (NIMS), accessed 15 Nov, 2025.

ML Pipeline Overview

Data Preprocessing
Clean and structure raw metallurgical data for ML readiness.

Split into Train/Test
Divide data to evaluate unbiased model performance.

Phase 1: Classification (CCT Type)
- Input: Composition (C, Mn, Si, Cr, Ni, Mo, B...)
- Model: Random Forest
- Output: CCT Type (1–6)

Phase 2: Regression (Hardness)
Inputs:
- Composition
- Cooling Time ($A_3 \rightarrow 773$ K)
- Transformation Times (Cp, Cf, C_2, Ce...)
- Predicted CCT Type

Model: Gradient Boosting Regressor
Output: Final Hardness (HV)

Evaluation (R^2, MSE, etc.)
Measure accuracy and error of ML predictions.

Prediction for new compositions
Generate hardness and CCT Type for unseen steels instantly

Sources: Zhu et al., “Machine Learning Prediction of Steel Hardness Using Composition-Based Features,” Journal of Materials Engineering and Performance, 2020.

Results: CCT Type Classification & Hardness Prediction

1
Model: Random Forest Classifier
Input: Chemical Composition
Output: CCT Diagram Type (1–6)
Performance Metrics:-
- Accuracy: 0.78
- F1-Score: 0.73

Some Input and Output values

Chemical Compositions [wt%]											CCT Dia. Type	
C	Si	Mn	Ni	Cr	Cu	Mo	V	Ti	Nb	B	Actual	Predicted
0.11	0.56	0.47	-	-	-	-	-	-	-	-	1	1
0.09	0.37	1.34	0.02	-	0.11	0.01	0.06	-	-	-	2	2
0.14	0.26	0.83	1.06	0.61	0.26	0.45	0.05	-	-	0.02	3	4

2
Model: Gradient Boosting Regressor
Input Features:
Composition, cooling time, transformation times, predicted CCT Type
Performance Metrics:-
- R^2 Score: 0.86
- RMSE: ~10.8 HV

Some Input and Output values

Chemical Compositions [wt%]											CCT Dia. Type			Hardness(HV)	
C	Si	Mn	Ni	Cr	Cu	Mo	V	Ti	Nb	B	Actual	Predicted	Cooling Time(sec)	Actual	Predicted
0.11	0.56	0.47	-	-	-	-	-	-	-	-	1	1	8	186	195
0.09	0.37	1.34	0.02	-	0.11	0.01	0.06	-	-	-	2	2	12	352	338
0.074	0.57	0.135	0.06	0.92	0.92	0.52	0.06	0.026	-	-	5	5	9	348	360

Future Work Model Improvements

Model Improvements
- Hyperparameter tuning
- Add metallurgical descriptors:
  - Carbon Equivalent (CE)
  - Hardenability factors
  - Alloy clustering indicators

Feature Expansion
- Include prediction of the starting times of phase transformations
- Add microstructure fraction prediction (F/P/B/M)

Deployment
- Build a GUI/web-based predictor
- Integrate visualization of CCT curves and predicted hardness

Long-Term Extensions
- Predict yield strength & tensile strength
- Apply model to other alloys

Conclusion

Summary

- Developed a computational ML-based pipeline to predict:
  - CCT Diagram Type
  - Final Hardness (HV)
- Leveraged the CCTD dataset (NIMS Japan)
- Achieved strong accuracy in both classification & regression
- Predictions aligned with metallurgical principles and transformation behavior

Impact

- Reduces reliance on costly experiments
- Enables fast screening of alloy compositions
- Supports computational metallurgy and accelerated alloy design

This work demonstrates that integrating domain knowledge with ML creates powerful tools for materials engineering.

References

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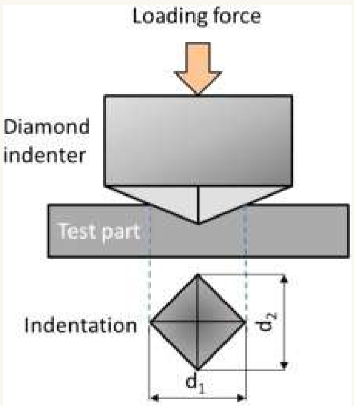

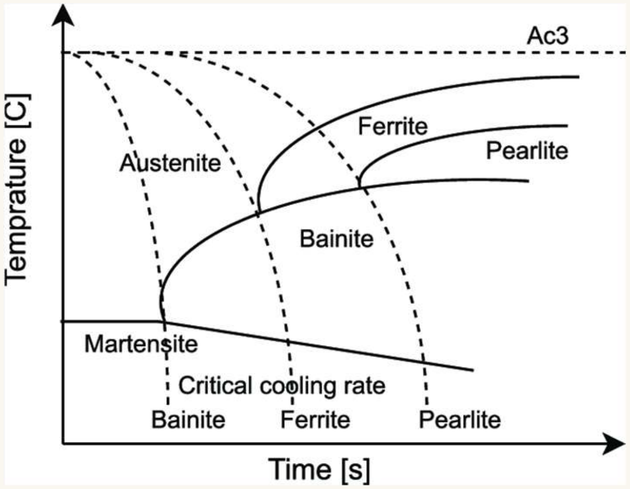

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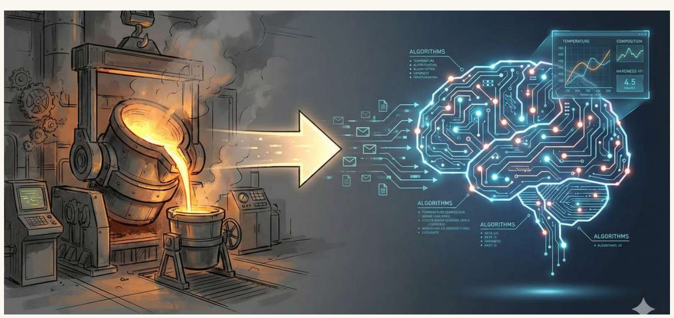

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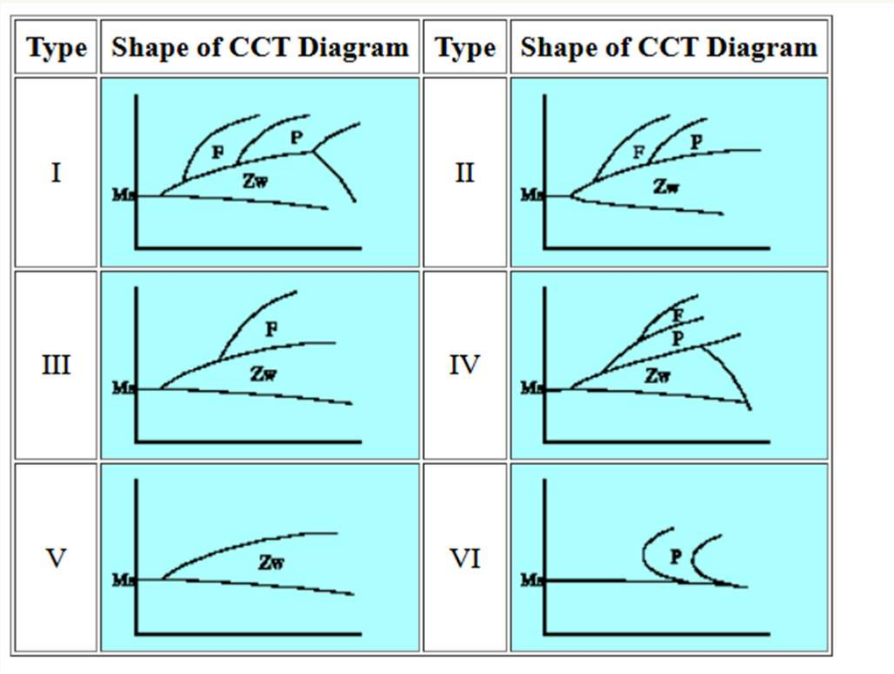

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