A Presentation on

Computational Materials Design and Solidification of TRIP Assisted Steel

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OUTLINE OF THE PRESENTATION

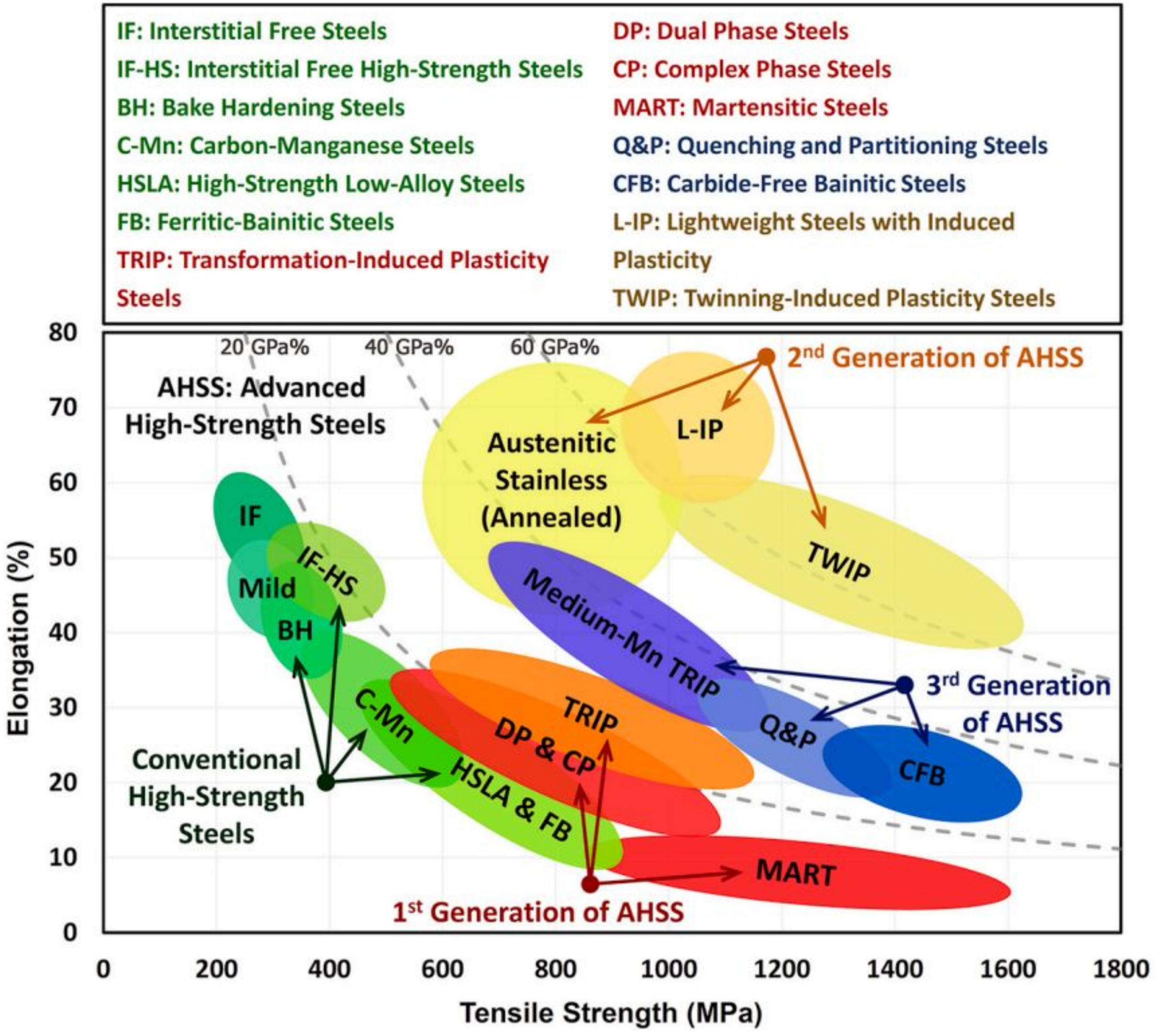
- Project Objective
  - Introduction to TRIP Steel
  - Enriching of Austenite with Carbon
  - Effect of Alloying Elements
  - Solidification Behavior
  - Dataset and Key Points
- Results

Project Objective

1. Develop a novel TRIP steel alloy composition: Explore combinations of inexpensive alloying elements (carbon, manganese, aluminum, silicon) using computational methods to maximize the Transformation-Induced Plasticity (TRIP) effect.

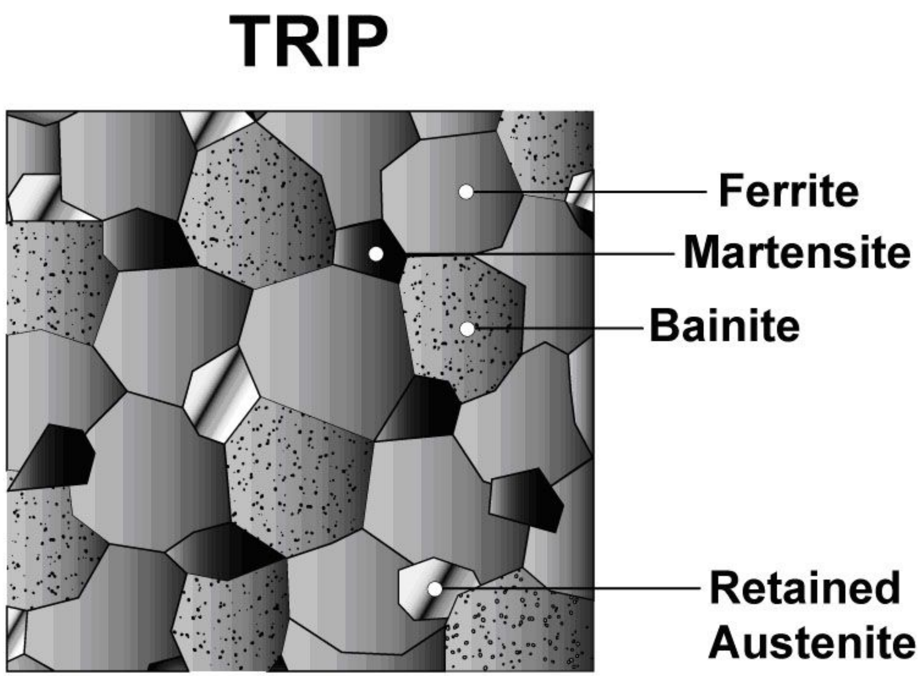
2. Optimize mechanical properties: Employ computational simulations to predict and optimize the strength, ductility, formability, and crashworthiness of the designed TRIP steel alloy for automotive applications.

3. Investigate microstructure-property relationships: Utilize computational tools to understand the interplay between microstructure (grain size, morphology, phase distribution) and the desired mechanical properties of the TRIP steel alloy.



Introduction to TRIP Steel

- TRIP Steel are a Class of High Strength steel alloys
- TRIP stands for "Transformation induced plasticity," which implies a phase transformation in the material, typically when a stress is applied.



Microstructure of TRIP Steel

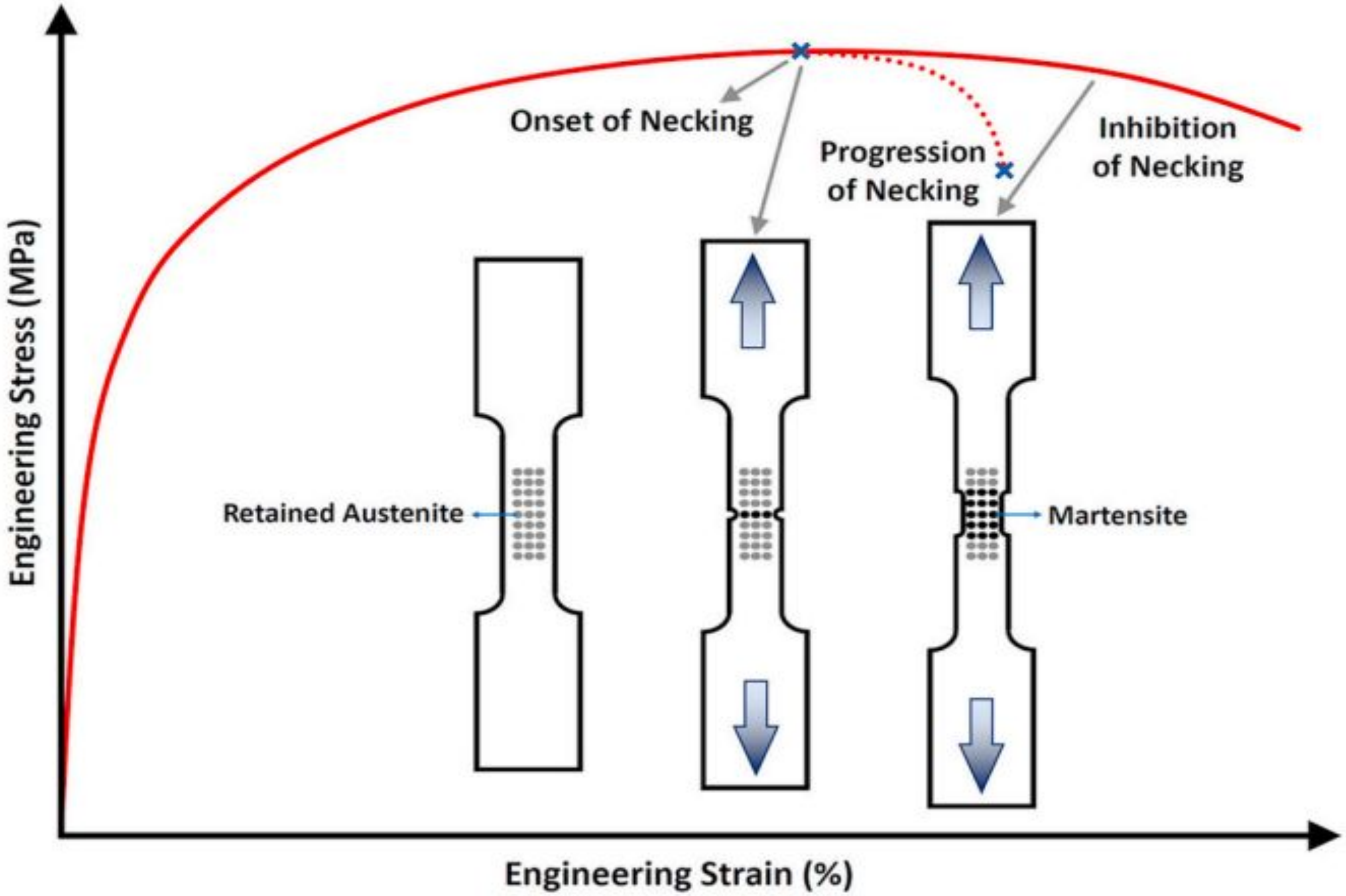
Properties

- High Strength and Toughness
- Formability
- Energy Absorption
- Lightweight Design
- Tailorable Microstructure

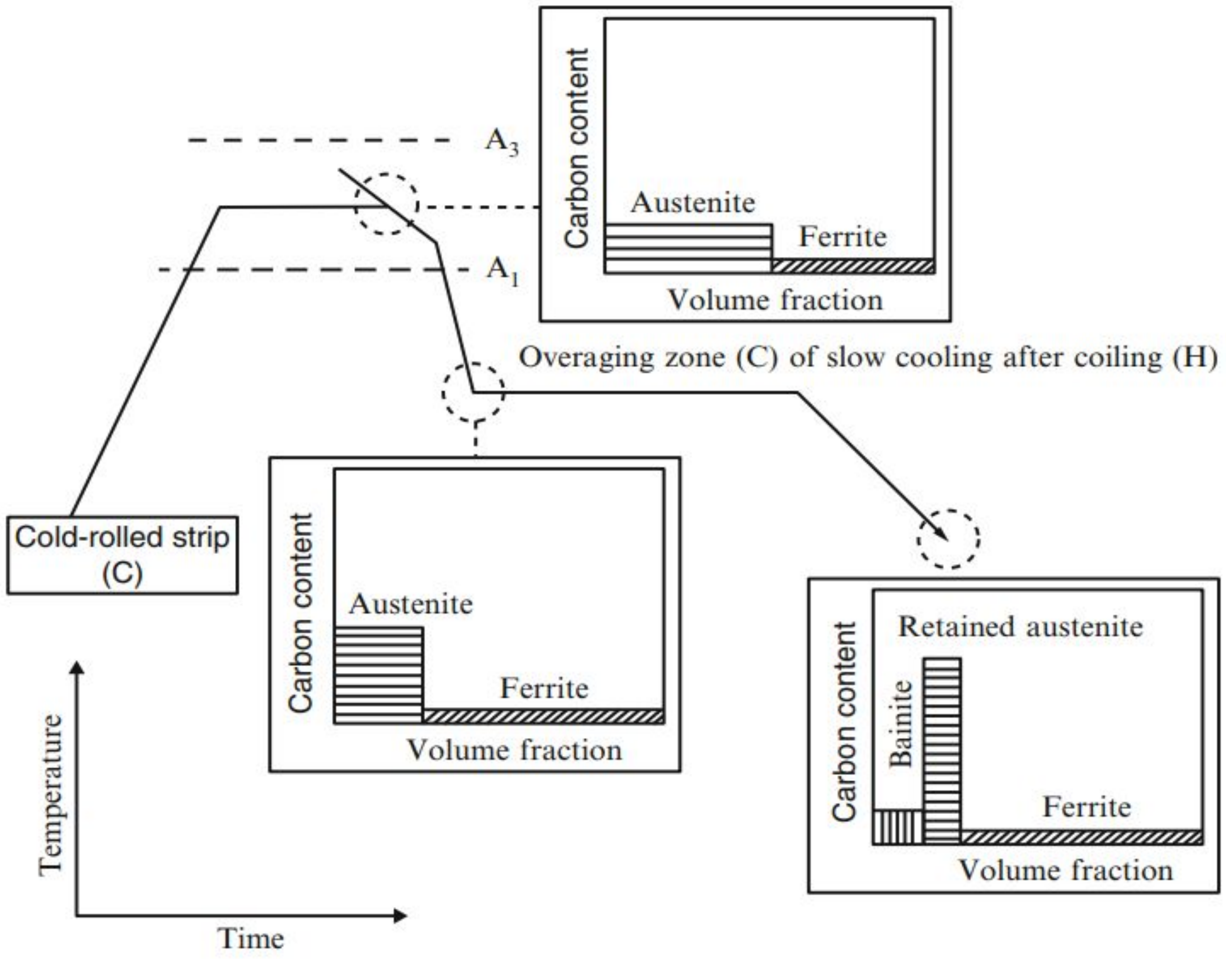
Applications

- Automotive Industry
- Construction and Infrastructure
- Aerospace Industry
- Advanced Engineering Structures
- Manufacturing and Machinery

TRIP Effect during Deformation



Enriching of Austenite with Carbon



Need of Ferrite Stabilisers!!!

Effect of Alloying elements

Mn
Potent stabilizer of austenite limited to 2.0%

C
Potent stabilizer

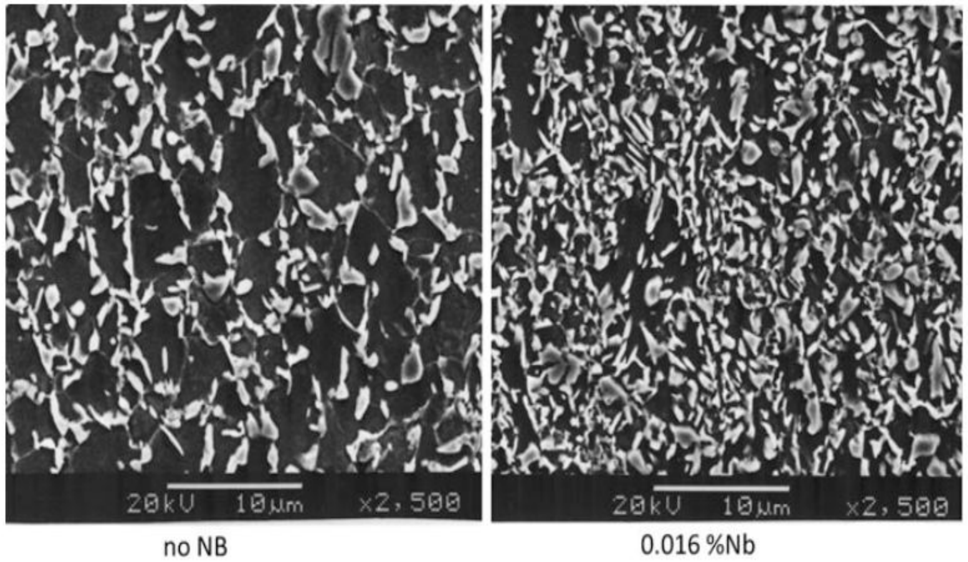
P
Increases retained austenite and its resistance to decomposition

Si
Restricts Carbide Precipitation

Cu
Enhances strength-ductility balance

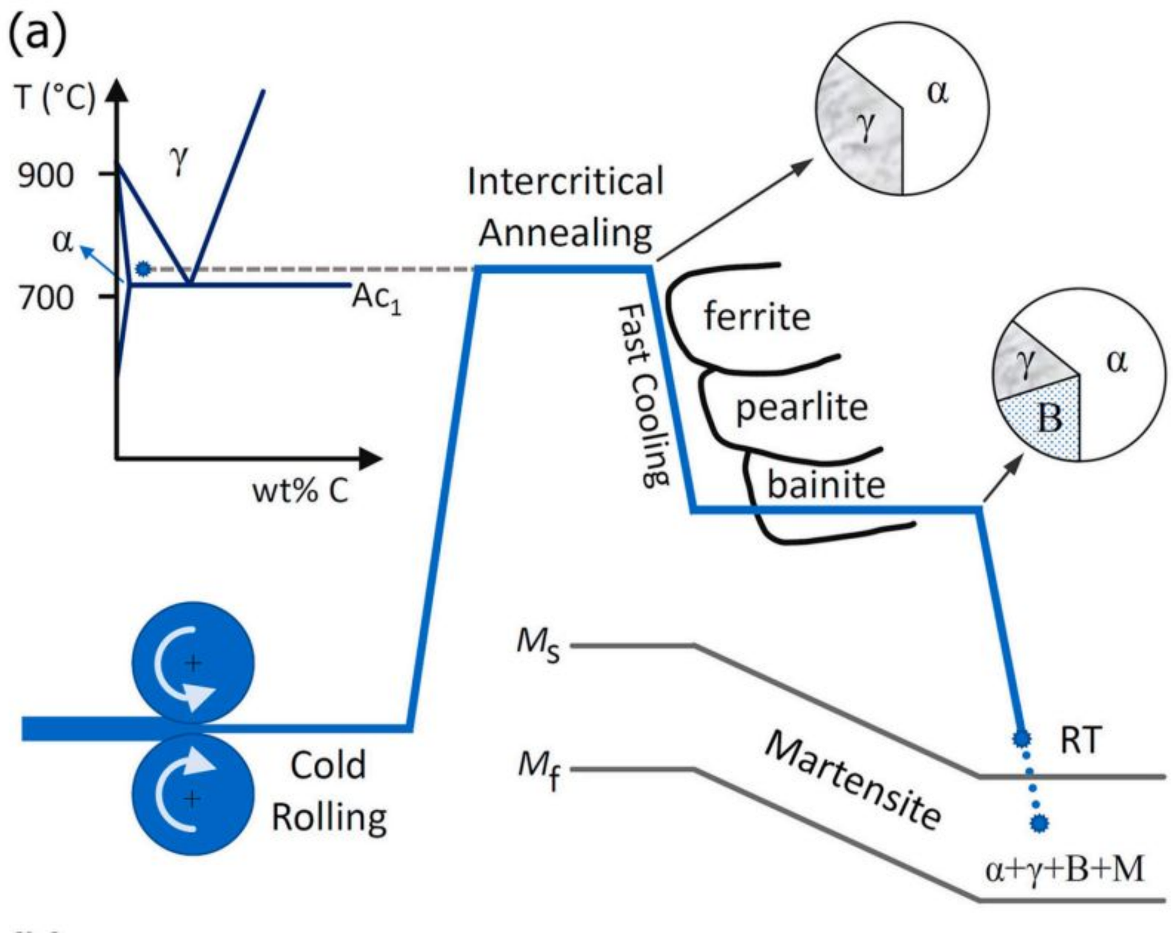
Al
More effective than Si in restricting Carbide Precipitation

Ti,V and Nb
Enhance strength-ductility balance



Effect of Nb on microstructure on TRIP780

Heat Treatment Cycle



Key Points

Takeaway 1

Retention of Austenite is crucial for designing TRIP Steels

Takeaway 2

Carbon content in retained austenite can be calculated from the lattice parameter of austenite. Longer austempering times increase carbon content in retained austenite.

Takeaway 3

The percentage of different phases can be controlled by using different heat treatments properly as per the composition of the alloy

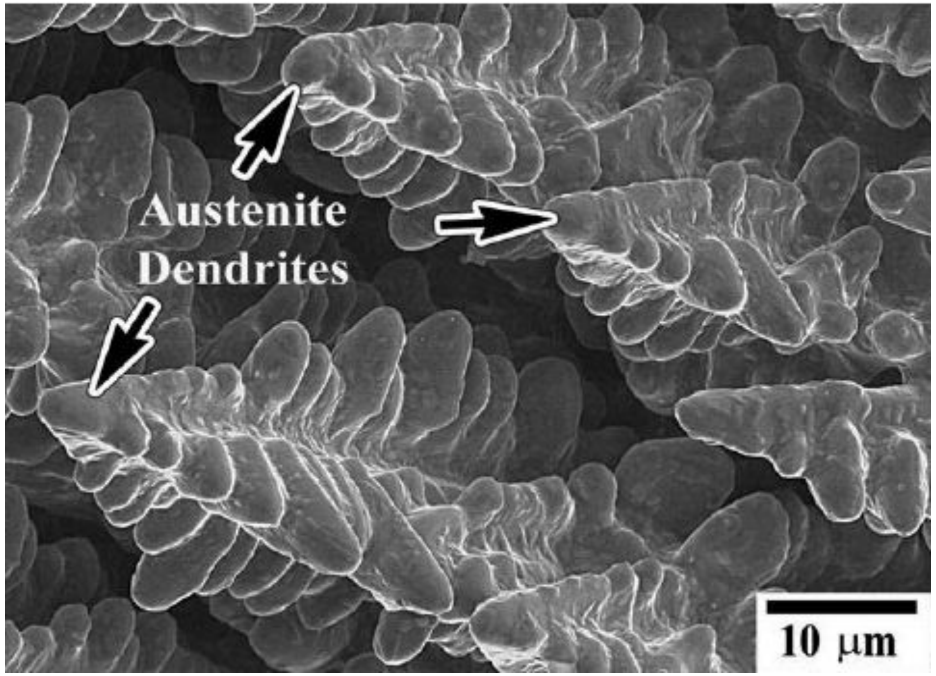
Impact Of Solidification

Solidification dictates the initial grain structure and distribution of alloying elements.

During solidification, the liquid metal solidifies into dendrites, which are finger-like structures.

Solidification dictates the initial grain structure and distribution of alloying elements.

The remaining liquid between the dendrites becomes enriched in certain alloying elements, particularly those with high partitioning coefficients (preference to stay in the liquid).



Segregation and Phase Formation

Alloying elements with high partitioning coefficients, like Mn, Ni, and C, get pushed ahead of the solidification front during dendrite growth.

This segregation creates localized regions with varying compositions within the microstructure.

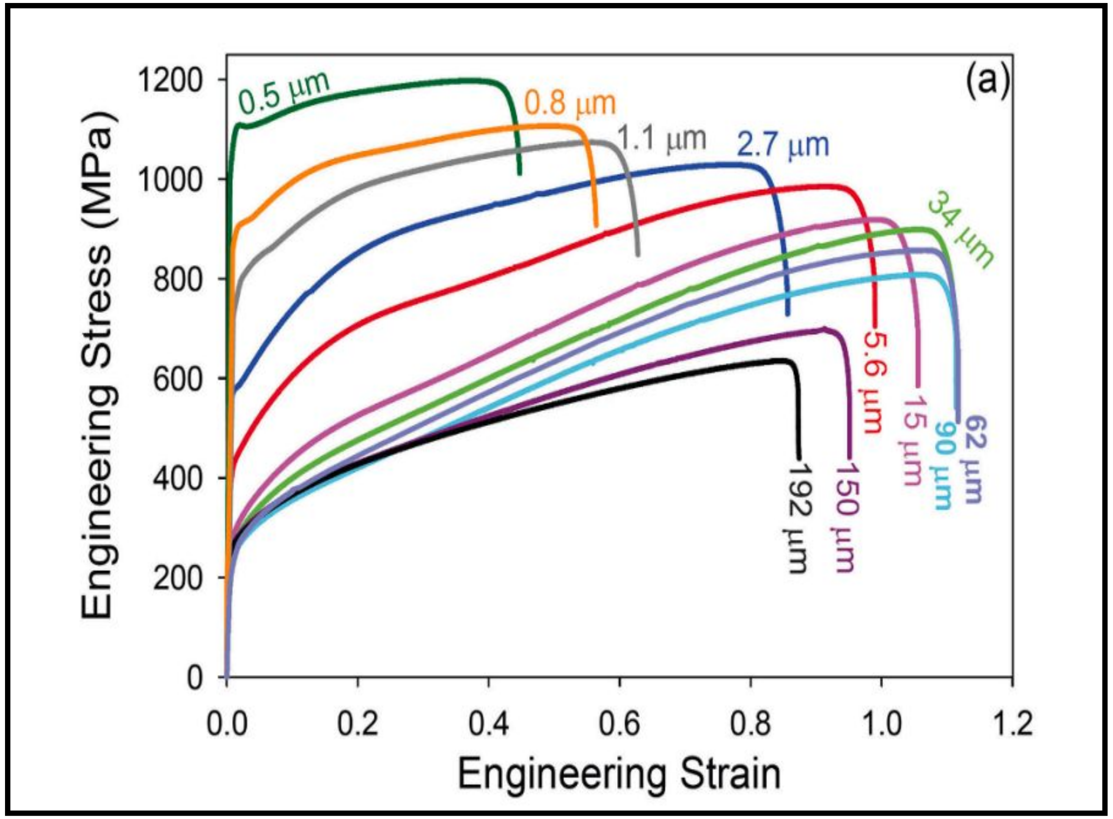
The composition variations influence the transformation temperatures of austenite to ferrite and bainite.

Grain Size and Microstructure

Solidification parameters like cooling rate and mold design influence the final grain size of the steel.

Finer grain sizes generally promote better mechanical properties, including higher strength and improved toughness.

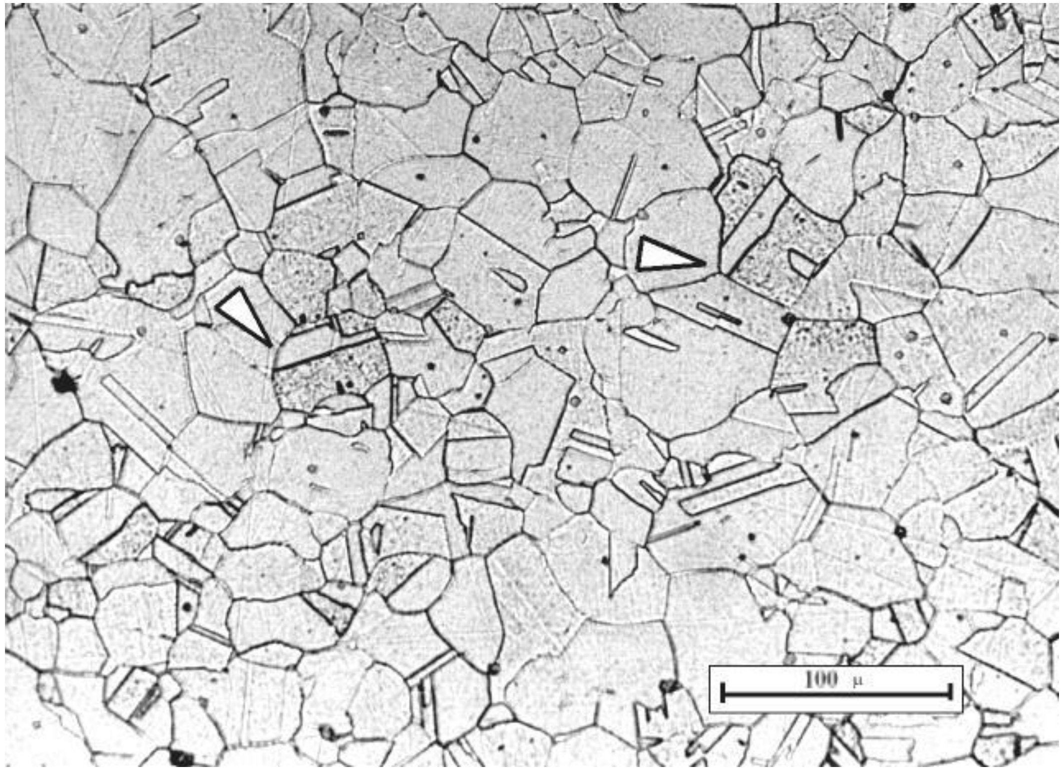
Finer grains provide more boundaries for nucleation of different phases, leading to a more dispersed and refined microstructure.



Stress-Strain Curve for different grain sizes

Formation of Non-Equilibrium Austenite

- **Non-equilibrium Austenite Formation**
- **Substitutional Solutes and Partitioning**
- **Incomplete Partitioning and Ferrite**
- **Impact on Ferrite**



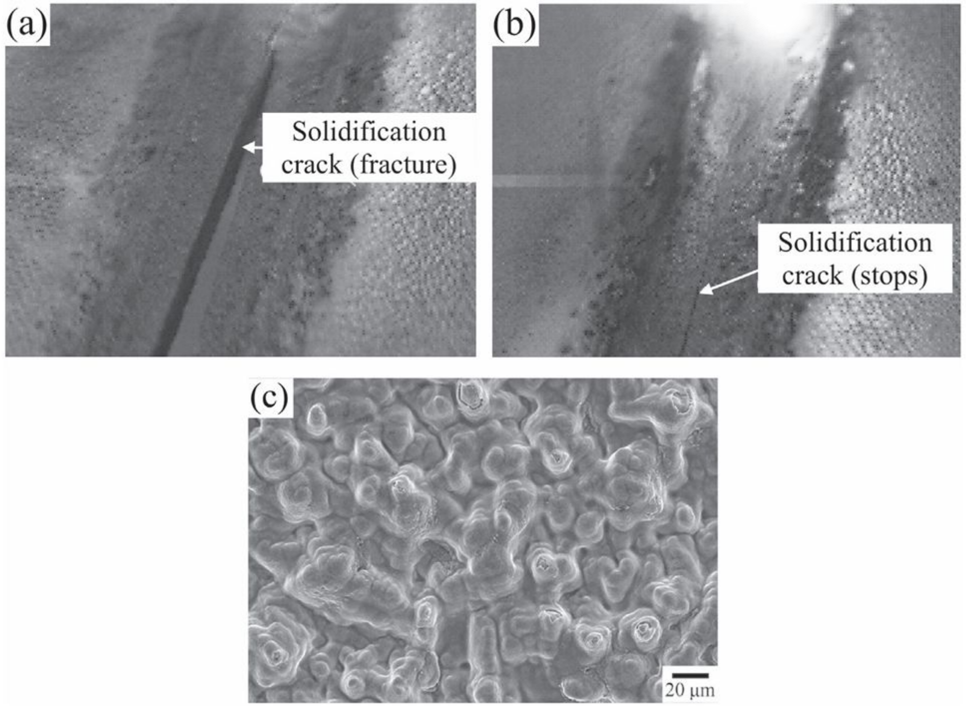
Essentially, the rapid solidification "freezes in" some of the substitutional solutes within the austenite, hindering its transformation to d-ferrite and leading to less of this phase in the cast microstructure.

Problem of Solidification Cracking

Reason for Solidification Cracking

1-The restraint, which is usually the mechanical or thermal stresses/strains

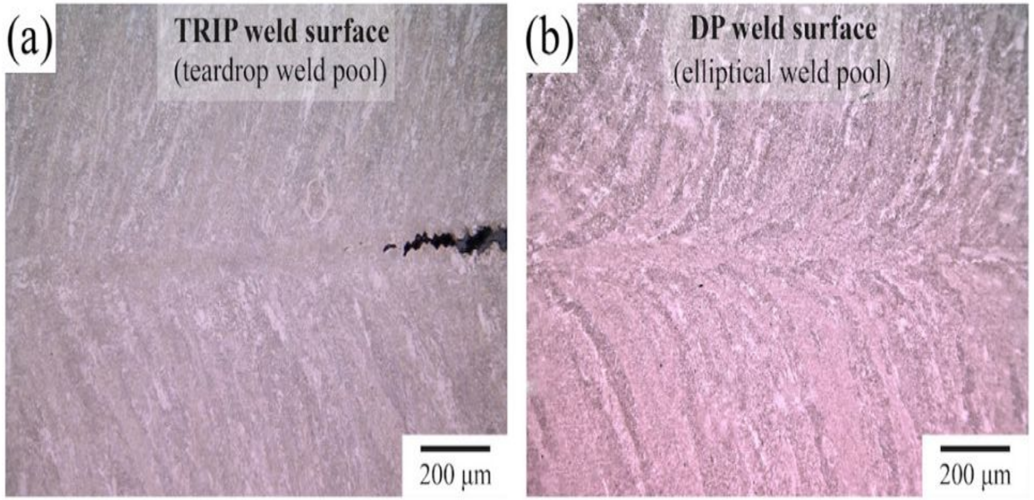
2- the solidifying microstructure. Metallurgical factors that affect the cracking susceptibility include solidification temperature range, solute segregation, surface tension and viscosity of the interdendritic liquid, liquid feeding tendency, grain morphology and dendritic coherency.



High speed camera images during welding of TRIP steel for, (a) case A and (b) case E in Table 2, (c) secondary electron micrograph of the fracture surface showing dendritic morphology, a typical feature of solidification cracking.

Problem of Solidification Cracking

TRIP steel with high P showed considerable segregation of phosphorus at the grain boundaries. Therefore, the solidification temperature range is extended considerably which is confirmed by the presence of inclusions.



The weld pool in TRIP steel has a teardrop shape.

Elliptical shape weld pool is better for solving the problem of solidification cracking.

Methodology and Work Done

- Prepared the dataset using literature available which contains compositions, Ultimate Tensile Strength, Yield Strength and percentage of different phases.
- Fixed the required UTS and YS and fixed the percentage of austenite, bainite and ferrite as per our requirement as 20/30% , 50% and 30/20% respectively.
- Predicted two compositions with the required properties.
- Using thermocalc and JmatPro Software found the percentage of phases and TTT curves both both compositions.

Dataset(updated to 80 from 50)

```
df.head(15)
```

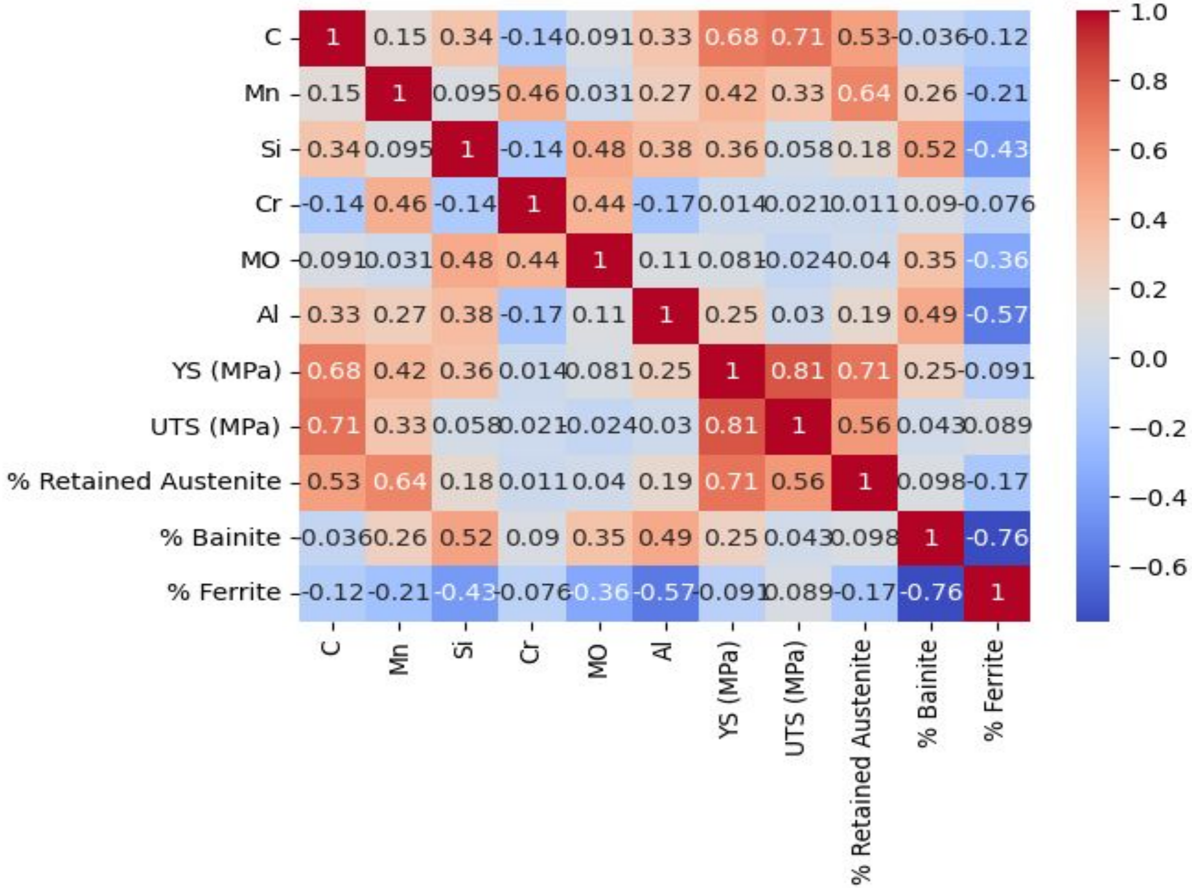
	C	Mn	Si	Cr	MO	Al	Cu	N	Zr	P	...	V	YS (MPa)	UTS (MPa)	% Retained Austenite	% Bainite	% Ferrite	TE	pse	ict	Paper Reference (Paper name)
0	0.39	2.8	2.8	1.2	1.2	1.5	0.0	0.0	0.0	0.0	...	0.0	860.0	1020.0	26.0	78.0	6.0	NaN	NaN	NaN	Singh, B., & Bhadeshia, H. K. D. H. (2019). TR...
1	0.32	2.4	2.4	1.0	1.0	1.3	0.0	0.0	0.0	0.0	...	0.0	880.0	1050.0	20.0	75.0	5.0	NaN	NaN	NaN	Miller, R. L. (2015). Ultrahigh strength steel...
2	0.34	2.5	2.5	1.1	1.1	1.4	0.0	0.0	0.0	0.0	...	0.0	930.0	1100.0	22.0	80.0	3.0	NaN	NaN	NaN	NaN
3	0.40	2.8	2.8	1.2	1.2	1.5	0.0	0.0	0.0	0.0	...	0.0	1080.0	1250.0	24.0	NaN	NaN	NaN	NaN	NaN	NaN
4	0.10	1.1	1.1	0.4	0.4	0.7	0.0	0.0	0.0	0.0	...	0.0	360.0	500.0	5.0	40.0	55.0	NaN	NaN	NaN	Han, J., & Li, Y. (2019). TRIP steels with high
5	0.11	1.2	1.2	0.4	0.4	0.7	0.0	0.0	0.0	0.0	...	0.0	380.0	520.0	6.0	45.0	49.0	NaN	NaN	NaN	Li, Y., & Wang, J. (2020). A review on the dev...
6	0.12	1.3	1.3	0.4	0.4	0.7	0.0	0.0	0.0	0.0	...	0.0	400.0	550.0	8.0	50.0	42.0	NaN	NaN	NaN	De Cooman, B. C. (1996). TRIP-aided steels: Hi...
7	0.13	1.5	1.5	0.5	0.5	0.8	0.2	0.0	0.0	0.0	...	0.0	420.0	570.0	9.0	53.0	38.0	NaN	NaN	NaN	NaN
8	0.15	1.5	1.5	0.5	0.5	0.8	0.0	0.0	0.0	0.0	...	0.0	430.0	590.0	10.0	60.0	30.0	NaN	NaN	NaN	Tomita, Y., Ushioda, S., Senuma, S., & Hatano,...
9	0.14	1.4	1.4	0.5	0.5	0.8	0.0	0.0	0.0	0.0	...	0.0	450.0	600.0	10.0	55.0	35.0	NaN	NaN	NaN	NaN
10	0.17	1.5	1.5	0.6	0.6	0.9	0.0	0.0	0.0	0.0	...	0.0	460.0	620.0	10.0	55.0	35.0	NaN	NaN	NaN	Fang, H., & Chen, K. (2021). TRIP steels with ...
11	0.18	1.6	1.6	0.6	0.6	0.9	0.0	0.0	0.0	0.0	...	0.0	480.0	650.0	12.0	60.0	28.0	NaN	NaN	NaN	Speer, J. G., De Cooman, B. C., & Matlock, D. ...
12	0.19	1.7	1.7	0.7	0.7	1.0	0.3	0.0	0.0	0.0	...	0.0	510.0	670.0	13.0	63.0	24.0	NaN	NaN	NaN	NaN
13	0.20	1.7	1.7	0.7	0.7	1.1	0.0	0.0	0.0	0.0	...	0.0	530.0	700.0	14.0	65.0	21.0	NaN	NaN	NaN	NaN
14	0.22	1.8	1.8	0.8	0.8	1.2	0.0	0.0	0.0	0.0	...	0.0	560.0	720.0	14.0	65.0	21.0	NaN	NaN	NaN	Speer, J. G., & Matlock, D. K. (2000). Design ...

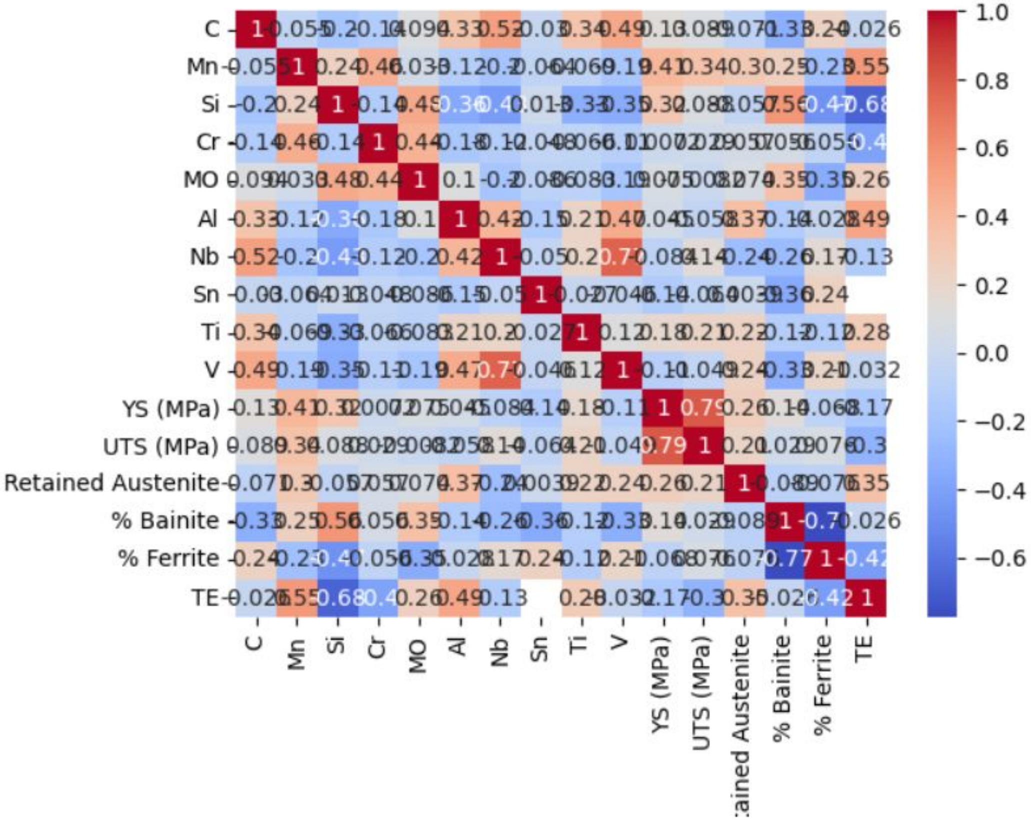
15 rows × 25 columns

Results

Correlation Heat Map

Using the Python libraries like Pandas and matplotlib we can create a Correlation Heatmap of the Data Set we have created through various research papers.





Results

Material Composition

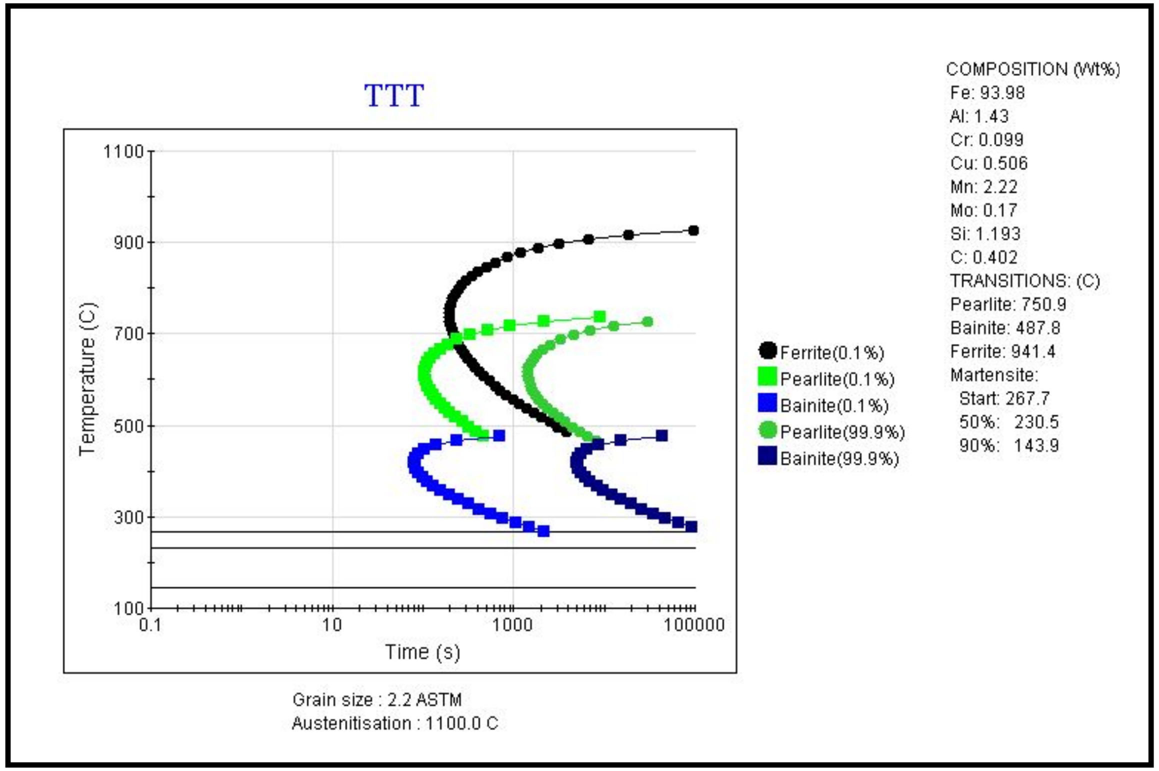
On using various different Machine Learning algorithms, We found that the best Machine learning model that works very well with the dataset is Random Forest and the compositions that were predicted can be found below:

Required Properties	C	Mn	Si	Cr	Mo	Al	Cu	Zr	P	S	Ni
Bainite-50 % RA - 20% Ferrite - 30%, UTS - 1300,YS-700	0.34	2.225	1.36	0.136	0.144	1.16	0.113	0.0002	0.0014	0.0004	0.0053
Bainite-50 % RA - 30% Ferrite - 20% UTS - 1300,YS-700	0.402	2.22	1.193	0.099	0.17	1.43	0.506	0	0.0008	0	0

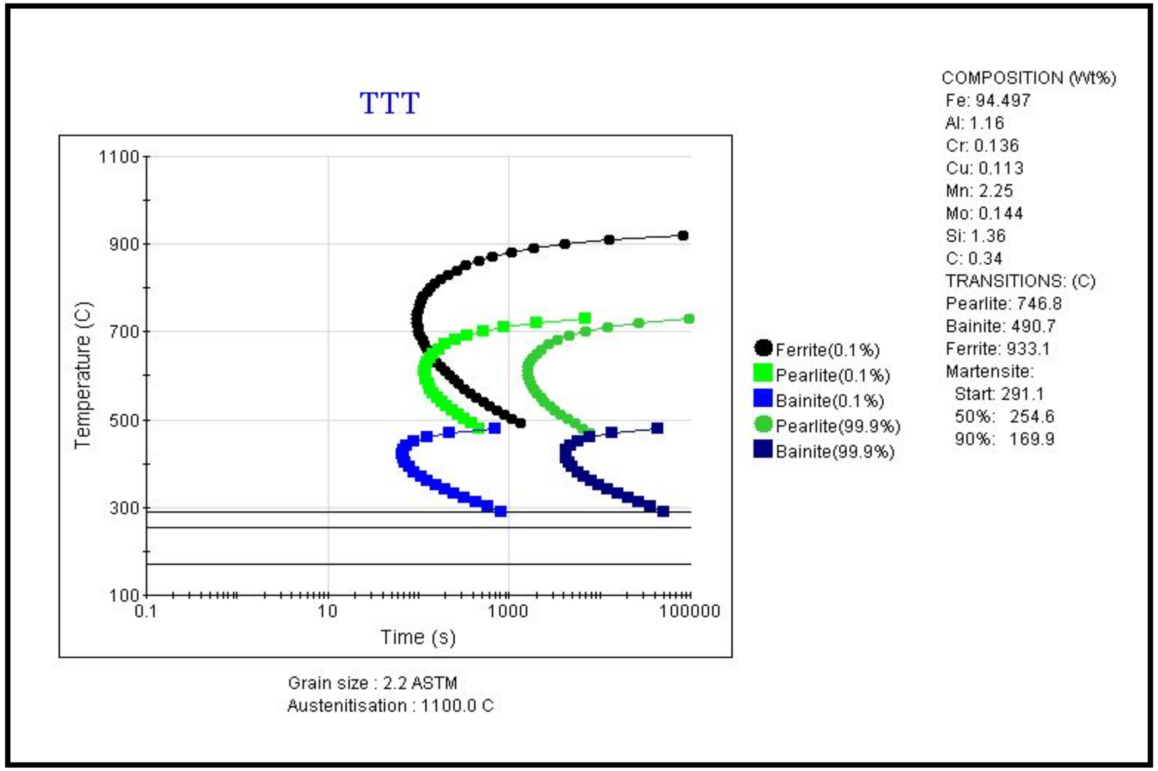
Results

Time Temperature Transformation Curves

The Time-Temperature-Transformation (TTT) curves were obtained using the JMatPro software which tells us about the heat treatments that we need to do for obtaining the required percentage of phases.



Curve for composition with C = 0.402



Curve for composition with C = 0.34

Conclusions

Creating the best TRIP steel involves carefully managing carbon, adding specific alloys, and using precise heat treatments.

1. Adjusting the amount of carbon gives strength without sacrificing the steel's ability to be shaped.
2. Adding elements like manganese, silicon, and aluminum fine-tunes how the steel transforms, helping create the desired TRIP effect.
3. The heat treatment process, including controlled rolling and quenching, determines the steel's structure, influencing important phases like ferrite, bainite, and retained austenite.

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THANK YOU

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