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Project Report:
FactSage Simulation Podcast

Influence of Carbon Allotropes on the Melting Point and Eutectic Behavior of the Ni–C Binary System

Presented by:	**Hafsa Raza**
Presented to:	**Prof. Philippe Ouzilleau**

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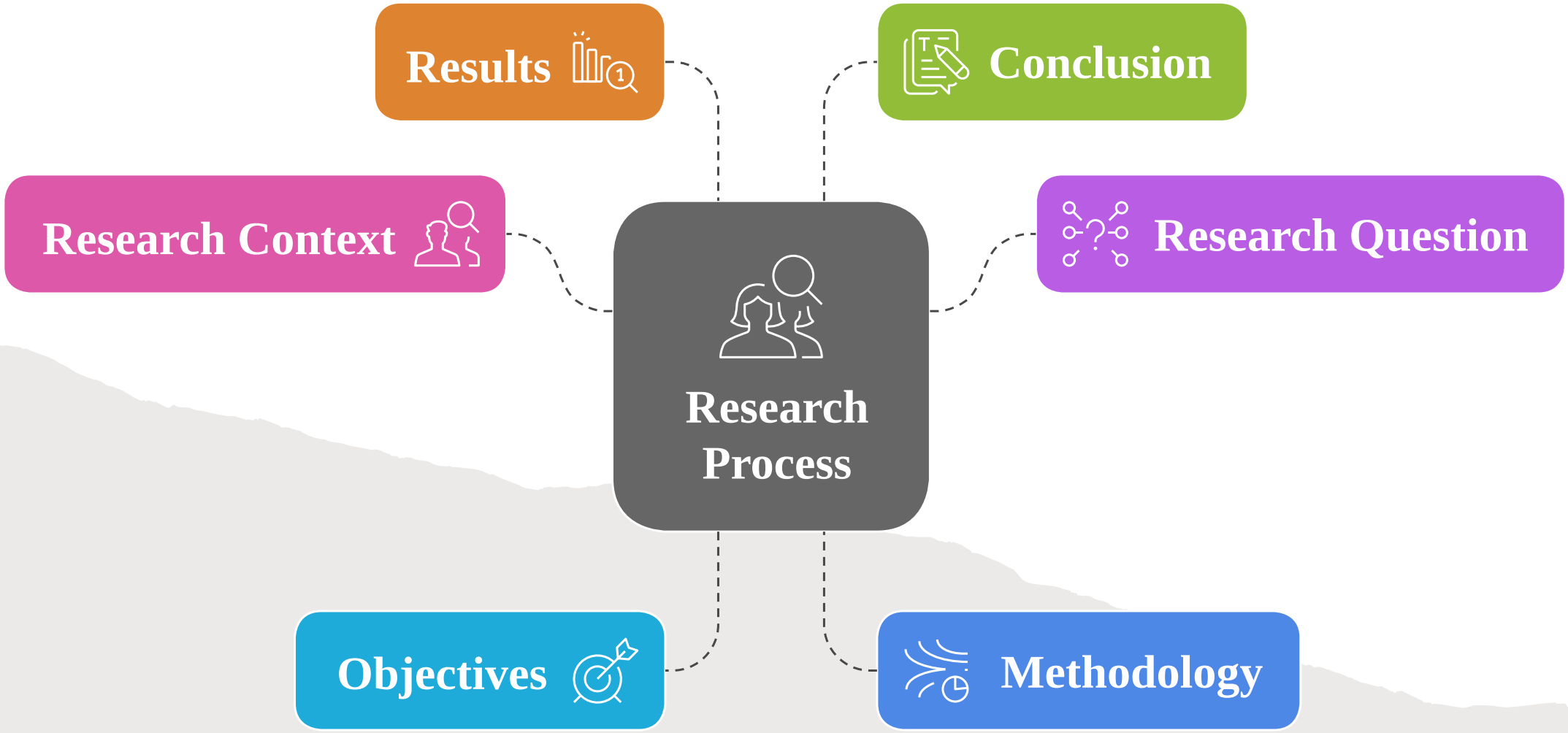
Project Overview



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Research Context and Literature Overview

- Ni–C system lacks stable carbides, making it ideal for thermodynamic studies.
- Nickel enables graphene growth via CVD by absorbing and releasing carbon.
- Carbon allotropes (graphite, diamond, graphene) affect phase stability.
- Using metastable carbon shifts eutectic temperature and solubility.
- Accurate phase modeling is key for carbon-based device fabrication.

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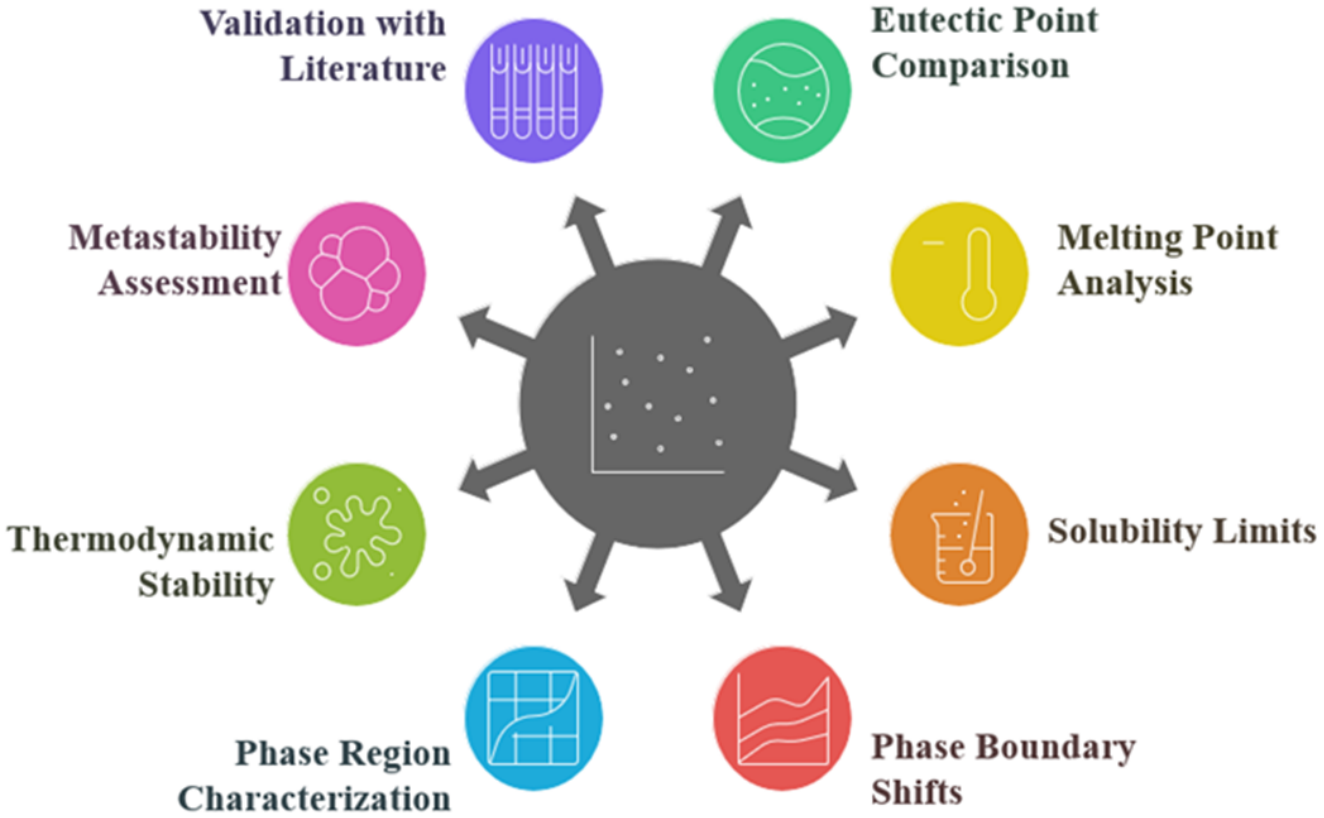
Research Question

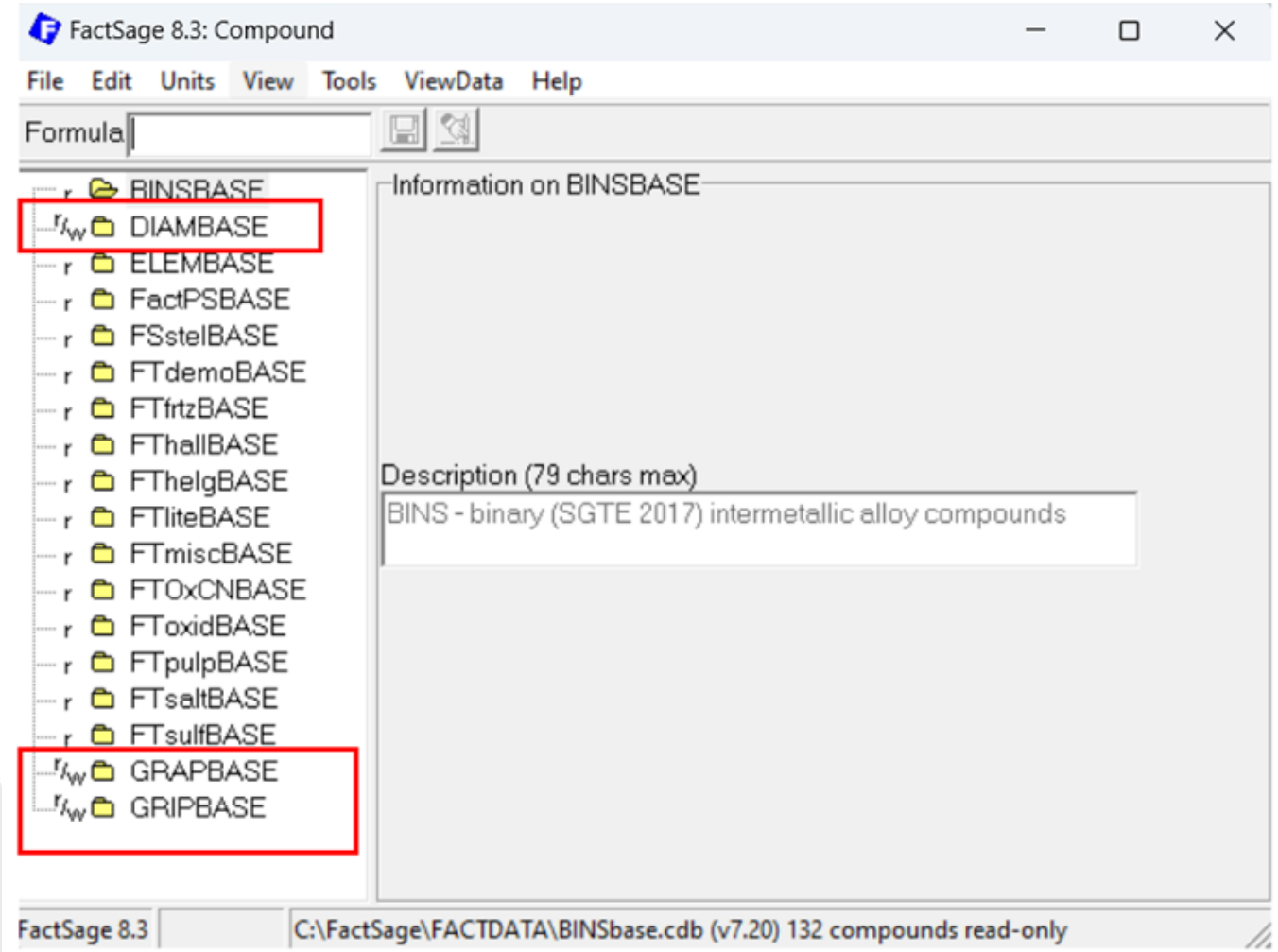
How do graphite, graphene, and diamond alter the melting point and eutectic features in the Ni–C phase binary diagram?

SPECIFIC OBJECTIVES



Methodology

Step 1:



Methodology

Step 2:

SGTE Databases

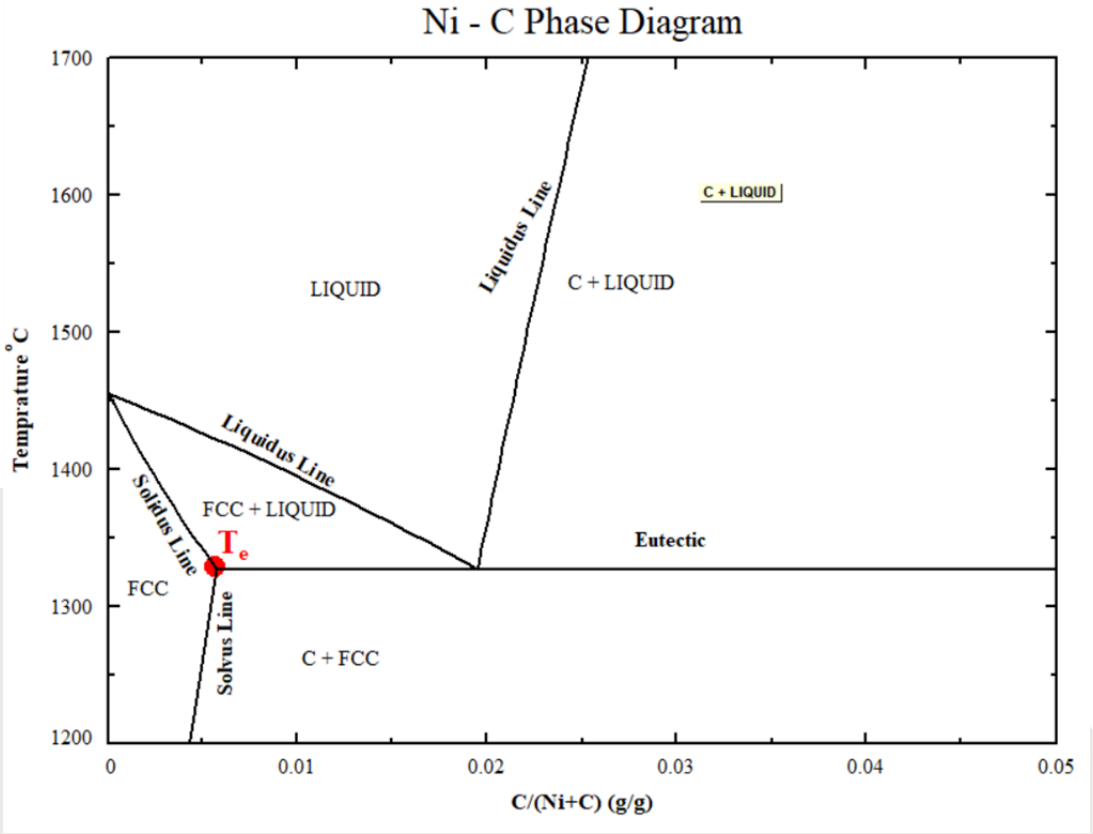
- SGTE stands for Scientific Group Thermodata Europe, an international consortium of thermodynamic experts.
- It offers experimentally validated and critically assessed thermodynamic data for solid, liquid, and gaseous phases.
- It includes comprehensive data for metals, alloys, and common non-metallic systems.
- SGTE does not provide thermodynamic functions for 2D materials like graphene, requiring manual data entry for such phases.

Example

- Eutectic point shifted from ~1326 °C (1.9 wt% C) with graphite
- To 2.5–3 wt% C, 20–30 °C lower with diamond

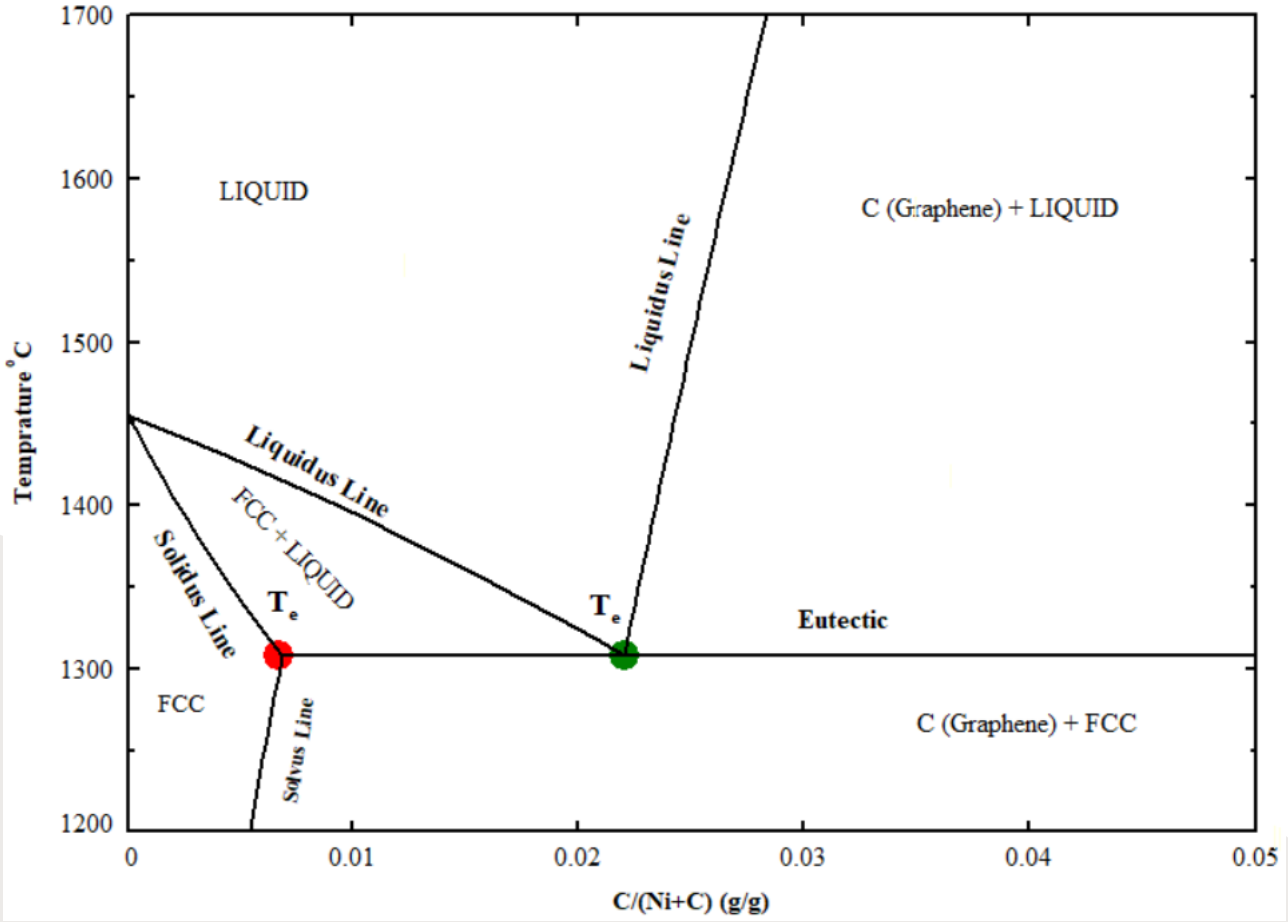
Presentation & Interpretation of Results

Ni-C binary Phase Diagram (Graphite)



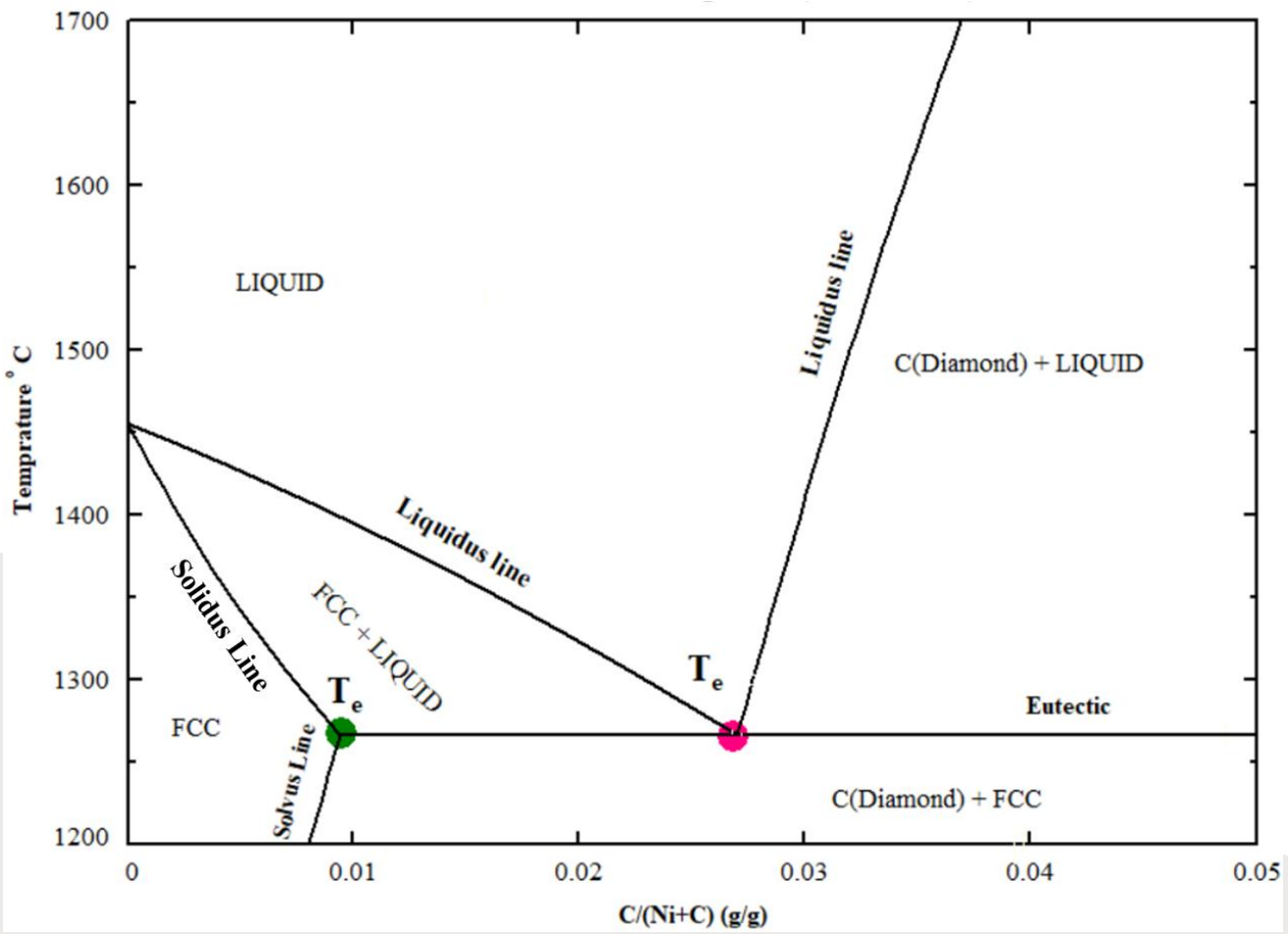
Presentation & Interpretation of Results

Ni-C binary Phase Diagram (Graphene)



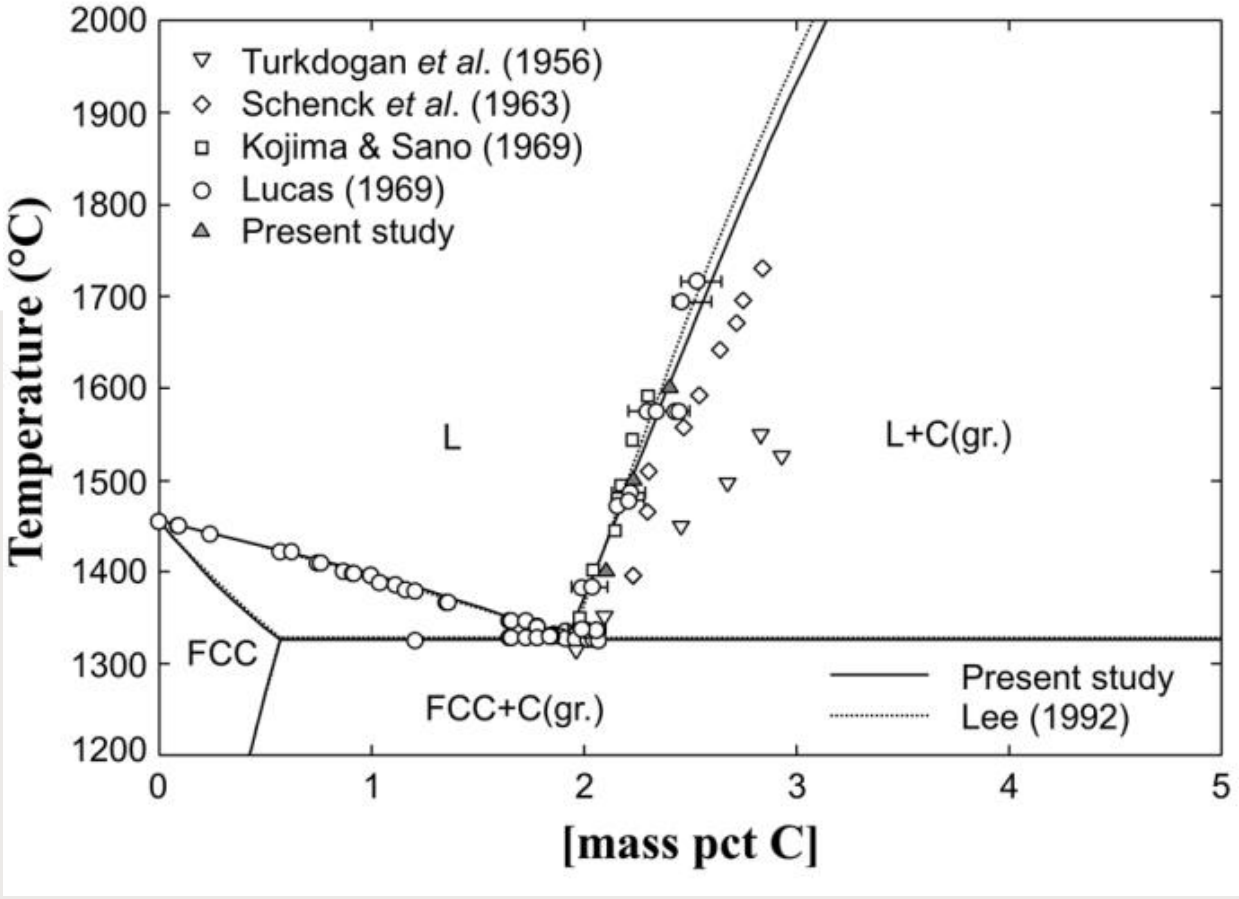
Presentation & Interpretation of Results

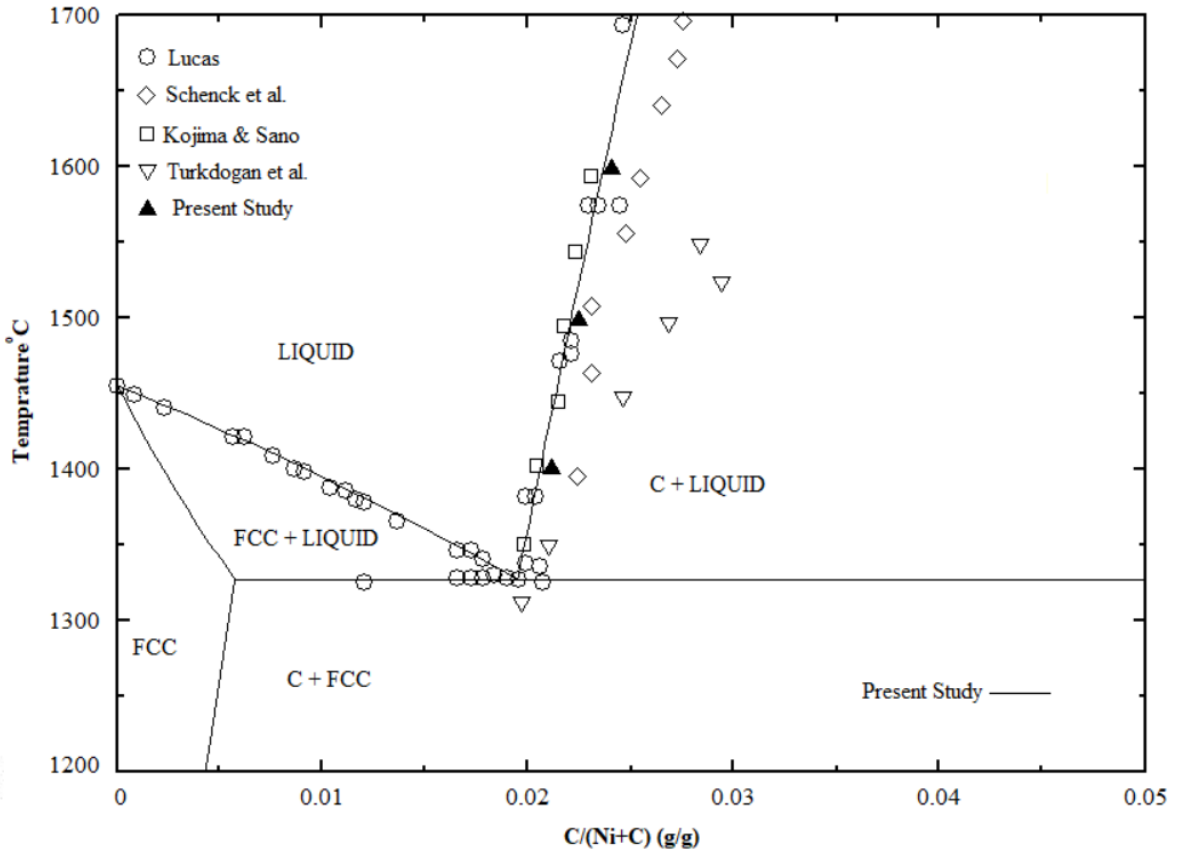
Ni-C binary Phase Diagram (Diamond)



Presentation & Interpretation of Results

Compare with the experimental findings:





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Conclusion

- The Ni–C system maintains a simple eutectic structure across all carbon allotropes.
- Graphite produces the highest eutectic temperature with the lowest carbon content.
- Diamond and graphene shift the eutectic to lower temperatures and higher C concentrations.
- The stability of the carbon phase critically influences phase equilibria and synthesis outcomes.