Lecture 6: Iron Carbides and Martensite

MIWUS - Mini Instant Winter University School
Computational Metallurgy Course

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Abstract

This lecture explores the complex world of iron carbides and their characterization through Mössbauer spectroscopy, building upon the thermodynamic foundations established in Lecture 5. We examine three complementary perspectives: (1) the characterization of iron carbides using Mössbauer Spectroscopy and DFT calculations, (2) thermodynamic assessment of the Fe-C system including metastable carbides by Naraghi et al., and (3) recent advances in thermodynamic modeling from the Jacob research group at TU Wien. The lecture prepares students for the advanced topics in steel transformations covered in Professor Harry Bhadeshia's course materials.

1 Introduction: The Iron Carbide Challenge

1.1 Historical Context and Ongoing Relevance

The study of iron carbides has been a central challenge in physical metallurgy since the pioneering work of Sorby in the 1860s. Despite nearly 160 years of investigation, fundamental questions remain unresolved in 2026:

- What is the precise nature of bainitic ferrite? Does it form as a supersaturated body-centered tetragonal (BCT) phase or body-centered cubic (BCC) phase with carbon in solution?
- What carbides are present during the tempering of martensite, and what is their formation sequence?
- How do transition carbides (-Fe_3C, -Fe_2C, -Fe_5C_2) relate thermodynamically to stable cementite (-Fe_3C)?
- What is the role of carbon ordering in martensite aging?

1.2 Personal Journey in Iron Carbides

As Professor Miani notes, he has been working on iron carbides since 1988 as a student. The topic remains fascinating because:

1. The bainite phase definition problem persists
2. New characterization techniques (Mössbauer spectroscopy, synchrotron XRD, atom probe tomography) continue to reveal new insights

3. Computational methods (DFT, CALPHAD) now complement experimental work
4. Industrial importance drives continued research

2 Part I: Mössbauer Spectroscopy of Iron Carbides

2.1 Introduction to Mössbauer Effect Spectroscopy (MES)

2.1.1 Physical Basis

Mössbauer Effect Spectroscopy is based on the recoilless emission and absorption of gamma rays by atomic nuclei bound in a solid. For ^{57}Fe, the technique provides:

- **Isomer shift (IS)**: Information about electron density at the nucleus, related to chemical bonding
- **Quadrupole splitting (QS)**: Information about symmetry of electric field gradient
- **Magnetic hyperfine field (B_{hf})**: Information about magnetic moment and magnetic ordering

2.1.2 Application to Iron Carbides

As highlighted in the Nature Communications paper by Jiang et al. (Scientific Reports 2016), MES is an excellent characterization technique for iron carbides because:

1. It distinguishes different iron sites in complex carbide structures
2. It provides magnetic information (Curie temperatures, magnetic moments)
3. It can be performed *in situ* during reactions or transformations
4. It is sensitive to small amounts of carbide phases

2.2 Computational Prediction of Mössbauer Parameters

2.2.1 DFT Methodology

The work by Jiang et al. demonstrates the power of combining density functional theory (DFT) calculations with experimental MES:

Computational Approach:

- Full-potential linearized augmented plane wave (FLAPW) method
- Various exchange-correlation functionals tested: LDA, GGA (PBE, PBEsol), GGA+U, meta-GGA, hybrid functionals
- Calculation of hyperfine parameters: B_{hf}, isomer shift, magnetic moments

Key Finding: PBEsol functional provides best agreement with experimental data for delocalized d-electron systems like iron carbides.

2.2.2 Iron Carbides Investigated

The complete iron carbide family:

Table 1: Iron carbides and their structures

Carbide	**Formula**	**Structure Type**
-Fe	Fe	BCC
’-FeC	FeC	Rock salt derivative
-Fe_3C	Fe_3C	Hexagonal
-Fe_2C	Fe_2C	Orthorhombic
-Fe_2C	Fe_2C	Monoclinic
-Fe_5C_2 (Hägg)	Fe_5C_2	Monoclinic
h-Fe_7C_3	Fe_7C_3	Hexagonal
-Fe_3C (Cementite)	Fe_3C	Orthorhombic
o-Fe_7C_3	Fe_7C_3	Orthorhombic
’-Fe_4C	Fe_4C	FCC derivative
”-Fe_4C	Fe_4C	Alternative structure
’-$Fe_{16}C_2$	$Fe_{16}C_2$	Ordered BCC

2.3 Experimental Validation

2.3.1 Synthesis of Pure Phases

The challenge in MES of iron carbides is obtaining single-phase samples. The Jiang et al. study synthesized:

-Fe_5C_2: Most stable under Fischer-Tropsch synthesis conditions

- Three distinct Fe sites: Fe1, Fe2, Fe3
- Hyperfine fields at room temperature: 18.3 T, 21.1 T, 10.8 T

-Fe_3C: Equilibrium carbide in Fe-C system

- Two distinct Fe sites
- Hyperfine fields at room temperature: 20.9 T, 19.4 T
- Curie temperature: 483 K

2.3.2 Temperature Dependence

The hyperfine field decreases with temperature according to:

$$B_{hf}(T) = B_{hf}(0\text{ K})\left(1-\frac{T}{T_C}\right)^{\beta} \tag{1}$$

where T_C is the Curie temperature and β is the critical exponent (mean field theory: $\beta = 0.5$).

2.4 Paalanen’s Work: Iron Carbides in Fischer-Tropsch Catalysis

2.4.1 Context and Motivation

Paasi Paalanen’s PhD thesis at Utrecht University (supervisor: Prof. Bert Weckhuysen) focused on iron carbides in Fischer-Tropsch synthesis (FTS). This work is highly relevant to steel metallurgy because:

- It provides precise identification protocols for iron carbides
- It demonstrates combined XRD + Mössbauer characterization

- It establishes formation temperature ranges for different carbides
- It shows how carbide formation depends on gas atmosphere and temperature

2.4.2 Carbide Formation Sequence

From Paalanen et al. (ChemCatChem 2020), the iron carbides form in order of increasing temperature during CO carburization:

1. **-$\mathbf{Fe_3C}$** (240-290°C): First carbide to form
2. **-$\mathbf{Fe_2C}$** (290-340°C): Intermediate carbide
3. **-$\mathbf{Fe_5C_2}$** (340-440°C): Hägg carbide, most stable in FTS
4. **-$\mathbf{Fe_3C}$** ($\geq$390°C): Cementite, equilibrium phase
5. **-$\mathbf{Fe_7C_3}$** (25 bar CO, 340°C): High-pressure conditions

2.4.3 Role of Na-S Promotion

Sodium-sulfur promotion affects:

- Increased Fe oxidation at low temperatures ($\leq$290°C)
- Preferential formation of -Fe_5C_2 over -Fe_3C at high temperatures
- No effect on fundamental carbide formation temperatures

2.5 Linear Relationship: B_{hf} vs. Magnetic Moment

A key finding from the DFT+experimental work:

$$B_{hf} = 12.81\ \mu_B + \text{offset} \tag{2}$$

where μ_B is the magnetic moment per iron atom. This provides a predictive tool for identifying carbides from Mössbauer spectra.

3 Part II: Thermodynamic Assessment by Naraghi et al.

3.1 Overview and Significance

The 2014 CALPHAD paper by Reza Naraghi, Malin Selleby, and John Ågren from KTH represents a comprehensive re-assessment of the Fe-C system with focus on:

1. Metastable carbides (Hägg, eta, epsilon)
2. Carbon ordering in martensite
3. Thermodynamic description valid from 0 K upwards
4. Non-stoichiometric cementite

3.2 Modeling Framework

3.2.1 Phase Descriptions

BCC Phase (Ferrite/Martensite): Sublattice model to describe carbon ordering:

$$\text{BCC: } (\text{Fe})_1(\text{C, Va})_1(\text{C, Va})_1(\text{C, Va})_1 \tag{3}$$

This multi-sublattice model allows description of:

- Disordered BCC (carbon randomly occupies octahedral sites)
- Zener ordered structure (carbon prefers one variant of octahedral sites)
- ”-$Fe_{16}C_2$ ordered structure

FCC Phase (Austenite): Standard two-sublattice model:

$$\text{FCC: } (\text{Fe})_1(\text{C, Va})_1 \tag{4}$$

Carbide Phases:

- Cementite (-Fe_3C): With off-stoichiometry capability
- Hägg carbide (-Fe_5C_2): Metastable phase
- Eta carbide (-Fe_2C): Metastable transition carbide
- Epsilon carbide (-Fe_3C): Metastable, often seen in tempering

3.3 Carbon Ordering in Martensite

3.3.1 Physical Basis

Fresh martensite is supersaturated with carbon. During early aging (room temperature to 200°C):

1. Carbon atoms redistribute from random octahedral sites
2. Zener ordering occurs: carbon preferentially occupies one variant
3. This causes measurable lattice parameter changes
4. Eventually forms ”-$Fe_{16}C_2$ ordered structure

3.3.2 Gibbs Energy Representation

At 300 K, the Gibbs energy curves show:

- $\mathbf{X}_s^1$: First spinodal point (critical carbon content)
- $\mathbf{X}_s^2$: Second spinodal point
- Between spinodal points: miscibility gap, tendency for decomposition

The critical carbon content for ordering varies in literature from 0.18 to 0.64 mass% C, reflecting modeling difficulties.

3.4 Metastable Carbides: Thermodynamic Stability

3.4.1 Gibbs Energy of Formation

Figure showing Gibbs energy of formation per mole of carbon:

$$\Delta G_f = G_{\text{carbide}} - n_{\text{Fe}} G_{\text{Fe}} - G_{\text{C(graphite)}} \tag{5}$$

Key observations:

- Cementite (-Fe_3C) is most stable at all temperatures
- Hägg carbide (-Fe_5C_2) is close in energy
- Eta carbide (-Fe_2C) has higher Gibbs energy
- All metastable carbides can form under appropriate kinetic conditions

3.5 Comparison with Previous Assessments

3.5.1 Improvements over Gustafson (1985)

The Naraghi assessment updates:

1. Incorporation of new low-temperature heat capacity data
2. Better description of carbon activity in austenite at high temperatures
3. Inclusion of metastable carbide models
4. Improved magnetic descriptions

3.5.2 Validation

The model reproduces:

- Eutectic temperature and composition
- Peritectic reaction
- Carbon solubility in ferrite and austenite
- Cementite precipitation during tempering
- Transition carbide formation sequences

3.6 Database Format and Adaptation

3.6.1 Original Format

The Naraghi database was developed for Thermo-Calc software. Key features:

- TDB (Thermodynamic Database) format
- GHSER functions for pure elements
- Magnetic model parameters (TC, BMAGN)
- Multi-component interaction parameters

3.6.2 Adaptation to Pandat

Assignment Task: Students will adapt this database for Pandat. Key considerations:

1. **Function definitions**: Pandat may use different GHSER reference states
2. **Magnetic parameters**: Syntax differences between Thermo-Calc and Pandat
3. **Phase names**: Ensure consistency
4. **Validation**: Compare calculated phase diagrams with published results

Comparison with Lecture 5 Database:

- Lecture 5 focused on high-pressure Fe-C (Brosh database)
- Naraghi focuses on metastable carbides at ambient pressure
- Both should give similar results for stable equilibria
- Differences in metastable extensions expected

4 Part III: Advanced Modeling by Jacob Group (TU Wien)

4.1 Research Focus at TU Wien

4.1.1 Key Contributions

The research group at TU Wien (including Aurélie Jacob, Erwin Povoden-Karadeniz) focuses on:

1. Revised thermodynamic description of Fe-Cr system
2. Thermodynamic prediction of bainite formation including BCT transformation
3. G-phase modeling in reactor pressure vessel steels
4. Interface-related precipitation mechanisms

4.2 Bainite Formation: The BCT Question

4.2.1 Experimental Evidence

Strong experimental evidence exists that bainitic ferrite forms as:

- Body-centered tetragonal (BCT) structure
- Supersaturated with carbon
- Carbon preferentially occupies octahedral sites along c-axis
- Creates tetragonal distortion: $c/a > 1$

4.2.2 Thermodynamic Modeling Approach

The Jacob group work provides:

Model Features:

- Incorporation of BCT as distinct phase from BCC
- Carbon-dependent tetragonality
- Driving force calculations for bainite transformation
- Comparison with martensite transformation

Implications:

- Resolves long-standing debate about bainite nature
- Explains carbon enrichment of austenite during transformation
- Predicts incomplete reaction phenomenon
- Connects with mechanistic models of bainite growth

4.3 Fe-Cr System: Improved -Phase Description

4.3.1 Sublattice Model for -Phase

Previous assessments had discrepancies in site fractions. The improved model:

$$\sigma\text{-phase: } (\mathrm{Cr, Fe})_{10}(\mathrm{Cr, Fe})_4(\mathrm{Cr, Fe})_{16} \tag{6}$$

Benefits:

1. Better agreement with experimental site occupancies
2. Improved prediction of -phase field boundaries
3. Foundation for multicomponent extensions (Fe-Cr-Ni, Fe-Cr-Mo)

4.3.2 Relevance to Steel Design

The -phase is critical in:

- Duplex stainless steels (embrittlement)
- High-temperature service (precipitation during aging)
- Weld heat-affected zones

Accurate thermodynamic description enables:

- Prediction of -phase solvus temperatures
- Optimization of heat treatment to avoid formation
- Design of -resistant compositions

4.4 Integration with Previous Lecture Topics

4.4.1 Connection to Lecture 5

Lecture 5 covered:

- High-pressure Fe-C (Brosh database)
- Computational steel design (Du-Schmid-Fetzer)
- MatCalc and Hallstedt-Noori databases

This lecture extends to:

- Metastable carbides and their characterization
- More detailed martensite/bainite models
- Experimental validation via Mössbauer spectroscopy

4.4.2 Unified Framework

All these databases share CALPHAD methodology but differ in:

1. **Scope**: Pressure range, phase coverage, element systems
2. **Optimization targets**: Different experimental datasets emphasized
3. **Application focus**: Geological vs. metallurgical vs. catalysis

5 Practical Application: Database Comparison Exercise

5.1 Objective

Students will compare predictions from:

1. Naraghi Fe-C database (adapted to Pandat)
2. Lecture 5 reference database
3. Commercial database (PanFe if available)

5.2 Test Calculations

5.2.1 Test 1: Martensite Tempering

Composition: Fe-0.8C (mass%)

Calculations:

- Quench from 850°C → martensite at room temperature
- Age at 150°C, 200°C, 250°C for various times
- Predict carbide types and fractions

Expected Results:

- 150°C: -Fe$_3$C precipitation
- 200-250°C: Transition from to -Fe$_3$C
- Carbon depletion in matrix

5.2.2 Test 2: Bainite Transformation

Composition: Fe-0.4C-2Mn-1Si (mass%)
Calculations:

- Isothermal transformation at 350°C, 400°C, 450°C
- Equilibrium carbide predictions
- Comparison of BCT vs. BCC models (if available)

5.2.3 Test 3: Non-stoichiometric Cementite

Composition: Fe-6.7C (mass%) = stoichiometric Fe_3C
Investigation:

- Does database allow off-stoichiometry?
- Calculate specific volume vs. composition
- Compare with Kayser experimental data (specific volume vs. carbon content)

5.3 Validation Against Experimental Data

5.3.1 Sources

- Paalanen Mössbauer data for carbide identification
- Bhadeshia's compilation of transformation temperatures
- Standard reference works (Metals Handbook, etc.)

5.3.2 Acceptance Criteria

- Temperature agreement within ±20°C for transformation temperatures
- Correct carbide sequence prediction
- Phase fraction trends consistent with experiments

6 Preparation for Bhadeshia Course

6.1 Course Structure

Professor Harry Bhadeshia's "Steels" course, delivered online in 2022 and now available on:

- YouTube: Bhadeshia123 Channel
- Cambridge University teaching materials: `https://www.phase-trans.msm.cam.ac.uk/teaching.html`
- Lecture notes: `https://www.phase-trans.msm.cam.ac.uk/2010/M21.pdf`

6.2 Relevant Topics from Theory of Transformations in Steel

From the textbook "Theory of Transformations in Steels" (2023 edition), chapters 8 and 9:

6.2.1 Chapter 8: Cementite

Topics covered:

- Crystal structure and symmetry
- Habit plane relationships with ferrite and austenite
- Thermodynamics and stability
- Precipitation mechanisms
- Role in pearlite, bainite, tempered martensite

Key Concepts for MIWUS Students:

1. Orientation relationships: Bagaryatskii, Pitsch
2. Coherency and semi-coherency
3. Coarsening kinetics

6.2.2 Chapter 9: Other Iron Carbides

Carbides discussed:

- -Fe_3C: Hexagonal transition carbide
- -Fe_2C: Orthorhombic carbide
- -Fe_5C_2: Hägg carbide
- -Fe_7C_3: Eckstrom-Adcock carbide

Critical Questions Addressed:

1. Are transition carbides truly metastable relative to cementite?
2. What are the transformation sequences during tempering?
3. How do alloying elements stabilize different carbides?

6.3 Integration with MIWUS Computational Approach

6.3.1 Computational Validation

Students will use databases to:

- Calculate driving forces for different carbide formations
- Predict which carbide forms under given conditions
- Compare with Bhadeshia's experimental compilations

6.3.2 Case Studies

Using both CALPHAD and Bhadeshia's phenomenological models:

1. **Tool Steel Tempering**: Predict carbide sequence in Fe-C-Cr-V
2. **Bainitic Steels**: Model carbon partitioning during transformation
3. **TRIP Steels**: Austenite stability and carbide precipitation

7 Conclusions and Next Steps

7.1 Key Takeaways

1. **Mössbauer spectroscopy** provides unique characterization of iron carbides through hyperfine interactions
2. **DFT calculations** now reliably predict Mössbauer parameters, enabling phase identification
3. **Thermodynamic databases** can incorporate metastable carbides and carbon ordering
4. **Bainite definition** remains an active research area, with BCT models showing promise
5. **Database comparison** reveals different optimization philosophies and application domains

7.2 Preparation for Next Lectures

7.2.1 Required Reading

1. Bhadeshia Chapters 8 & 9 from Theory of Transformations in Steels
2. Naraghi et al. CALPHAD paper (2014)
3. Jiang et al. Nature Scientific Reports (2016) on Mössbauer
4. Paalanen PhD thesis (selected chapters)

7.2.2 Computational Assignments

1. Adapt Naraghi database to Pandat format
2. Run test calculations comparing different databases
3. Validate against experimental tempering data
4. Prepare presentation on database comparison findings

7.3 Looking Forward: Steel Course Topics

From Bhadeshia's M21 lecture notes, upcoming topics will include:

- Martensite crystallography and morphology
- Bainite transformation kinetics
- Tempering mechanisms
- Mechanical properties-microstructure relationships

The computational thermodynamic foundation from MIWUS will support understanding of these transformation phenomena.

Acknowledgments

This lecture synthesizes contributions from:

- Professor Harry Bhadeshia (Cambridge University) for decades of fundamental research on steel transformations and for making his course materials openly available
- Dr. Reza Naraghi (now at Thermo-Calc) for thermodynamic assessments during his PhD at KTH
- Dr. Aurélie Jacob (TU Wien) for advanced modeling of steel phases
- Dr. Paasi Paalanen and Prof. Bert Weckhuysen (Utrecht University) for detailed iron carbide characterization
- The CALPHAD and Mössbauer spectroscopy communities for open data sharing

References

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Online Resources

- MIWUS Course Materials: `https://www.gotrawama.eu/miwus26/`
- Bhadeshia Teaching Page: `https://www.phase-trans.msm.cam.ac.uk/teaching.html`
- Bhadeshia YouTube Channel: `https://www.youtube.com/playlist?list=PLj4YiOgq320onCH7PDcSX1AN`
- Paalanen PhD Thesis: `https://dspace.library.uu.nl/handle/1874/400080`
- Nature SR Paper: `https://www.nature.com/articles/srep26184`

A Appendix A: Mössbauer Spectroscopy Parameters

A.1 Hyperfine Interactions Summary

Table 2: Typical Mössbauer parameters for iron carbides at room temperature

Phase	**IS (mm/s)**	**QS (mm/s)**	B_{hf} **(T)**	T_C **(K)**
-Fe (BCC)	0.00	0.00	33.0	1043
-Fe_3C	0.18-0.25	0.00-0.04	20.2-20.9	483
-Fe_5C_2	0.20-0.27	0.00	10.8-21.1	520-543
-Fe_3C	0.21-0.24	0.00	17-19	–
-Fe_2C	0.22	0.00	16-18	–

Note: IS = Isomer Shift, QS = Quadrupole Splitting, B_{hf} *= Hyperfine Field,* T_C *= Curie Temperature*

B Appendix B: Database Adaptation Guide

B.1 Thermo-Calc to Pandat Conversion

B.1.1 Common Syntax Differences

1. **GHSER Functions:**
   - Thermo-Calc: `GHSERFE#`
   - Pandat: May require explicit definition or different naming
2. **Magnetic Parameters:**
   - Thermo-Calc: `TC(PHASE,ELEMENT;0)`
   - Pandat: Check specific syntax in manual
3. **Excess Parameters:**
   - Both use similar Redlich-Kister polynomials
   - Check order of interaction parameters

B.1.2 Validation Checklist

After conversion, verify:

1. Database loads without errors
2. Pure element reference states match
3. Binary phase diagrams reproduce literature
4. Invariant reactions (eutectic, peritectic) at correct T and composition
5. Metastable extensions behave as expected

C Appendix C: Assignment Details

C.1 Database Comparison Project

C.1.1 Deliverables

1. **Technical Report** (15-20 pages):
    - Introduction: Importance of iron carbides in steels
    - Methodology: Database conversion procedure
    - Results: Comparative calculations
    - Discussion: Strengths and limitations of each database
    - Conclusions: Recommendations for different applications
2. **Converted TDB Files:**
    - Naraghi database in Pandat format
    - Documentation of all modifications made
    - Test scripts demonstrating calculations
3. **Comparative Plots:**
    - Fe-C phase diagram from each database
    - Temperature vs. carbide fraction during tempering
    - Gibbs energy of formation for all carbides
4. **Presentation:** 15-minute presentation of findings

C.1.2 Grading Rubric

C.2 Timeline

- Week 1: Database acquisition and preliminary conversion
- Week 2: Test calculations and debugging
- Week 3: Comprehensive comparison and analysis
- Week 4: Report writing and presentation preparation

Table 3: Grading criteria for database comparison assignment

Criterion	**Weight**
Database conversion accuracy	25%
Quality of comparative calculations	25%
Critical analysis and insights	20%
Validation against experimental data	15%
Report quality and presentation	15%
Total	**100%**

D Appendix D: Computational Tools Reference

D.1 Software for Mössbauer Analysis

- **MossWinn**: Windows-based fitting software for Mössbauer spectra
- **Recoil**: Versatile Mössbauer spectral analysis software
- **VESTA**: Visualization of crystal structures for carbides

D.2 CALPHAD Software

- **Pandat**: CompuTherm's software (3-element free version)
- **Thermo-Calc**: Commercial software with student licenses
- **OpenCalphad**: Open-source alternative
- **PyCalphad**: Python library for thermodynamic calculations

D.3 DFT Codes for Hyperfine Calculations

- **WIEN2k**: All-electron LAPW code (used by Jiang et al.)
- **VASP**: Plane-wave pseudopotential code
- **Quantum ESPRESSO**: Open-source plane-wave code
- **CASTEP**: Plane-wave code with hyperfine capabilities