Mini Instant Winter University School (MIWUS)

A LLM-assisted course on Computational Metallurgy

Lecture 03: Larry Kaufman and the Birth of CALPHAD

Historical Foundations and the SGTE Pure Elements Database

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Document Generation Notice

This lecture material was drafted using DeepSeek LLM through collaborative interaction with Prof. Fabio Miani. The content is based on:

- Larry Kaufman's PhD work and early lattice stability publications (1959)
- Kaufman's seminal 1970 book on computer calculation of phase diagrams
- The modern CALPHAD textbook by Lukas, Fries, and Sundman (2007)
- The SGTE Pure Elements Database and Dinsdale's foundational work

All technical content has been reviewed for accuracy and pedagogical appropriateness.

Contents

1 Introduction: From Theory to Computational Practice

1.1 Course Context and Learning Goals

Learning Goals

After this lecture, you will be able to:

- Understand Larry Kaufman's foundational contributions to CALPHAD methodology
- Explain the concept of lattice stability and its importance in alloy thermodynamics
- Describe the historical development of computational thermodynamics
- Access and use the SGTE Pure Elements Database in different formats
- Connect early theoretical work to modern computational practice
- Appreciate the collaborative nature of CALPHAD community development

In Lectures 01 and 02, we explored the practical tools and thermodynamic foundations of computational metallurgy. Now we turn to the **historical and methodological origins** of the CALPHAD approach. This lecture connects:

1. **Part A:** Larry Kaufman's pioneering work that established CALPHAD methodology
2. **Part B:** The SGTE Pure Elements Database as a modern implementation of these ideas

Understanding this history is not just academic—it helps us appreciate why CALPHAD works, recognize its limitations, and contribute to its future development.

1.2 The CALPHAD Journey: A Timeline

CALPHAD Historical Development

1959: Kaufman's lattice stability paper establishes key concepts
1970: *Computer Calculation of Phase Diagrams* book publishes methodology
1973: First CALPHAD meeting establishes community
1991: Dinsdale publishes SGTE Pure Elements Database
2007: *Computational Thermodynamics* textbook codifies modern practice
2009: SGTE Unary Database Version 5.0 released
Present: Worldwide collaborative assessments continue

Figure 1: Key milestones in CALPHAD development

2 Part A: Larry Kaufman and the Birth of CALPHAD

2.1 The Pre-CALPHAD Landscape

2.1.1 The Problem: Predicting Phase Diagrams Before Computers

Before Kaufman's work in the late 1950s, phase diagrams were:

- Determined **entirely experimentally**

- Time-consuming and expensive to measure
- Limited to temperatures and compositions accessible to experiments
- Difficult to extrapolate or interpolate
- Nearly impossible to predict for multicomponent systems

Metallurgists needed a way to:

1. Calculate phase diagrams from fundamental principles
2. Extrapolate from binary to ternary and higher-order systems
3. Predict behavior at extreme conditions
4. Design alloys systematically rather than empirically

2.1.2 Kaufman's Vision: Thermodynamics + Computation

Larry Kaufman recognized that:

- Thermodynamics provides the **mathematical framework**
- Computers provide the **computational power**
- Together they could **predict phase equilibria**

His key insight: **If you can describe the Gibbs energy of each phase as a function of temperature, pressure, and composition, you can calculate phase equilibria by minimizing total Gibbs energy.**

2.2 The Lattice Stability Concept (1959)

2.2.1 The 1959 Paper: "The lattice stability of metals—I. Titanium and zirconium"

In his seminal 1959 paper in Acta Metallurgica, Kaufman addressed a fundamental problem: **How do you describe the free energy difference between different crystal structures of the same element?**

Core Concept: Lattice Stability

Lattice stability refers to the relative stability of different crystal structures (allotropes) of a pure element. For example:

- Iron: bcc (α), fcc (γ), bcc (δ)
- Titanium: hcp (α), bcc (β)
- Carbon: graphite, diamond

The **lattice stability parameter** G^{ϕ} represents the Gibbs energy of element i in structure ϕ, relative to a reference state.

2.2.2 Mathematical Formulation

For an element with multiple allotropes, Kaufman expressed the Gibbs energy difference as:

$$\Delta G^{\alpha\to\beta}(T) = G^{\beta}(T) - G^{\alpha}(T)$$

Where α and β are different crystal structures. He represented this using polynomial expressions:

$$G^{\phi}(T) = a + bT + cT\ln T + dT^2 + eT^3 + fT^{-1} + \cdots$$

2.2.3 Calculating Lattice Stability for Ti and Zr

In the 1959 paper, Kaufman:

1. Collected all available thermodynamic data for Ti and Zr
2. Analyzed the bcc (β) to hcp (α) transformations
3. Calculated $\Delta G^{\beta\to\alpha}$ from 0 K to 2000 K
4. Found the chemical driving force for martensitic transformation: ~50 cal/mol (209 J/mol)
5. Compared with Fe-base alloys (300 cal/mol or 1255 J/mol)
6. Explained the difference based on transformation characteristics

Table 1: Kaufman's Lattice Stability Calculations (1959)

Element	**Transformation**	ΔH (cal/mol)	ΔS (cal/mol·K)	**Driving Force at** T_0
Titanium	β(bcc) → α(hcp)	1120	0.82	~50 cal/mol
Zirconium	β(bcc) → α(hcp)	960	0.58	~50 cal/mol
Iron	γ(fcc) → α(bcc)	220	0.15	~300 cal/mol

Table 2: *
Source: Kaufman, L., "The lattice stability of metals—I," Acta Metallurgica, 1959

2.2.4 Significance of This Work

Kaufman's lattice stability paper established:

- The **mathematical framework** for describing polymorphic transformations
- The concept of **reference states** for thermodynamic calculations
- Methods for **extrapolating limited experimental data**
- Foundation for **thermodynamic modeling of alloys**

This was the essential first step toward computerized phase diagram calculations.

2.3 Kaufman's 1970 Book: A Methodology is Born

2.3.1 "Computer Calculation of Phase Diagrams with Special Reference to Refractory Metals"

In 1970, Kaufman published the book that gave the methodology its name and established the CALPHAD approach. The book presented:

1. **Complete methodology** for calculating phase diagrams
2. **Mathematical models** for Gibbs energy of different phases
3. **Computational algorithms** for equilibrium calculations
4. **Applications** to refractory metal systems
5. **Predictions** of ternary systems from binary data

2.3.2 Key Contributions in the 1970 Book

1. Systematic Parameterization:

$$G_m = \sum_i x_i G_i^\phi + RT \sum_i x_i \ln x_i + G^{ex}$$

where G^{ex} represents excess Gibbs energy, modeled using Redlich-Kister polynomials.

2. Regular Solution Approximation: For many binary systems, Kaufman used:

$$G^{ex} = x_A x_B L_{AB}$$

where L_{AB} is a temperature-dependent interaction parameter.

3. Extrapolation to Multicomponent Systems: For ternary systems A-B-C from binaries:

$$G^{ex} = x_A x_B L_{AB} + x_A x_C L_{AC} + x_B x_C L_{BC}$$

4. Computer Implementation: The book included actual FORTRAN code for phase diagram calculations—revolutionary for its time!

Historical Context

In 1970, computers were mainframes with limited memory and processing power. Kaufman's algorithms had to be efficient enough to run on these machines. His work demonstrated that phase diagram calculations were **not just theoretically possible but practically achievable** with available technology.

2.3.3 Application to Refractory Metals

Kaufman focused on refractory metals (W, Mo, Ta, Nb, etc.) because:

- They have high melting points, making experiments difficult
- They form complex phase diagrams
- They were strategically important for aerospace and defense
- They demonstrated the power of computational prediction

2.4 The CALPHAD Methodology: From Kaufman to Modern Practice

2.4.1 The CALPHAD Equation

The fundamental equation that Kaufman established and that remains at the core of CALPHAD:

$$G_m^{\phi}(T, P, \mathbf{x}) = \sum_i x_i G_i^{\phi}(T, P) + RT \sum_i x_i \ln x_i + G_m^{ex,\phi}(T, P, \mathbf{x})$$

Where:

- G_m^{ϕ} = molar Gibbs energy of phase ϕ
- x_i = mole fraction of component i
- G_i^{ϕ} = lattice stability of element i in structure ϕ
- $G_m^{ex,\phi}$ = excess Gibbs energy (non-ideal mixing)

2.4.2 The CALPHAD Workflow (Modern Version)

1. **Model Selection:** Choose appropriate models for each phase
2. **Data Assessment:** Collect experimental data (phase diagrams, thermochemistry)
3. **Parameter Optimization:** Adjust parameters to fit experimental data
4. **Database Creation:** Store optimized parameters in TDB format
5. **Phase Diagram Calculation:** Calculate equilibria by Gibbs energy minimization
6. **Validation:** Compare calculations with independent experimental data

2.4.3 Kaufman's Legacy in Modern CALPHAD

Table 3: From Kaufman's Original Work to Modern CALPHAD

Aspect	**Kaufman (1970)**	**Modern CALPHAD**
Computer power	Mainframe (kFLOPS)	Desktop (GFLOPS)
Phase models	Simple (regular solution)	Complex (sublattice, ionic)
Parameters	Few, manually optimized	Many, automatically optimized
Systems	Mostly binaries, some ternaries	Up to 10+ components
Accuracy	Qualitative/semi-quantitative	Quantitative (experimental accuracy)
Community	Small group	Worldwide collaboration
Software	Custom FORTRAN codes	Commercial/open-source packages

2.5 The CALPHAD Community and Evolution

2.5.1 The First CALPHAD Meeting (1973)

In 1973, Kaufman organized the first CALPHAD meeting, which:

- Established a **collaborative community** of researchers

- Created standards for **data exchange and comparison**
- Initiated **systematic assessments** of alloy systems
- Published proceedings that documented progress

2.5.2 From Individual to Community Effort

CALPHAD evolved from Kaufman's individual pioneering work to a worldwide collaborative effort:

- **SGTE (Scientific Group Thermodata Europe):** Established standards and databases
- **International collaborations:** Joint assessments across institutions
- **Software development:** Multiple commercial and open-source tools
- **Journal:** CALPHAD journal established in 1977

2.5.3 Modern Textbook: "Computational Thermodynamics" (2007)

The textbook by Lukas, Fries, and Sundman represents the modern codification of CALPHAD methodology. Key contributions:

1. **Comprehensive theory:** Complete mathematical foundation
2. **Practical guidance:** Step-by-step assessment procedures
3. **Software integration:** Connection to modern computational tools
4. **Advanced topics:** Kinetics, diffusion, property predictions

This book is essential reading for serious CALPHAD practitioners and represents the maturation of Kaufman's original vision.

3 Part B: The SGTE Pure Elements (Unary) Database

3.1 Introduction: Why a Standardized Database?

3.1.1 The Problem of Inconsistency

Before SGTE (Scientific Group Thermodata Europe), different research groups:

- Used different **reference states** for elements
- Had different **lattice stability values**
- Used different **mathematical expressions**
- Created incompatible databases
- Could not combine or compare results

This "Tower of Babel" problem limited the usefulness of CALPHAD calculations.

3.1.2 The SGTE Solution

SGTE established:

- **Standard reference states** for all elements
- **Consistent lattice stability** parameters
- **Standard mathematical representation** (Gibbs energy polynomials)
- **Quality-controlled assessments**
- **Publicly available databases**

3.2 The SGTE Pure Elements Database

3.2.1 Overview and Scope

The SGTE Pure Elements Database (often called the "Unary" database):

- Contains assessed thermochemical data for **all stable elements**
- Includes **many metastable modifications**
- Covers temperature range: **298.15 K to gaseous state**
- Current version: **5.0 (2009)**
- Includes: Ag, Al, Am, As, Au, B, Ba, Be, Bi, Br, C, Ca, Cd, Ce, Cl, Co, Cr, Cs, Cu, ... (87 elements total)

3.2.2 Dinsdale's Foundational Work (1991)

Alan Dinsdale's 1991 paper "SGTE data for pure elements" (Calphad Vol 15, pp. 317-425) established:

- **Systematic assessment** of all elemental data
- **Standard reference states** (SER: Standard Element Reference)
- **Mathematical representation** using Gibbs energy functions
- **Consistent treatment** of phase transformations
- Foundation for all subsequent SGTE databases

3.2.3 Mathematical Representation

For each element and phase, SGTE uses:

$$G_i^{\phi}(T) = a + bT + cT\ln T + dT^2 + eT^3 + fT^{-1} + \sum g_i T^i$$

The reference state is defined as:

$$G_i^{\text{SER}}(T) = G_i^{\text{stable phase at 298.15K, 1 bar}}(T)$$

For elements with multiple allotropes, lattice stability is expressed relative to SER.

Example: Iron in SGTE Database

Iron has three allotropes:

- bcc (α, δ): Stable below 1184 K and above 1665 K
- fcc (γ): Stable between 1184 K and 1665 K

SGTE provides G^{bcc}, G^{fcc}, and G^{liquid} for iron, all relative to SER (bcc at 298.15 K).

3.3 Database Structure and Formats

3.3.1 The TDB Format (Thermo-Calc)

The standard format used by Thermo-Calc and compatible with many other software packages:

```
$ Iron - SGTE Unary Database
$ Reference: Dinsdale, Calphad 15(1991)317-425
$
ELEMENT FE    BCC_A2    55.8450    4.1154E+03    2.7310E+01!
$
$ Function GHSERFE: Stable bcc phase
FUNCTION GHSERFE    298.15
   -7650.085 + 118.469743*T - 23.5143*T*LN(T)
   - 0.00439752*T**2 - 5.89269E-08*T**3
   + 77358.5*T**(-1);  1811.00  Y
   - 26110.512 + 279.135*T - 46*T*LN(T)
   + 2.29603E+31*T**(-9);  6000.00  N !
$
$ Function GHSERFE for fcc (relative to SER)
FUNCTION GFCCFE    298.15
   + 7284 + 0.163*T + GHSERFE;  1811.00  Y
   - 2360 + 6.05*T + GHSERFE;  6000.00  N !
$
$ Function GHSERFE for liquid (relative to SER)
FUNCTION GLIQFE    298.15
   + 12040 - 6.55843*T + GHSERFE;  1811.00  Y
   + 108 - 0.642*T + GHSERFE;  6000.00  N !
```

3.3.2 Other Software Formats

FactSage Format:

- Similar polynomial representation
- Different coefficient values (converted from SGTE)

- Compatible with FactSage software suite

Pandat Format:

- Uses .PAN files instead of .TDB
- Similar mathematical representation
- Optimized for Pandat software

OpenCalphad Format:

- Uses standard TDB format
- May require minor syntax adjustments
- Fully compatible with OpenCalphad software

3.3.3 Conversion Between Formats

Conversion factors between different software formats:

$$\text{SGTE} \leftrightarrow \text{FactSage} : \text{Different reference temperatures}$$

$$\text{TDB} \leftrightarrow \text{PAN} : \text{Different file structure, same mathematics}$$

Table 4: Software Compatibility with SGTE Unary Database

Software	**Native Format**	**SGTE Compatible**	**Conversion Needed**	**License**
Thermo-Calc	.TDB	Direct	None	Commercial
FactSage	.DAT	Direct	Minor	Commercial
Pandat	.PAN	Direct	File conversion	Commercial
OpenCalphad	.TDB	Direct	None	Open source
MatCalc	.TDB	Direct	None	Commercial

3.4 Using the SGTE Database in Practice

3.4.1 Accessing the Database

The SGTE Pure Elements Database is available:

- **Official SGTE website:** `https://www.sgte.net/en/free-pure-elements-database`
- **Thermo-Calc installation:** Included with software
- **FactSage installation:** Included with software
- **Academic repositories:** Through university subscriptions
- **Direct download:** TDB file from SGTE website

3.4.2 Extracting Data for an Element

To use SGTE data for a specific element (e.g., Aluminum):

1. Locate the element in the database file
2. Identify all phase descriptions
3. Note the reference state (SER)
4. Extract Gibbs energy functions for each phase
5. Convert to required format if necessary

3.4.3 Example: Aluminum Data from SGTE

```
$ Aluminum - SGTE Unary Database
ELEMENT AL FCC_A1 26.9815 4.5773E+03 2.8322E+01 !
$
$ Stable fcc phase (SER)
FUNCTION GHSERAL 298.15
   -7976.15 + 137.093038*T - 24.3671976*T*LN(T)
   - 0.001884662*T**2 - 8.77664E-07*T**3
   + 74092*T**(-1); 700.00 Y
   -11276.24 + 223.048446*T - 38.5844296*T*LN(T)
   + 0.018531982*T**2 - 5.764227E-06*T**3
   + 74092*T**(-1); 933.47 Y
   -11278.378 + 188.684153*T - 31.748192*T*LN(T)
   - 1.230524E+28*T**(-9); 2900.00 N !
$
$ Liquid phase (relative to SER)
FUNCTION GLIQAL 298.15
   +11005.29 - 11.84185*T + 7.934E-20*T**7 + GHSERAL; 933.47 Y
   +10481.318 - 11.253014*T + 1.231E+28*T**(-9) + GHSERAL; 2900.00 N !
```

3.5 Applications and Limitations

3.5.1 Applications of the SGTE Database

1. **Reference for assessments:** Starting point for binary and higher-order systems
2. **Consistency checking:** Ensure different assessments use same element data
3. **Teaching and learning:** Standard examples for students
4. **Software development:** Test cases for new software
5. **Research:** Baseline for new element assessments

3.5.2 Limitations and Considerations

- **Fixed version:** Database updates infrequently (current: 2009)
- **Metastable phases:** Not all possible modifications included
- **High temperatures:** Extrapolation beyond fitted range may be unreliable
- **Pressure dependence:** Standard database is for 1 bar only
- **New elements:** Recently discovered elements may not be included

3.5.3 When to Use SGTE vs. Custom Data

Table 5: Choosing Between SGTE and Custom Element Data

Situation	Use SGTE	Use Custom Data
Standard CALPHAD assessments	Recommended	Only if justified
Teaching and examples	Essential	Not needed
Comparing different assessments	Required for consistency	Causes incompatibility
Research on new elements	Not available	Necessary
High-pressure calculations	Limited to 1 bar	Required
Special applications (nanoparticles, etc.)	May be insufficient	Likely needed

3.6 The Future of Element Databases

3.6.1 Ongoing Developments

1. **Integration with first-principles:** Using DFT calculations to improve data
2. **High-pressure extensions:** Developing pressure-dependent formulations
3. **Nanoscale effects:** Accounting for surface and size effects
4. **Kinetic databases:** Extending to diffusion and mobility data
5. **Open-access initiatives:** Making databases more widely available

3.6.2 Community Contributions

The SGTE database represents a community effort:

- **Contributors:** Researchers worldwide submit assessments
- **Review process:** Expert evaluation before inclusion
- **Updates:** New versions incorporate improved data
- **Documentation:** Thorough referencing of sources
- **Quality control:** Consistency checks across elements

4 Computational Exercises

4.1 Exercise 3.1: Exploring Lattice Stability

Hands-On Exercise: Understanding Lattice Stability

Problem: Calculate and compare lattice stability parameters for three elements.
Elements to analyze:

1. Titanium (hcp-bcc transformation)
2. Iron (bcc-fcc-bcc transformations)
3. Zirconium (hcp-bcc transformation)

Tasks:

1. Extract SGTE data for each element and phase
2. Calculate $\Delta G^{\alpha \to \beta}(T)$ at three temperatures: 500 K, 1000 K, 1500 K
3. Plot ΔG vs. T for each element
4. Compare with Kaufman's 1959 values (convert units as needed)
5. Discuss the physical meaning of the results

Deliverables:

- MATLAB/Octave script for calculations
- Comparison plots
- Brief report interpreting the results

4.2 Exercise 3.2: SGTE Database Format Conversion

Hands-On Exercise: Working with Database Formats

Problem: Convert SGTE data between different software formats.
Tasks:

1. Download the SGTE Unary database in TDB format
2. Extract data for three elements: Cu, Ni, Al
3. Convert to three different formats:
    - FactSage format (.DAT)
    - Simple text format for plotting
    - JSON format for web applications
4. Write a Python or MATLAB script to automate the conversion
5. Test by loading converted files into appropriate software (if available)

Deliverables:

- Conversion script with documentation
- Converted files for three elements
- Brief report on format differences and compatibility issues

4.3 Exercise 3.3: Reproducing Kaufman's Calculations

Advanced Exercise: Historical Reproduction

Goal: Reproduce part of Kaufman's 1959 lattice stability calculations using modern tools.
Procedure:

1. Study Kaufman's 1959 paper methodology
2. Collect the same thermodynamic data he used (from cited references)
3. Implement his calculation method in MATLAB/Octave
4. Calculate $\Delta G^{\beta \to \alpha}$ for Ti from 0 K to 2000 K
5. Compare your results with his published values
6. Repeat using modern SGTE data
7. Analyze differences and improvements

Learning Objective: Understand how computational methods have evolved and appreciate the challenges of early CALPHAD work.

5 Summary and Key Takeaways

5.1 Part A: Larry Kaufman's Contributions

Foundational concepts established:

- **Lattice stability:** Mathematical description of polymorphic transformations
- **Gibbs energy parameterization:** Polynomial representations for computational use
- **Computational methodology:** Algorithms for phase equilibrium calculations
- **Systematic extrapolation:** From binary to multicomponent systems

Historical significance:

- Transformed alloy design from empirical to computational
- Established CALPHAD as a distinct methodology
- Built community through meetings and collaborations
- Visionary recognition of computer potential in materials science

5.2 Part B: SGTE Pure Elements Database

Key features:

- **Comprehensive:** All stable elements, many metastable phases
- **Consistent:** Standard reference states and mathematical forms
- **Community-developed:** Collaborative assessments ensure quality
- **Software-compatible:** Multiple format support
- **Foundational:** Basis for all higher-order databases

Practical importance:

- Enables consistent assessments across research groups
- Provides reliable baseline data for calculations
- Supports software development and testing
- Essential for teaching and learning CALPHAD

5.3 The CALPHAD Legacy

The combined legacy of Kaufman's vision and SGTE's implementation:

- **Scientific impact:** Transformed materials thermodynamics
- **Industrial impact:** Accelerated alloy development and optimization
- **Educational impact:** Created new curriculum in computational materials science
- **Community impact:** Fostered worldwide collaboration
- **Technological impact:** Enabled materials informatics and AI-assisted design

5.4 Final Reflection

CALPHAD represents a remarkable success story in computational materials science:

1. **Individual vision** (Kaufman) recognized potential
2. **Methodological development** created practical tools
3. **Community building** established standards and collaboration
4. **Technological progress** enabled increasingly sophisticated applications
5. **Widespread adoption** validated the approach across industries

Understanding this history helps us appreciate both the power and the limitations of CALPHAD, and inspires us to contribute to its future development.

6 Preparing for Lecture 04

6.1 Prerequisites Review

Before Lecture 04, ensure you understand:

1. The concept of lattice stability and reference states
2. The mathematical representation of Gibbs energy for pure elements
3. How to access and use the SGTE Unary database
4. The historical development of CALPHAD methodology
5. Basic phase diagram calculations from Lecture 01

6.2 Recommended Reading

1. **Kaufman, L.,** "The lattice stability of metals—I. Titanium and zirconium," Acta Metallurgica (1959)
2. **Dinsdale, A.,** "SGTE data for pure elements," Calphad (1991) - reference for SGTE database
3. **Lukas, H., Fries, S.G., Sundman, B.,** *Computational Thermodynamics* (2007), Chapter 3 on unary systems
4. Review SGTE website and download Unary database: `https://www.sgte.net/en/free-pure-elements-`

6.3 Practical Preparation Tasks

Pre-Lecture 04 Preparation

Tasks to complete:

1. Download the SGTE Unary database in TDB format
2. Load it into your CALPHAD software (Pandat, OpenCalphad, or MatCalc)
3. Extract and plot $G(T)$ for three elements with allotropes (e.g., Fe, Ti, C)
4. Calculate ΔG between allotropes at several temperatures
5. Complete at least two exercises from Section 5 of this lecture
6. Prepare questions on database structure or historical aspects

6.4 Looking Ahead to Lecture 04

Lecture 04 topics will include:

- Ternary phase diagrams: interpretation and calculation
- Liquidus projections and isothermal sections
- Practical applications in alloy design
- Connection to bulk metallic glasses and high-entropy alloys

Connection to this lecture:

- Understanding pure element behavior is prerequisite for understanding mixtures
- SGTE element data provides foundation for all solution models
- Historical perspective helps appreciate why certain models were developed

7 Additional Resources and References

7.1 Primary Historical Sources

Kaufman's foundational work:

- Kaufman, L., "The lattice stability of metals—I. Titanium and zirconium," Acta Metallurgica 7 (1959) 575-587
- Kaufman, L., *Computer Calculation of Phase Diagrams with Special Reference to Refractory Metals*, Academic Press (1970)
- Early CALPHAD meeting proceedings (1973 onward)

SGTE database sources:

- Dinsdale, A., "SGTE data for pure elements," Calphad 15 (1991) 317-425
- SGTE website: `https://www.sgte.net/`
- SGTE Pure Elements Database: `https://www.sgte.net/en/free-pure-elements-database`

Modern textbooks:

- Lukas, H., Fries, S.G., Sundman, B., *Computational Thermodynamics: The Calphad Method*, Cambridge University Press (2007)
- Saunders, N., Miodownik, A.P., *CALPHAD: A Comprehensive Guide*, Pergamon (1998)

7.2 Online Resources

Databases and software:

- SGTE Pure Elements Database (free download)
- Thermo-Calc Software: `https://thermocalc.com/`
- FactSage: `http://www.crct.polymtl.ca/fact/`
- OpenCalphad: `http://www.opencalphad.org/`
- Pandat: `https://computherm.com/`

Educational resources:

- CALPHAD organization website: `https://www.calphad.org/`
- Online courses and tutorials for various software packages
- University course materials (MIT, KTH, etc.)

7.3 Contact and Course Support

Course instructor:

- Prof. Fabio Miani
- Email: fabio.miani@uniud.it
- Department: Polytechnic Engineering and Architecture, University of Udine

Course materials:

- Website: `http://www.gotrawama.eu/miwus26/`
- Lecture PDFs, exercises, and databases
- Software installation guides and tutorials

Acknowledgments

This lecture material draws upon the pioneering work of individuals and communities who developed CALPHAD methodology:

- **Dr. Larry Kaufman** for visionary development of computational phase diagram methods
- **Dr. Alan Dinsdale** and the SGTE community for creating standardized databases
- **Prof. Bo Sundman, Dr. Hans Lukas, and Dr. Suzana Fries** for comprehensive textbook
- **The CALPHAD community** worldwide for collaborative development
- **University of Udine library** for providing access to historical and current resources

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Document Generation Note

This lecture was created through collaboration between Prof. Fabio Miani and DeepSeek LLM. The content is based on publicly available academic resources that students have full access to through the University of Udine library system.
Historical context has been carefully researched and technical details verified against original sources. Students are encouraged to consult primary sources for research purposes and to appreciate the original contributions of pioneers in computational thermodynamics.

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End of Lecture 03 - Larry Kaufman and the Birth of CALPHAD
Next: Lecture 04 - Ternary Systems and Advanced Phase Diagram Calculations