

**Dr. Fan Zhang, FASM
President
CompuTherm, LLC
Middleton, WI
Trustee (2024-2027)**



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Dr. Fan Zhang is the president of CompuTherm, one of the leading software developers in the field of computational thermodynamics and kinetics using the CALPHAD method. She is responsible for the company's long-term strategic planning in research and development, product development, service, and commercialization.

Dr. Fan Zhang joined CompuTherm as a materials scientist right after graduating from the University of Wisconsin-Madison in 1997. In the early years of her career, Dr. Zhang mainly focused on developing thermodynamic databases for various metal alloy systems using the CALPHAD method. After a few years, she started developing her leadership skills when she served as the principal investigator of several small business innovative research (SBIR) programs sponsored by the US air force research laboratory. Dr. Zhang has authored and co-authored more than 130 peer-review papers. She has been invited to give invited presentations numerous times at various conferences in the field of materials science and ICME.

Dr. Zhang is actively involved in professional services. She has served as Associate Editor of Journal of Phase Equilibria and Diffusion since 2009. She is a member of the ASM Alloy Phase Diagram Committee, a member of ASM Content & Data Products Council, a member and past chair of TMS Alloy Phase Committee.

Dr. Fan Zhang completed her bachelor (1987) and master (1990) education in physical chemistry in metallurgy at University of Science and Technology Beijing (USTB), China. She received her Ph.D degree in materials science and engineering in 1997 from the University of Wisconsin-Madison.

Abstract: The CALPHAD Method and Its Applications in Materials Science and Metallurgical Practices

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Abstract:

As once remarked by Sir William Hume Rothery “Phase diagram is the beginning of wisdom-not the end of it”. Indeed, phase diagrams, serving as the foundational tools for understanding numerous phenomena in physical metallurgy, are usually referred to as roadmaps for alloy design. Traditionally, phase diagrams were derived solely from experimental methods, suitable for binary and simple ternary systems, but inadequate for complex multi-component systems. Yet, multi-component phase diagrams are crucial in modern materials design since multiple elements are often needed to tailor material properties to meet the diverse requirements of various applications.

The CALPHAD (Calculation of Phase Diagram) method was introduced in 1970 by Prof. Larry Kaufman for calculating self-consistent phase diagrams. This methodology involves constructing a thermodynamic database, comprising Gibbs energy functions for all the phases in a system. With this database, phase equilibria and thermodynamic properties can be calculated at any composition and temperature, making CALPHAD the premier method for multi-component phase diagram calculation with acceptable accuracy for practical applications. In recent years, CALPHAD method has expanded beyond its original scope of phase diagram calculation. Firstly, by coupling with kinetic models, it has been employed to simulate diffusion-controlled physical metallurgy phenomena, including solidification, homogenization, diffusion, and precipitation. Secondly, integration with methods like the phase field method (PFM) enables the simulation of phase transformation and microstructural evolution in complex multi-component alloys. Thirdly, by interfacing with finite element method (FEM) software, it facilitates the simulation of microstructure evolution of complicated alloys during conventional manufacturing processes, such as forging and rolling.

Undoubtedly, CALPHAD has been instrumental in accelerating materials design and development. In this presentation, we will explore various applications across a range of alloy systems, including aluminum alloys, nickel-based superalloys, titanium alloys, high-entropy alloys and more.