Hillert Materials Modeling Colloquium series XII

Professor John Ågren

Evolution of thermodynamic modeling in Sweden and KTH - its industrial impact

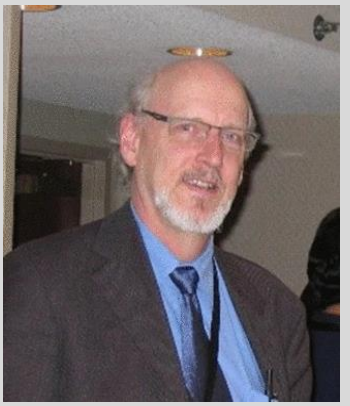
Phase diagrams and thermodynamics have been used to analyze metallurgical and materials phenomena for more than a century but not much of practical calculations were performed before computers became more widely available in the 1960's. At that time Mats Hillert at KTH was probably first in Sweden and among the first worldwide to use computers for thermodynamic calculations. Together with Larry Kaufman in US and others he developed the CALPHAD method during the early 1970's. At the same time one of Mats colleagues at KTH, Lars Gunnar Sillén professor in inorganic chemistry, made calculations on aqueous solutions. One of Sillén's students was Gunnar Eriksson who became professor and later developed the famous softwares SOLGAS and SOLGASMIX.

Later in the 70's, when computers became more common and less expensive, the development became intensive. The Thermo-Calc code was developed by students in Mats' group. Meanwhile other codes were developed worldwide but Thermo-Calc was the most general and flexible one. At that time the interest in ab-initio quantum mechanical calculations was initiated because some data was difficult to determine experimentally. A discussion with physicists was initiated.

It soon became evident that Thermo-Calc could be a very efficient tool in materials industry. The first company to use the code in Sweden was Sandvik and internationally the Japanese Nippon Steel.

The talk will discuss this development and give some practical examples.

Tuesday, 25 April 2023, 3:00 pm, MSE KTH, Zoom
https://kth-se.zoom.us/j/63437879504 (Meeting ID: 634 3787 9504)



John Ågren holds a PhD from the Royal Institute of Technology (KTH) in Stockholm, Sweden, 1981 and afterwards he has been staying at ManLabs Inc. in US and at MPI in Dusseldorf. He was appointed full Professor in physical metallurgy at KTH 1991. He has launched and been the director of several excellence centres at KTH and is one of the developers of the softwares Thermo-Calc and DICTRA. He is one of the founding fathers of the company Thermo-Calc software AB and is the chairman of the directory board since 2001.

Ågren is a member of the Royal Swedish Academy of Engineering Sciences, NAE (US National Academy of Engineering) and a Fellow of ASM. He has received numerous awards, e.g. the Hume-Rothery award from TMS, the ASM Gold medal and the Gibbs Award.

Ågren has published more than 200 journal articles within the areas of phase transformations, diffusion and thermodynamics with an emphasis towards modelling and simulations. Ågren's expertise covers a wide range of materials such as steels, super alloys, cemented carbides as well as topics like powder-metallurgical processing and heat treatment of steels.

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