

## The 2017 NIMS Award goes to Dr. John Ågren, Dr. Bo Sundman, and Dr. Kiyohito Ishida

9 August 2017

National Institute for Materials Science (NIMS)

### Overview

National Institute for Materials Science (NIMS) (President: Kazuhito Hashimoto) has selected the following three winners for the NIMS Award this year.



**Dr. John Ågren**  
(Royal Institute of Technology,  
Sweden)



**Dr. Bo Sundman**  
(Royal Institute of Technology,  
Sweden)



**Dr. Kiyohito Ishida**  
(Tohoku University)

The three awardees have advanced the field of computational thermodynamics and developed thermodynamic calculation software, both of which are fundamental in structural material design. These developments, as well as the results of their studies on alloy design and practical applications, play the role of a chart and compass to advance technologies for materials development and study materials behavior under various usage environments. They are the fundamental and universal tools in use by materials researchers worldwide. In particular, in the field of structural materials, these tools have contributed to the development of a multitude of exceptional steel materials, heat-resistant alloys, and light alloys. These tools are widely regarded as great achievements in the field of “structural materials,” which is the theme of the NIMS Award 2017. The award ceremony and award winning lectures will be held on the first day of “NIMS WEEK 2017,” which is scheduled over three days, from Wednesday, October 4th to Friday, October 6th, at the International Congress Center in Tsukuba, Japan.

### 【NIMS Award】

Since 2007, the “NIMS Award,” an international award, has been given to researchers with outstanding achievements in the development of scientific technologies for application in various substances and materials.

As for NIMS Award 2017, top scientists were nominated from various countries worldwide, in line with this year’s theme, “structural materials.” A committee of unbiased scholarly experts carried out a rigorous, final selection process.

### 【NIMS WEEK】

NIMS Week is an “academic symposium and business forum” that is held annually, hosted by NIMS. It is a week in which one can experience “MEGA Evolution of Materials” events include lectures by the recipients of the NIMS Awards, who are world-class materials researchers, exhibitions of state-of-the-art materials that will soon be in practical use, and private consultations where one can interact personally with researchers.

In 2016, more than 1,500 people belonging to various domestic and foreign enterprises and public research institutes attended the event. Over the years, this event has sparked a number of collaborations and practical applications. In 2017, the largest ever “open house for enterprises” will be held, and 76 research laboratories will be open for public.

**NIMS WEEK 2017**  
**Winners of NIMS Award 2017**

Awardee 1: **Dr. John Ågren** (Royal Institute of Technology, Sweden, Professor)

Awardee 2: **Dr. Bo Sundman** (Royal Institute of Technology, Sweden, Professor Emeritus)

Awardee 3: **Dr. Kiyohito Ishida** (Tohoku University, Professor Emeritus)

**Awardee 1**

Dr. John Ågren (Royal Institute of Technology, Sweden, Professor)

**【Research field】** Computational thermodynamics

**【Title of research result】** Development of kinetic simulation packages for computational thermodynamics

**【Summary of research result】**

Dr. John Ågren was a key member in the development of the software “DICTRA,” a pioneering kinetic computational software based on thermodynamics. This software has enabled kinetic simulations that are indispensable to the prediction of microstructure formation in practical materials, such as simulations of complicated precipitation behavior, grain growth, and diffusion controlled phase transformations in multicomponent systems. The software and databases by Sundman is for static computations, such as stable/metastable phase equilibrium calculations; however, the DICTRA has greatly contributed to the expansion of the practical applicable range of computational thermodynamics from the field of statics into that of dynamics. The software DICTRA, developed by Ågren, requires the Gibbs energy function as one of fundamental parameters. This is evaluated based on statistical thermodynamics and is provided through Thermo-Calc and thermodynamic databases, which was developed by Sundman. At present, these two programs are essential for microstructure simulations and theoretical foundations for property prediction in structural materials. Currently, both pieces of software are used in many universities and enterprises, and it has been shown that they are highly useful as the main tools in ICME for the development of new materials.

**Awardee 2**

Dr. Bo Sundman (Royal Institute of Technology, Sweden, Professor Emeritus)

**【Research field】** Computational thermodynamics

**【Title of research result】** Development of thermodynamic calculation packages for computational thermodynamics

**【Summary of research result】**

Dr. Bo Sundman was a key member in the development of software “Thermo-Calc,” a pioneering thermodynamic calculation software. Thermo-Calc has enabled computations of complex phase equilibria and thermodynamic quantities in multicomponent systems. As a result, the analysis of phase equilibria in practical alloy systems has improved tremendously. In addition, the development of thermodynamic databases for multicomponent systems has enabled estimations of phase equilibria even in metastable systems based on the thermodynamic quantities obtained from stable systems. Studies that use this software have immensely contributed toward enhancing the utility of the method of computational thermodynamics in alloy development. The software and databases developed by the awardee and others are the basic data and parameters required for dynamic simulations of diffusions and reactions on the software “DICTRA,” which was developed by Ågren. At present, these two programs are essential in both roles (statics and dynamics), namely as microstructure simulations for structural materials and theoretical foundations for property prediction. Currently, both software packages are used in many universities and various companies, and it has been shown that they are highly useful as the core tools in ICME (Integrated Computational Materials Engineering) for the development of new materials.

**【Influence of achievements by Dr. Ågren and Dr. Sundman on academic and industrial worlds】**

Results from both research laboratories were incorporated in the commercial computational codes of Thermo-Calc/DICTRA, and their usage in industry is promoted. The number of license holders in Japan is several hundred in universities and enterprises, and that for DICTRA is several dozen in various fields. In particular, in the field of structural materials, those codes are making significant contributions to the prediction of precipitation behavior and equilibrium phases for Fe-based alloys and Ni-based alloys. For example, they were used in SIP-MI (Strategic Innovation promotion Program-Materials Integration) projects, and they have been playing important roles in integration systems being developed. It is expected that their importance and practical applicability will further increase in the future.

**Awardee 3**

Dr. Kiyohito Ishida (Tohoku University, Professor Emeritus)

**【Research field】** Structural materials

**【Title of research result】** Alloy design and development of structural materials based on thermodynamics of phase diagrams and microstructure

**【Summary of research result】**

Dr. Kiyohito Ishida conducted basic, applied research on alloy design and the structure control of materials, based on phase diagrams and microstructure of alloys. He has contributed to society by leading this field internationally, developing a number of new materials, and putting them into practical use. He experimentally determined the phase diagrams of a number of practically important alloy systems such as steel materials, micro solders, copper alloys, cobalt alloys, nickel alloys, and more. He also conducted the thermodynamic analysis for each multicomponent alloy, and developed thermodynamic databases of alloy phase diagrams, which are widely useful for material development. In addition, he performed basic research on material structures, such as grain growth, precipitations, magnetic transformations, and martensitic transformations. He has presented much of his research results in famous international journals, such as *Nature* and *Science*. Furthermore, making full use of the simulations and the databases of alloy phase diagrams that were developed based on his basic research results, he has successfully developed several new alloys, such as unleaded free-cutting steel, Co-based super heat-resistant alloys, Cu-Ni-Al-based high-strength and high-conductivity alloys, Cu-Al-Mn-based shape memory alloys, and more, and has put them into practical use.

**【Influence of achievements by Dr. Kiyohito Ishida on academic and industrial worlds】**

As a pioneer of alloy design and new material development utilizing multicomponent computational phase diagrams, he has highlighted the importance of the CALPHAD method and simulation methods, both within and outside of Japan. He also largely contributes to university-industry cooperation. For example, he started the 172nd Committee on Alloy Phase Diagrams as a University-Industry Cooperative Research Committee in the Japan Society for the Promotion of Science, and he encouraged, ahead of the world, Japanese enterprises to introduce these methods, which contributed to the realization of high-level technology and high-level competitiveness. He also led a research project titled, “Development of the Integrated Design System for Materials Microstructure and Properties” as the research director from 2003 to 2009 in CREST, which is a Strategic Basic Research Program in the Japan Science and Technology Agency. This was a pioneering study on “Materials Integration,” which is currently acquiring significant attention due to the Materials Genome Initiative (MGI). In that research project, he has recently discovered Co-based heat-resistant alloys. This research, as evidenced by many workshops on new heat-resistant alloys held in the US and European countries, has triggered a lot of subsequent research activities and development in overseas countries other than Japan. He has successively held prestigious positions, such as the President of the Japan Institute of Metals and Materials and Vice chairman of Alloy Phase Diagram International Commission (APDIC). He has largely contributed to the research and development of structural materials, development of human resources, and international cooperation, both domestically and internationally.

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