Prof. P. Rama Rao

Prof. P. Rama Rao is a distinguished Indian metallurgist, materials scientist, and science administrator known for his extensive contributions to research, national institutions, and science policy. He made significant contributions to physical metallurgy, high-strength steels, and materials research in India.

He served as a Professor at BHU, Director of the Defence Metallurgical Research Laboratory (DMRL), Secretary of the Department of Science and Technology (DST), Chairman of the Atomic Energy Regulatory Board (AERB), and Vice-Chancellor of the University of Hyderabad. He also played a key role in shaping India's science and technology policy.

He is a recipient of the Padma Shri, Padma Bhushan, Padma Vibhushan, and the Shanti Swarup Bhatnagar Prize for his outstanding contributions to science and engineering.

IIM Metallurgy Materials Engineering

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भारतीय प्रौद्योगिकी संस्थान हैदराबाद
Indian Institute of Technology Hyderabad

Department of Materials Science and Metallurgical Engineering, IIT Hyderabad
and
Indian Institute of Metals Hyderabad Chapter
in association with Student Affiliated Chapters of Hyderabad

Cordially invite you to the Celebration of

IIM 80th Foundation Day
&
IIM National Metallurgists' Day

FIRST LECTURE OF THE

Prof. P. Rama Rao Distinguished Lecture Series

By

Prof. Shrikant Lele

Distinguished Professor, IIT BHU, Varanasi

On

Computational Thermodynamics of Alloys

Feb 24, 2026 | 11 AM | LH3, MSME, IITH

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We look forward to your gracious presence to celebrate this event.

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Indian Institute of Technology Hyderabad

ABSTRACT OF THE TALK:

One of the principal aims of metallurgical engineering is to develop alloys with improved properties and/or enhanced functionalities. These properties or functionalities depend primarily on the atomic structure of the phases present and their distribution in the microstructure of the alloy at chosen conditions of temperature and pressure. Our focus is on understanding the stability of various phases as a function of composition and temperature. Gibbs showed that the phase or combination of phases with the least Gibbs energy among all competing phases is the stable state of the alloy. The Gibbs energy can be determined experimentally through thermodynamic measurements or theoretically using Density Functional Theory calculations for a particular combination of composition and temperature.

For predictions of phase stability, it is convenient to have an analytical expression for the Gibbs energy which is a continuous function of composition and temperature. The Gibbs energy of mixing depends primarily on configurational contributions and secondarily on changes in vibrational states and volume. Ordered structures need more complex treatment. Observation of the regularity of the enthalpies of mixing of disordered solutions led to the regular solution model. More complex behaviour required extension to various polynomials such as the Redlich-Kister or Legendre polynomials for binary alloys and their generalization for ternary and quaternary alloys. The coefficients which appear in these expressions serve as model parameters devoid of any physical basis. They must be determined by fitting to experimental or first-principles data. The practical advantage of such expressions is that expressions for quinary and higher order systems are simple additive combinations of those for their lower order subsystems. This procedure which has come to be called the Calphad method has shown great utility in the design of newer alloys with as many as a dozen or more components. A deficiency in this approach is the fact that the model parameters for a particular alloy system are not universal, for example, the parameters for a binary system applicable to say Aluminium and Titanium base multicomponent alloys can be significantly different.

Physically based models such as Guggenheim's quasi-chemical model and Kikuchi's cluster variation method (CVM) for the configurational entropy account for short range order in alloys. A complementary model for the configurational enthalpy of mixing is provided by the cluster expansion (CE) method. The cluster expansion is a bilinear sum of the products of configurational variables (called correlation functions) and their coefficients (Cluster Expansion Coefficients) which serve as model parameters. The choice of correlation functions and the resulting cluster expansion are not unique and thus the model parameters are also not unique. Thus, they are not suited for storing directly in a database. However, they are physically equivalent and one set of parameters can be transformed to another. These CECs are expected to be universally applicable for a system independent of the multicomponent supersystem of which it is a part.

Widespread use of CE-CVM requires a standardized expansion so that the CECs can be used without transformations. We present a cluster expansion in terms of a chosen set of independent cluster variables (CVs). The CVs represent the fractions of corresponding cluster configurations in the alloy. The choice of CVs ensures that the CECs are inherited from a subsystem in a supersystem without any transformation. Such a set of CECs is suitable for incorporation in a universal database. A CE-CVM model for a better representation of the Gibbs energy of ordered structures is briefly discussed.

Prof. Shrikant Lele

ABOUT SPEAKER:

Professor Shrikant Lele, Formerly Rector and Professor of Metallurgy, Banaras Hindu University, Varanasi has contributed to the advancement of the structure and thermodynamics of materials. His early work on diffraction effects of stacking faults in close-packed structures is internationally well known. He has done, for the first time, an analysis of dislocation reactions and the energetics of various types of stacking faults in the four-layer double hexagonal close-packed (dhcp) structure. Another major contribution by him is the unique application for diffraction methods to the study of solid-state transformations among the small-period polytypes of SiC. He has formulated six dimensional models for the structures of decagonal quasicrystals which predicted the layer spacing in such structures which was independently confirmed by experiments. He has studied electron diffraction patterns from quasicrystals for determining the nature of defects from the diffuse spots in such patterns.

Prof. Lele's contributions towards the thermodynamics of liquids using the RAS (Regular Associated Solution) and its implications for the formation of metastable structures after solidification are significant. His recent work on determining thermodynamic properties of multicomponent alloys using the cluster variation method (which accounts for short range order) is unique both in scope and content. Prediction of the stability of different phases in such alloys, which is important for development of newer alloys, is thus made possible.

Prof. Lele is a Fellow of the Indian National Science Academy, Indian Academy of Sciences, National Academy of Sciences (India), National Academy of Engineering, Hon Member of the Indian Institute of Metals and Life Member of the Electron Microscope Society of India. He is a recipient of National Metallurgist's Day Award (1984) and SS Bhatnagar Prize (1987).