INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

Special Seminar

Prof. Dr. G. Cacciamani

Dipartimento di Chimica e Chimica Industriale
Università di Genova, Italy

Wednesday, November 14, 2:00 p.m.
ICAMS seminar room 0.08

Thermodynamic modelling of intermetallic systems with structural ordering: Co-Ni-Ti as an example

Structural ordering, possibly combined with magnetic ordering, is a well known phenomenon often occurring in alloy systems relevant to key technological materials such as superalloys, magnetic alloys, alloyed aluminides, etc.

The Compound Energy Formalism (CEF), usually applied in the Calphad method, is especially suitable for the development of thermodynamic models based on the crystal structure of the modelled phases. In particular, groups of ordered phases deriving from the same disordered structure may be described by a single multi-sublattice model, the different ordered structures resulting from the sublattice occupations. In this way, among other advantages, either first and second order phase transitions as well as site occupancies and order parameters may be calculated as a function of the state variables.

The CEF modelling of a number of ordered phases (especially those based on the fcc and bcc lattices) will be discussed, with emphasis on the role of the coordination number and geometry. The application to the modelling and assessment of the Co-Ni-Ti system will be presented as an example.