8th. World Congress on Computational Mechanics (WCCM8)
5th. European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008)
June 30 – July 5, 2008
Venice, Italy

MULTISCALE METHODS IN COMPUTER MATERIALS SCIENCE

MACIEJ PIETRZYK[1], PETER D. HODGSON[2] AND TADEUSZ BURCZYNSKI[3]

[1]Akademia Gorniczo-Hutnicza
Mickiewicza 30, 30-059 Krakow, Poland
pietrzyk@metal.agh.edu.pl www.miti.agh.edu.pl

[2]Deakin University
Geelong, Victoria 3217, Australia
phodgson@deakin.edu.au www.deakin.edu.au/cmfi

[3]Silesian University of Technology
Konarskiego 18a, 44-100 Gliwice, Poland
Tadeusz.Burczynski@polsl.pl www.kwmimkm.polsl.pl

Key words: Multi Scale Modelling, Computer Materials Science, Digital Materials, Finite Element Method, Cellular Automata, Molecular Dynamics, Modelling Industrial Problems.

ABSTRACT

Numerical modelling of materials during processing, manufacturing and exploitation is common in industry and research. The Finite Element Method (FEM) is widely used to simulate a particular deformation, thermomechanical or heat treatment process. Applications of the FEM vary from modelling of simple tests to the complex behaviour of entire structures (e.g. aeroplanes, buildings, implants). FEM has recently been combined with discrete methods, such as Monte Carlo (MC), Cellular Automata (CA), Molecular Dynamics (MD), etc to handle events that occur at the micro and nano scales. Through this FEM can now replicate real phenomena that occur in materials on different length and time scales. This enables complex analysis of material behaviour, including modelling of discontinuities and stochastic processes.
Contributions in the following areas are invited:
- Conventional multi scale approaches based on the FE (XFEM, GFEM).
- Theoretical basis of various applications of multi-scale techniques, e.g. Monte Carlo (MC), Cellular Automata (CA), Molecular Dynamics (MD). Alternative multi scale methods: e.g. combination of CA-FE methods, Neuro-Fuzzy Cellular Automata – Finite Element technique (nF-CAFE) or Neuro Expert Cellular Automata–Finite Element models (NESCAFE).
- Applications of multi scale modelling to industrial problems such as ingot melting, casting, welding, laser treatment, fusion welding, forging, friction stir welding, drawing, flow/spin forming, flat and shape rolling, ring rolling, stretch forming, deep drawing, semi-solid metal-working, highly filled material processing, injection moulding, blow or compression moulding, vapour deposition, molecular beam epitaxy, joining etc.
- Solving microstructural problems, crack propagation, strain localization, microstructure evolution, solidification, phase transformation, influence of the strain path etc.
- Application of the mutli scale modelling to functionally graded materials, nano layers, sandwich materials etc.
- Multi scale approaches based on the mesh free methods, particle-in-cell and other particle methods and development of new multi scale approaches.