Computational Approach to Materials Science and Engineering - Web course

COURSE OUTLINE

To take a computational approach to concepts in materials science and engineering

COURSE DETAIL

Part I -- Preliminaries	
Module 1: Introduction	(I hour)
Part II -- Tools of the trade: a short tutorial introduction	
Module 1: The C programming language	(3 hours)
Module 2: gnuplot – the plotting freeware	(2 hours)
Module 3: GNU Octave for computations and plotting	(3 hours)
Module 4: Scilab: the scientific computation package	(2 hours)
Module 5: Some miscallaneous freeware	(4 hours)
Part III -- Dealing with data	
Module 1: Plotting	(2 hours)
Module 2: Fitting	(3 hours)
Module 3: Interpolation	(3 hours)
Module 4: Numerical integration	(3 hours)
Module 5: Numerical differentiation	(3 hours)
Part IV – Structure, Thermodynamics and Phase Transformations	

NPTEL

http://nptel.iitm.ac.in

Metallurgy and Material Science

Pre-requisites:

Exposure to Introductory engineering mathematics, introductory materials science and introductory programming courses is preferred.

Additional Reading:

- Given in each chapter

Hyperlinks:

- http://www.gnu.org/software/octave/
- http://gcc.gnu.org/codingconventions.html

Coordinators:

Dr. M.P. Gururajan
Department of Metallurgical Engineering and Materials ScienceIIT Bombay

Dr. Prita Pant
Department of Metallurgical Engineering and Materials ScienceIIT Bombay

Module 1: Structure and defects	(3 hours)
Module 2: Regular solution model	(2 hours)
Module 3: Diffusion and precipitate growth kinetics	(4 hours)
Module 4: Spinodal decomposition	(4 hours)
Module 5: Ordering	(2 hours)
Module 6: Molecular dynamics simulations	(optional – 5 hours)
Module 7: Monte Carlo simulations: phase separation and ordering	(optional – 5 hours)
Module 8: Solidification	(optional – 5 hours)

References:

- Materials Science and Engineering, V Raghavan, Prentice-Hall India, 2004
- Advanced Engineering Mathematics, E Kreyzig, Wiley-India,1999