# Carnegie Mellon
## Materials Science and Engineering Seminar Series

# G. Malcolm Stocks

Oak Ridge National Laboratory
Group Leader, Materials Theory Group

*"Fundamental Studies of Defects in Structural Materials: Dislocations and Displacement Cascades"*

**Friday, Feburary 18, 2011**
**10:30 AM Seminar in Scaife Hall 125**

The extent to which the collective effects of defects can be manipulated and controlled yields the combination of materials properties – strength, toughness, resistance to degradation in extreme chemical and radiation environments – needed in advanced structural materials for energy applications. In the fist part of this presentation, I shall outline progress towards experimental characterization of dislocations and radiation induced displacement cascades that are of sufficiently high spatial and temporal resolution that we will be able to probe the structure and interactions of defects at the level of unit events. In the second part, I will discuss recent advances in the theory and modeling of magnetism that are allowing us to treat the evolution of the spin degrees of freedom (spin dynamics) on the same *ab initio* footing as the ionic degrees of freedom are dealt with in modern *ab initio* molecular dynamics studies. I will show results for the finite temperature magnetic state of Fe as well as calculations that address the importance of the disruption of the magnetic state of Fe caused by the introduction of defects such as dislocations and displacement cascades that are based on large scale (~10,000 atom) models and the use of order-N electronic structure methods that can take advantage of the modern petaflop class computers.

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**Dr. G. Malcolm Stocks** is an ORNL Corporate Fellow and Group Leader of the Materials Theory Group (MTG) in the Materials Science and Technology Division (MSTD) at the Oak Ridge National Laboratory. In addition he is the Director of the *"Energy Frontier Research Center for Defect Physics in Structural Materials"* (*"Center for Defect Physics"* (CDP for short). The CDP is one of 46 Department of Energy *"Energy Frontier Research Centers"* (EFRC) that aim to address basic science challenges for future energy technologies. Dr. Stocks' major research activities include first principles electronic structure theory, theory of magnetism, alloy theory, strongly correlated electron physics, and the application of parallel algorithms and computers. He has contributed to the development of a number of first principles electronic structure, most specifically the Korringa-Kohn-Rostoker Coherent-Potential-Approximation (KKR-CPA) approach for calculating the electronic and ground state properties of random substitutional alloys as well as the linear scaling (order-N) Locally Self-consistent Multiple Scattering (LSMS) method for performing electronic structure calculations on systems comprising many thousands of atoms. Dr. Stocks is a fellow of the American Physical Society, has published more than 230 papers, is co-editor of five research volumes, and has won numerous honors and awards. Most notably he has twice received the Gordon Bell Prize for his contributions to the use of massively parallel computing in science.