

MAR11-2010-008749

Abstract for an Invited Paper
for the MAR11 Meeting of
the American Physical Society

Kinetic Monte Carlo with fields: diffusion in heterogeneous systems

JOSE ALFREDO CARO, Los Alamos National Laboratory

It is commonly perceived that to achieve breakthrough scientific discoveries in the 21st century an integration of world leading experimental capabilities with theory, computational modeling and high performance computer simulations is necessary. Lying between the atomic and the macro scales, the meso scale is crucial for advancing materials research. Deterministic methods result computationally too heavy to cover length and time scales relevant for this scale. Therefore, stochastic approaches are one of the options of choice. In this talk I will describe recent progress in efficient parallelization schemes for Metropolis and kinetic Monte Carlo [1-2], and the combination of these ideas into a new hybrid Molecular Dynamics-kinetic Monte Carlo algorithm developed to study the basic mechanisms taking place in diffusion in concentrated alloys under the action of chemical and stress fields, incorporating in this way the actual driving force emerging from chemical potential gradients. Applications are shown on precipitation and segregation in nanostructured materials. Work in collaboration with E. Martinez, LANL, and with B. Sadigh, P. Erhart and A. Stukowsky, LLNL. Supported by the Center for Materials at Irradiation and Mechanical Extremes, an Energy Frontier Research Center funded by the U.S. Department of Energy (Award # 2008LANL1026) at Los Alamos National Laboratory

[1] B. Sadigh et al. to be published

[2] E. Martinez et al. J. Comp. Phys. 227 (2008) 3804-3823