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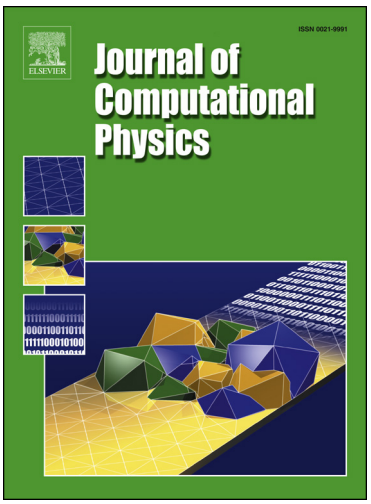

Cluster dynamics modelling of materials: A new hybrid deterministic/stochastic coupling approach

Pierre Terrier, Manuel Athènes, Thomas Jourdan, Gilles Adjanor, Gabriel Stoltz

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Cluster dynamics modelling of materials: a new hybrid deterministic/stochastic coupling approach.

Pierre Terrier[a,b], Manuel Athènes[b], Thomas Jourdan[b,*], Gilles Adjanor[c], Gabriel Stoltz[a]

[a] *Université Paris-Est, CERMICS (ENPC), INRIA, F-77455 Marne-la-Vallée, France*
[b] *DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, F-91191 Gif-sur-Yvette, France*
[c] *EDF R&D, Département Matériaux et Mécanique des Composants, Les Renardières, F-77250 Moret sur Loing, France*

Abstract

Deterministic simulations of the rate equations governing cluster dynamics in materials are limited by the number of equations to integrate. Stochastic simulations are limited by the high frequency of certain events. We propose a coupling method combining deterministic and stochastic approaches. It allows handling different time scale phenomena for cluster dynamics. This method, based on a splitting of the dynamics, is generic and we highlight two different hybrid deterministic/stochastic methods. These coupling schemes are highly parallelizable and specifically designed to treat large size cluster problems. The proof of concept is made on a simple model of vacancy clustering under thermal ageing.

Keywords: Cluster dynamics, Fokker-Planck equation, Langevin dynamics, Markov process, stochastic simulations

1. Introduction

The microstructural evolution of materials under thermal ageing or irradiation involves complex processes, such as nucleation, growth and coarsening of precipitates or bubbles, that occur on different time scales. The computer simulation of such processes triggered the development of efficient methods able to deal with very different time scales [1–17].

*Corresponding author. Tel.: +33 169087344
Email address: thomas.jourdan@cea.fr (Thomas Jourdan)