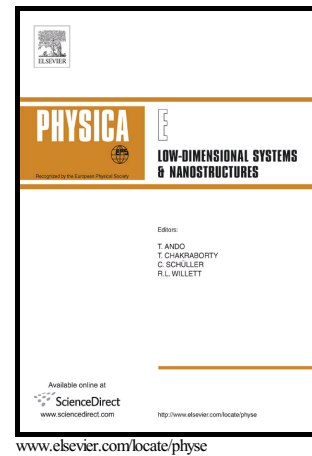


Author's Accepted Manuscript

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PII: S1386-9477(17)31119-0
DOI: <http://dx.doi.org/10.1016/j.physe.2017.09.005>
Reference: PHYSE12905

To appear in: *Physica E: Low-dimensional Systems and Nanostructures*

Received date: 26 July 2017
Accepted date: 5 September 2017

Cite this article as: Alexander Tarasenko, Analytical approach for collective diffusion: One-dimensional lattice with the nearest neighbor and the next nearest neighbor lateral interactions, *Physica E: Low-dimensional Systems and Nanostructures*, <http://dx.doi.org/10.1016/j.physe.2017.09.005>

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Analytical approach for collective diffusion: One-dimensional lattice with the nearest neighbor and the next nearest neighbor lateral interactions

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Abstract

Diffusion of particles adsorbed on a homogeneous one-dimensional lattice is investigated using a theoretical approach and MC simulations. The analytical dependencies calculated in the framework of approach are tested using the numerical data. The perfect coincidence of the data obtained by these different methods demonstrates that the correctness of the approach based on the theory of the non-equilibrium statistical operator.

Keywords: Lattice gas systems; Kinetic Monte Carlo simulations; Diffusion and migration

1 Introduction

The theoretical investigations of the diffusive mass transfer processes attract much attention. They control a multitude of the physico-chemical phenomena. But the complexity of the real systems makes their study quite difficult. Therefore, it is not surprising that a wide variety of models have been developed for this purpose. In the lattice gas (LG) models the stochastic movement of the particles (atoms, ions, molecules) in a continuous space is replaced by the particle jumps over the sites of a lattice with definite dimension and symmetry. The problem is considerably simplified and for some cases the investigation of the migration is reduced to the solution of the ordinary diffusion equation. Also the calculations of the diffusion coefficients can be carried out to the final point and the

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