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The Open-Access Journal for the Basic Principles of Diffusion Theory, Experiment and Application

Surface Diffusion of Particles over the Bivariate Trap Lattices

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Abstract

We investigate the diffusion of particles on heterogeneous lattices with two kinds of non-equivalent sites. General analytical expressions for the chemical and jump diffusion coefficients have been derived in the case of strong inhomogeneity. We have calculated coverage dependencies of the diffusion coefficients and other necessary thermodynamic quantities for some representative values of the lateral pairwise interaction between the particles. The analytical data have been compared with the numerical data obtained by the kinetic Monte Carlo simulations. Almost perfect agreement between the respective results has been found.

Keywords: Lattice gas, Diffusion, kinetic Monte Carlo simulations.

1. Introduction

We have investigated migration of particles over a number of inhomogeneous lattices. There are the 1-D chain with alternating deep and shallow sites, 2-D honeycomb, square, triangular and dice lattices and 3-D simple cubic lattice. Such systems display specific peculiarities which qualitatively affect the diffusion as compared to the similar homogeneous lattices. The lattice inhomogeneity causes specific correlation between the slow and fast particle jumps. It is shown that the character of the particle migration depends crucially on the jump frequencies of particles occupying the deep and shallow sites. If these frequencies differ considerably, the particles perform pairs of strongly correlated jumps.

2. Model and Hamiltonian

In the following we consider an ideal regular lattice with coordination number z. There are deep, **d**, and shallow, **s** sites, arranged in alternating order. Let us consider the particle migration on an inhomogeneous lattice in detail. All particles tend to occupy **d** sites resulting in either the empty **s** sites and partially filled **d** sites, or the completely filled **d** sites and partially **s** sites. The inhomogeneity imposes rather specific correlation between the particle jumps. Any migration event starts by a slow jump which transfers a particle to a shallow site and creates an unstable local non-equilibrium configuration with the occupied **s** site and empty **d** site. There are two fast decay ways for this configuration. Either the particle jumps to any of the nearest neighbor (NN) empty **d** sites or the **d** site is filled by a particle from any filled NN **s** sites. As creation and decay of the intermediate non-equilibrium configuration take place on largely different time scales, their combination ought to be considered as the central entity of the diffusion process. The particle jumps collect into pairs: any slow jump is followed immediately by a fast jump. Such jump pairs are the most frequent events and they govern the particle migration.

Despite of the fact that the individual jumps are statistically uncorrelated, the lattice inhomogeneity imposes a strong pair-wise correlation between slow and fast jumps. We obtain the analytical expressions for the chemical diffusion coefficients for the inhomogeneous lattices mentioned above and checked them by kinetic MC simulations. The perfect agreement between the respective results has been found in the whole coverage region and wide temperature region for the repulsive and attractive lateral interaction between the particles.

3. Conclusions

We have shown that the model of jump pairs works rather well in the inhomogeneous lattices. It forms a sound basis for the quantitatively correct description of the particle diffusion in such systems. It should be noted that the expressions for the diffusion coefficients are obtained without any fitting parameters.

It should be noted that this approach is quite general. We do not use any specific features of the inhomogeneous systems like dimensionality, symmetry, and interaction potential. The inclusion of the fast jumps into the slow jumps substantially reduces the complex dynamics of the particle system. The significant simplification of the particle migration on the basis of this model permits to develop the simple analytical expressions for the chemical diffusion coefficient which are valid for different inhomogeneous lattices.

The proposed model of jump pairs gives reasonable and natural explanation of the peculiar characteristics of the diffusion in the inhomogeneous lattices mentioned above. The proposed model of jump pairs gives reasonable and natural explanation of the peculiar characteristics of the diffusion in the inhomogeneous lattices mentioned above. The analytical expressions are quite simple. The calculations of the diffusion coefficients is reduced to the calculations of some thermodynamic quantities, which is simpler by many orders of magnitude, as compared to the numeric MC simulations.

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