Monte Carlo study of transport phenomena in surface binary alloys

A. De Virgiliis and K. Binder

Institut für Physik, Johannes Gutenberg Universität, Staudingerweg 7,
55099 Mainz (Germany). Email: devirgia@uni-mainz.de

1. Introduction

In this work the transport properties of lattice-gas models of two species of particles with repulsive interactions and different transitions rates are studied. The Onsager coefficients and the interdiffusion are directly estimated from numerical simulations of the mobilities.

2. The ABV model

We consider a square $L \times L$ lattice with periodic boundary conditions and each site can be taken by an A-atom, an B-atom, or stay vacant. For a fixed, small vacancy concentration $c_v=0.04$ this model shows an order-disorder transition at a temperature $T=0.91$ (in units of T_c (Ising))

3. Simulation of tracer diffusion, Onsager coefficients and interdiffusion

In order to study diffusion properties, we introduce different jump rates $_A$ and $_B$ of the particles to empty sites. The self-diffusion coefficients are obtained from mean-square displacements of tagged particles. For the calculation of the Onsager coefficients we impose chemical potential gradients either on the A or on the B atoms to create steady-state currents in the system. Thus these coefficients are directly estimated from the mean displacements along the direction of the applied gradient. The interdiffusion constant D_{int}, which describes how a weak deviation of the concentration difference between A and B from its average value spreads out, is obtained by applying a wavevector-dependent chemical potential difference to the system, to prepare an initial state where a concentration wave is present. At time $t=0$, this perturbation is switched off, and then one simply watches the decay of the concentration wave in time.

4. Conclusion

We observed a strong influence of the ordering on most of the transport properties of the model. The interdiffusion cannot be explained neither by the slow-mode [3] nor by the fast-mode theories[4]. The estimated Onsager coefficients are well reproduced by an aproximation making use of the tracer diffusion coefficients [2].
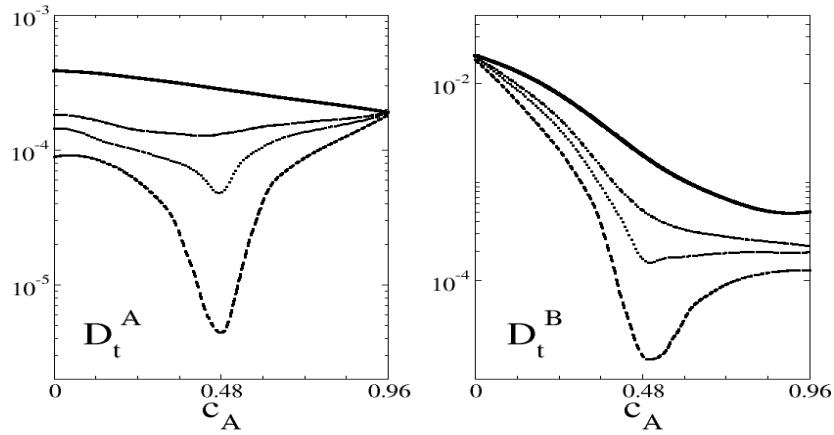
Fig. 1. Tracer diffusion coefficients, as a function of the concentration c_A. The temperatures are: *T=0.6* (dashed), *T=Tc =0.91* (doted) and *T=1.2* (dot-dashed) [1]. The top thick line indicates the noninteracting, infinite temperature limit (random alloy).
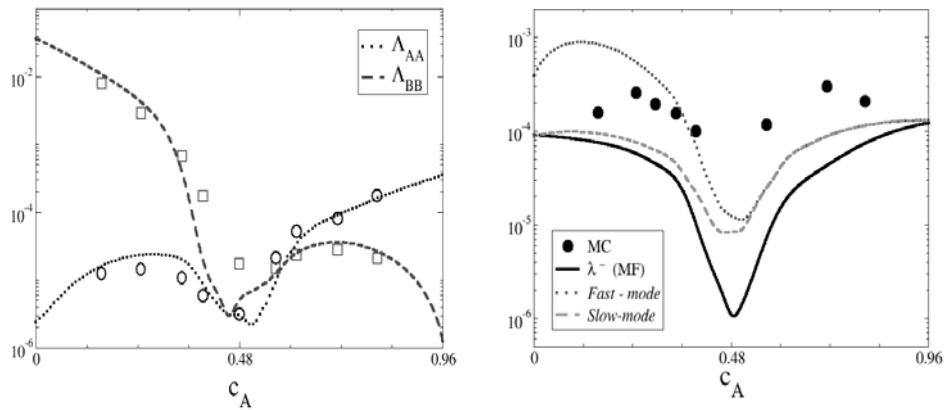

Fig. 2. Left: Onsager coefficients at T=0.6. The lines are results from the simulations and the points corresponds to estimations of an aproximate theorie [2]. Right: interdiffusion coefficient. The points are results from the simulations[1] and the lines corresponds to different aproximated theories [3,4].

References

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