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LETTER TO THE EDITOR

Finite-size scaling study of non-equilibrium percolation

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Abstract. Induced by phase separation in the lattice gas model a transient percolation phenomenon occurs for concentrations c exceeding a critical curve $c_p^{(corr)}(T, t)$, which depends both on temperature T and on the time t passed after the quench to a state inside the miscibility gap. A finite-size scaling analysis of extensive Monte Carlo data is carried out to locate $c_p^{(corr)}(T, t)$ and to show that the critical behaviour of this percolation transition is consistent with random percolation, contrary to previous suggestions.

When a binary mixture is quenched from an initial state that is macroscopically homogeneous to a final state inside the miscibility gap, the resulting inhomogeneous patterns which form due to the onset of phase separation (Gunton *et al* 1983) may either have the character of isolated 'droplets' well separated from each other, or of an interconnected 'percolating' network of the minority atomic species on the background of the majority 'phase'. The transition between these two types of topologies is not identical to random percolation (Stauffer 1985), however, since the kinetics of cluster formation during phase separation is a transient non-equilibrium phenomenon where long range spatial correlations develop.

This transition has recently been studied for the lattice gas model with nearest-neighbour interaction (Binder 1980, Heermann *et al* 1987, Hayward *et al* 1987). Here a 'cluster' (or 'droplet') is defined geometrically as in random percolation, by requiring that each site belonging to a cluster must be occupied and be a nearest neighbour of at least one other occupied site belonging to this cluster. Considering a 'quenching experiment' at fixed concentration c which starts with an initially random occupation of sites consistent with the chosen concentration (temperature $T \to \infty$ in the lattice gas), the system is initially not percolating for $c < c_p^{(random)}$, the critical concentration for random site percolation ($c_p^{(random)} \approx 0.312$ for the simple cubic lattice). Hayward *et al* (1987) suggested a kind of 'gelation transition': as time proceeds, by random diffusion monomers (or small clusters) hit the large clusters which thereby grow and they eventually coalesce to form an infinite network at a time $t_{crit}(c, T)$. This means, on the other hand, that a system for $c < c_p^{(corr)}(T, t)$ is non-percolating, while for $c > c_p^{(corr)}(T, t)$ it percolates (we here denote the inverse function of the critical time $t_{crit}(c, T)$ in the plane of variables c and t as $c_p^{(corr)}(T, t)$ because this is a correlated percolation problem). However, although Hayward *et al* (1987) could not analyse the time dependence of $c_p^{(corr)}(T, t)$ quantitatively, they speculated that the critical exponents of this non-equilibrium percolation transition differ from those of random percolation; this dynamic percolation problem then would form a new 'universality class'.

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In the present work, we attempt to clarify this problem by extensive Monte Carlo simulations, which are analysed by finite-size scaling methods (Kirkpatrick 1979, Binder 1987). By this method, we are able to show that the curve $c_p^{(corr)}(T, t)$ has a minimum in the (c, t) plane (figure 1). Thus at $T = 0.3\,T_c$ we find a significant regime of c, namely $0.1718 \leqslant c \leqslant 0.312$, where the dynamic percolation transition alluded to above occurs: clusters gel together into a percolating net. However, for $0.171\,89 \leqslant c < c_p^{(corr)}(T, \infty)$ this percolating net exists only as a transient phenomenon (see also Heermann 1984), for a finite range of time $t_{crit}^{(1)}(c, T) < t < t_{crit}^{(2)}(c, T)$. We have not attempted to estimate quantitatively the asymptotic value $c_p^{(corr)}(T, \infty)$, to which $c_p^{(corr)}(T, t)$ tends for $t \to \infty$, since this would require prohibitively large amounts of computer time. Already for $c = 0.18$ $t_{crit}^{(2)}(c, T = 0.3\,T_c)$ is about 360 time units, which means that the effort to study this percolation transition requires much more time than a study of the random percolation problem, where each configuration is generated in a single filling of the lattice, without any evolution in time.

Despite the obviously transient characters of this new kind of percolation transition, we do not confirm the non-standard exponent estimates of Hayward *et al* (1987): rather within reasonable statistical errors, our exponent estimates agree with the random percolation exponents! We interpret this finding by the fact that during 'spinodal decomposition' (Gunton *et al* 1983) only finite-ranged correlations are created.

In the following, we sketch the main points of the analysis that lead to these conclusions (see Lironis 1988 for more details). Following Kirkpatrick (1979) the critical concentration $c_p^{(corr)}(T, t)$ is found from a finite-size analysis of the 'spanning probability' $P_{sp}(L, c, t)$ that a cluster occurs in the system which spans from one boundary of the $L \times L \times L$ system to the opposite boundary (and requiring this spanning property in all these spatial directions). For $L \to \infty$, $P_{sp}(L, c < c_p^{(corr)}(T, t), t) \to 0$, $P_{sp}(L, c > c_p^{(corr)}(T, t), t) = 1$. Therefore the finite-size scaling assumptions (Barber 1983,

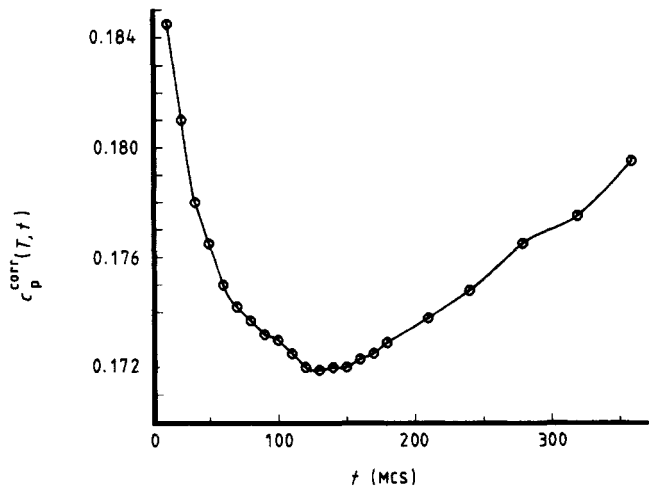

Figure 1. Critical curve $c_p^{(corr)}(T = 0.3\,T_c, t)$ in the concentration (c)-time (t) plane, for the simple cubic nearest-neighbour lattice gas model which evolves in time through random nearest-neighbour exchanges of occupation variables (i.e. the kinetic Ising model of Kawasaki (1972)). Note that $c_p^{(corr)}(T, t = 0) = c_p^{(random)} = 0.312$ is off scale here. The state of the system is percolating above the curve shown and not percolating below. Time is measured in units of Monte Carlo steps (MCS) per lattice site.

Binder 1987) imply for P_{sp}

$$P_{sp}(L, c, t) = \tilde{P}_{sp}(\delta c L^{1/\nu}) \qquad \delta_c \equiv c - c_p^{(corr)}(T, t),\ L \to \infty \tag{1}$$

where $\tilde{P}_{sp}(\mathcal{S})$ is the appropriate scaling function and ν the critical exponent of the connectedness length. Since (1) implies, that for $c = c_p^{(corr)}(T, t)$ all curves $P_{sp}(L, c, t)$ must have a common intersection point $\tilde{P}_{sp}(0)$, the critical concentration can be found without any assumption on critical exponents (figure 2). It is seen that $c_p^{(corr)}(T, t)$ can be estimated with a relative error of less than 10^{-3}, which is nearly an order of magnitude better precision than that of Hayward *et al* (1987).

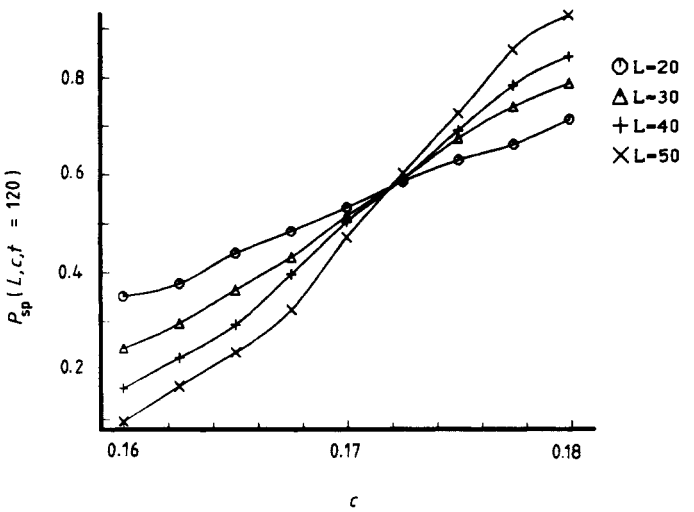

Figure 2. Plot of the spanning probability $P_{sp}(L, c, t = 120)$ against c for four different lattice linear dimensions. The abscissa of the common intersection point yields $c_p^{(corr)}(T = 0.3T_c,\ t = 120) \approx 0.1720$. All times are measured in MCS per site.

Figure 3 tests the scaling property of (1) more fully as well as the standard finite-size scaling relations for the percolation probability $P_\infty(L, c, t)$ and percolation susceptibility $\chi(L, c, t)$,

$$P_\infty(L, c, t) = L^{-\beta/\nu}\tilde{P}_\infty(\delta c L^{1/\nu}) \tag{2a}$$

$$\chi(L, c, t) = L^{\gamma/\nu}\tilde{\chi}(\delta c L^{1/\nu}). \tag{2b}$$

Here P_∞ is defined as the fraction of occupied sites that belong to the largest cluster in the system, and $\chi = \Sigma_s' s^2 n_s(c)/c$, $n_s(c)$ being the concentration of clusters containing s sites, and the largest cluster is excluded from the sum. While these data refer to periodic boundary conditions, a cluster counting and subsequent finite-size scaling analysis has also been performed for free boundary conditions. In all cases similar quality of 'data collapsing' on the scaling functions is obtained as shown in figure 3. The final exponent estimates are

$$\nu \approx 0.88 \pm 0.06 \qquad \beta \approx 0.42 \pm 0.02 \qquad \gamma \approx 1.74 \pm 0.06. \tag{3}$$

Within the quoted error bars these numbers agree with the hyperscaling relation $3\nu = \gamma + 2\beta$ and with the corresponding exponents for the random percolation problem

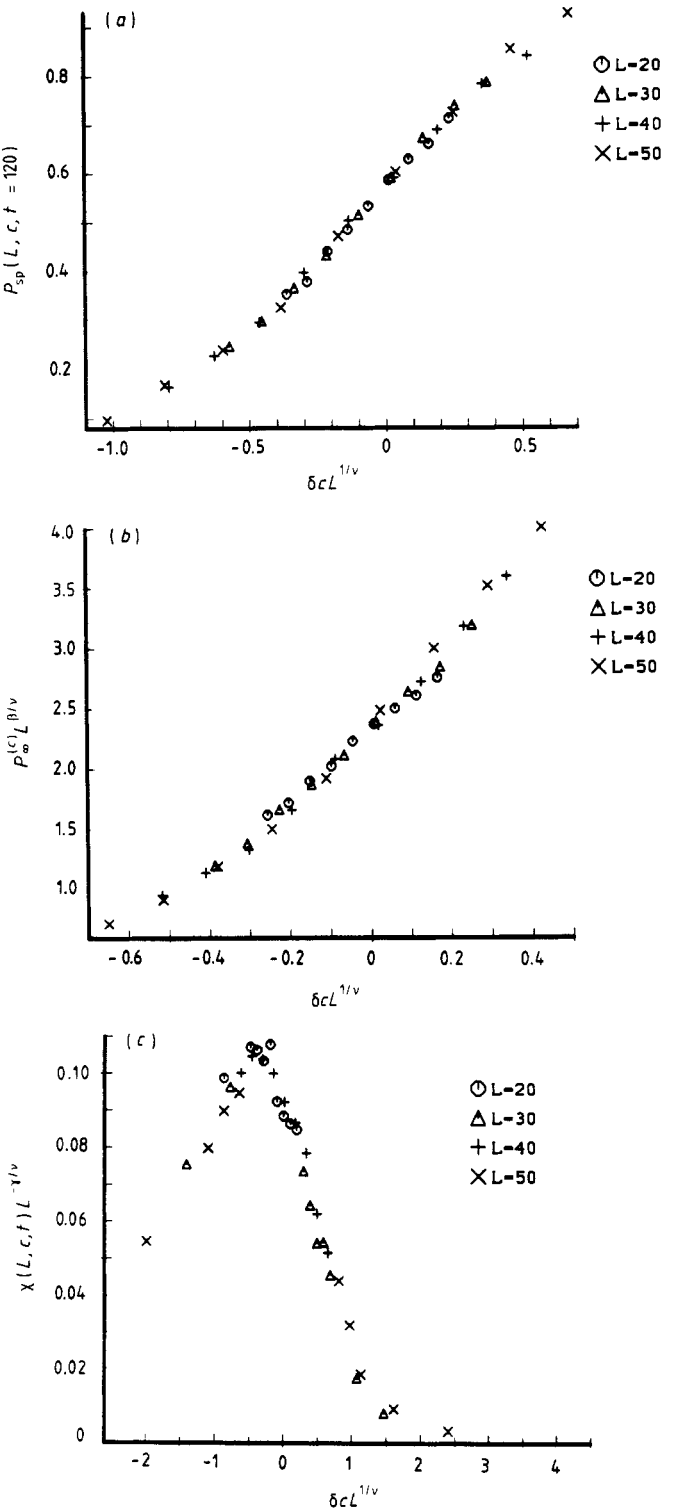

Figure 3. (*a*) Finite-size scaling plot of the spanning probability data of figure 2, using $\nu = 0.91$. (*b*) Finite-size scaling plot of $P_\infty(L, c, t = 120)$ using $\beta = 0.43$, $\nu = 0.91$. (*c*) Finite-size scaling plot of $\chi(L, c, t = 120)$ using $\gamma = 1.74$, $\nu = 0.82$.

(Stauffer 1985). The estimate $\nu \approx 0.7$ due to Hayward *et al* (1987) is definitely ruled out—this work was hampered by a too low statistical accuracy, although the 'raw data' for $P_\infty(L, c, t)$ were qualitatively similar to those used here (Lironis 1988). Also in the present case the statistical fluctuations are too large to prevent us from including more subtle effects (such as corrections to finite-size scaling, etc) into the analysis.

In the spirit of figure 2, the phase diagram figure 1 implies that we must see two intersections in $P_{sp}(L, c, t)$ if we analyse it at fixed c as a function of t (e.g. figure 4). The strong statistical scatter of our data confuses somewhat the analysis, but, imposing the condition that the value of the intersection point should be universal $\{\tilde{P}_{sp}(0) \approx 0.57\}$, the diagram given in figure 1 can be deduced by repeating the analysis shown in figure 2 for other times.

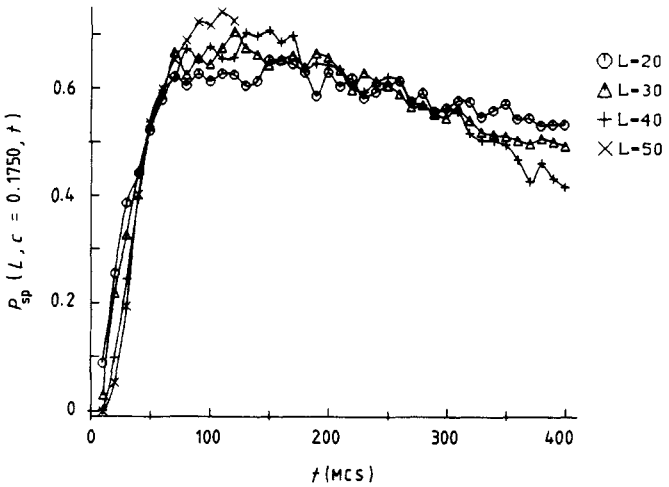

Figure 4. Spanning probability $P_{sp}(L, c = 0.175, t)$ against t for four different lattice linear dimensions. Note a first intersection at $t \approx 60$ and a second one at $t \approx 240$.

Apart from the questions about the universal properties of the percolation transition, one can also study the microscopic dynamic processes involved in this coalescence of clusters. For example, we have found that the decrease in the fraction of sites contained in 'dangling ends' with time (Lironis 1988) reflects the coarsening of the cluster structure, though the detailed kinetic mechanisms are not yet understood. It is also interesting that for small cluster sizes one observes a depletion of less stable cluster sizes (e.g. $s = 3, 5$) in comparison with neighouring ones which are more stable ($s = 4, 6$) due to a more compact configuration (figure 5). This observation indicates that faithful dynamical modelling of the 'cluster dynamics' processes, as has been proposed by various authors (Binder 1977, Binder *et al* 1978, Langer and Schwartz 1980, Kampmann and Wagner 1984), is more difficult than previously thought.

In summary, the 're-entrant' character of dynamic percolation during phase separation of lattice gas models of binary alloys has been quantitatively established, for the first time (figure 1); contrary to previous suggestions we find that this transition falls into the universality class of random percolation. While the critical exponents thus pose no problem, it is still unclear as to what extent dynamic percolation shows up in the scattering function, and also the detailed 'cluster dynamics' processes remain to be clarified.

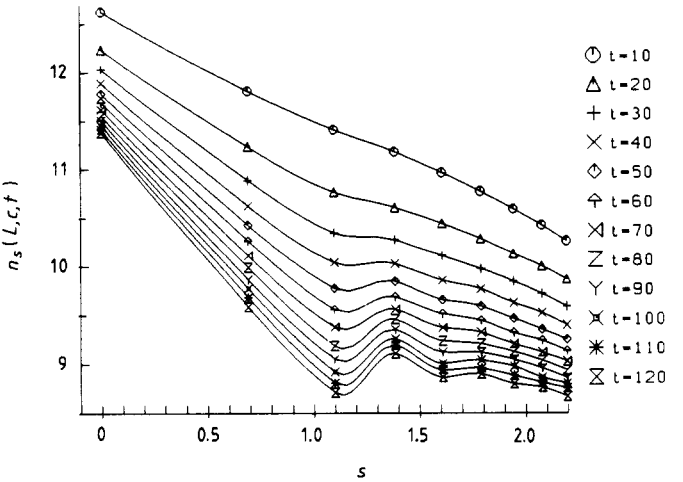

Figure 5. Cluster size distribution $n_s(L = 50, c = 0.15, t)$ against lg s for 12 times as indicated in the figure. Note the maximum which develops for $s = 4$.

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