COMPUTER SIMULATION STUDY OF ENCOUNTER EFFECTS ON PHASE SEPARATIONS

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Many theoretical and numerical attempts have been made to understand the late-stage dynamics of phase separations in off-critically quenched binary systems [1]. However, in spite of its importance, an effect of encounters among droplets has been neglected in previous works, except for a phenomenological theory by Davies et al [2]. When two droplets meet, the greater of them absorbs the lesser, and their total volume is conserved. In fact, in computer simulations such encounters always occur whatever initial conditions one chooses, when the total volume fraction (denoted by Q) is greater than 0.2 [1,3]. Thus, to study the phase separation dynamics at higher volume fractions, one must take into account such an encounter mechanism into the theory as well as the Ostwald ripening mechanism.

To include such encounter effects, we have extended the droplet model for the phase separation dynamics in off-critically quenched binary systems [4]. The droplet model equation is written in terms of radii of droplets and their center of mass positions with the constraint of the total mass conservation, and can describe not only the late-stage dynamics but also the early-stage dynamics after nucleation stage [3]. Based on the model equation, we have presented the systematic theory and the computer simulations for crossover phenomena of the phase separation dynamics at lower volume fractions. In particular, we have shown that there exists three characteristic stages (or mechanism), that is, the single-body growth mechanism (diffusion-controlled stage), the many-body growth mechanism (intermediate stage), and the Ostwald-ripening mechanism (coarsening stage) [3]. Encounter effect is incorporated into the model as follows [4]. When the sum of two droplet radii is greater than the intervortex distance plus $.10^{-2} < a > (\tau)$ with the average droplet radius $< a >$ at time τ, these two droplets are interpreted to coalesce. At that time these two droplets are replaced with one new droplet at the center of mass position for these droplets with its volume being the sum of two droplets volume.

Performing large scale simulations, we have found four characteristic stages with three crossovers at higher volume fractions [4]. In Fig.1 we show the average droplet radius $< a >$ as a function of time τ for various volume fractions. We can see that the growth exponent in the intermediate stage

for $Q = 0.4$ is different from that for $Q = 0.1$. Similar behavior has been obtained for the dymanic structure function. The encounter effect is thus found to strong influence a transition from the diffusion-controlled to the coarsening stage. Moreover, the late stage scaling functions for the droplet size distribution function and the structure function at larger volume fractions are found to differ from those predicted by the theory without the encounter effect.

References

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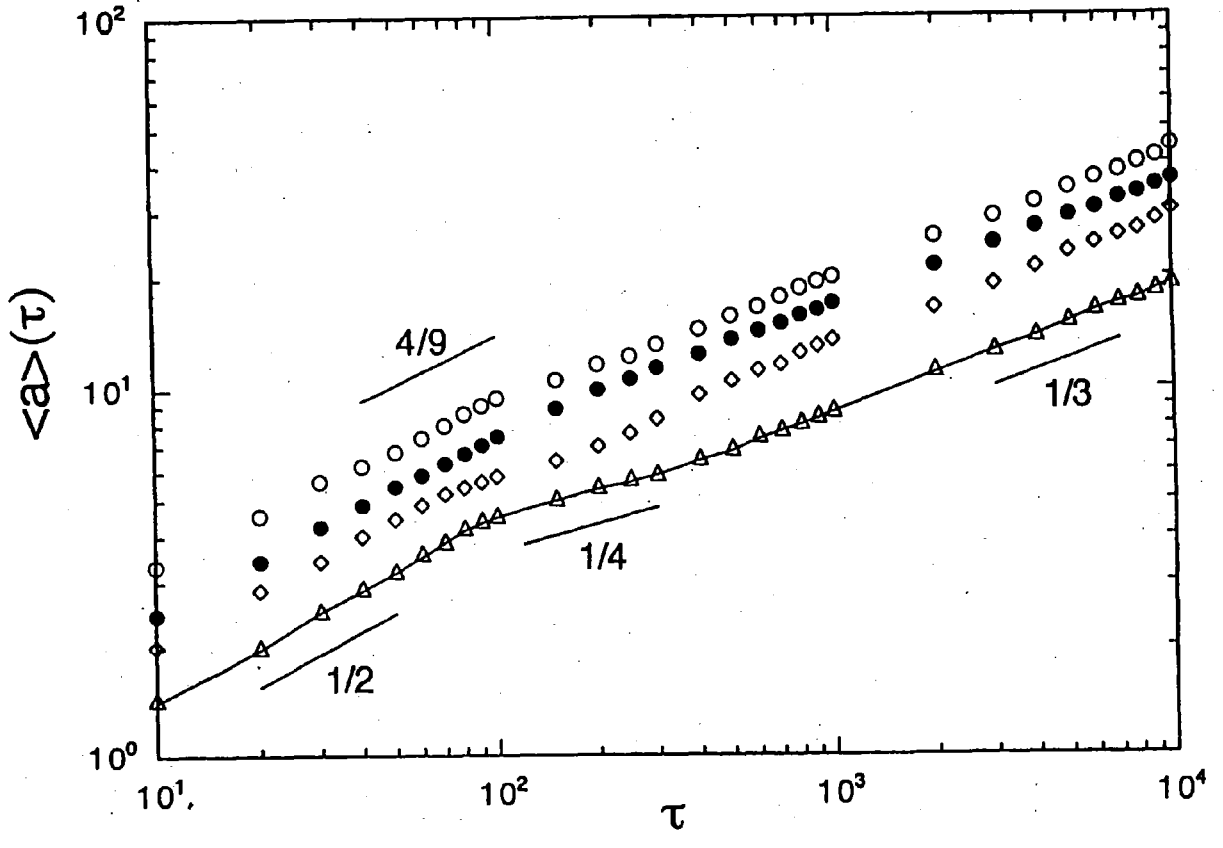

Fig.1 A log–log plot of the average droplet radius $< a > (\tau)$ versus τ. Shown are the simulation data for $Q = 0.1(\triangle)$, $0.2(\diamond)$, $0.3(\bullet)$, and $0.4(\circ)$. with slopes indicated. The solid line represents the theoretical result for $Q = 0.1$ without the encounter effect.