Comment on "Aging Effects in a Lennard-Jones Glass"

In a recent Letter, Kob and Barrat [1] reported results of molecular dynamics simulations for the off-equilibrium dynamics in a binary Lennard-Jones (LJ) glass. The main conclusions of their work was (i) they find aging in this glassy system and (ii) they find a *simple* aging scenario close to a t/t_w scaling, which is very reminiscent of comparable studies in spin glasses. In this Comment, we would like to emphasize that a different aging scenario, known under the name *activated dynamics* scaling, is much more appropriate for the system under consideration than the one proposed by Kob and Barrat [1].

For this reason we repeated the simulation by Kob and Barrat, using exactly the same potential (Lennard-Jones for a binary mixture), the same parameters (same diameters, mixture, density, and temperatures), and the same quenching procedure ($T_i = 5, T_f = 0.4$), however, with much larger systems ($32\,768 = 32^3$ particles) and similar times (2×10^6 time steps, one time step corresponding to 0.01 LJ units). The aging properties of the system manifest themselves in the two-time autocorrelation function

$$C_q(t + t_w, t_w) = \frac{1}{N} \sum_i e^{iq[r_i(t+t_w) - r_i(t_w)]}, \qquad (1)$$

where $r_i(t)$ is the position of particle i at time t and the absolute value of q corresponds to the first maximum in the structure function. We averaged C_q over 100 randomly distributed vectors. The function (1) was evaluated after every ten time steps, and 5^n (n such that $t \in [5^n, 5^{n+1}]$) measurements were averaged over to improve statistics. We convinced ourselves that different quenching procedures with identical initial and final temperatures, T_i and T_f, lead to the same scaling behavior.

In [1] it has been suggested that $C_q(t + t_w, t_w)$ obeys

$$C_q(t + t_w, t_w) \sim \tilde{c}(t/t_r) \qquad (2)$$

with a relaxation time $t_r \propto t_w^\alpha$. We checked this *ansatz* for our data and display the result in the inset of Fig. 1; surprisingly, we find an exponent $\alpha \sim 1.1$, very close to one (corresponding to simple t/t_w scaling) but different from the one $\alpha = 0.88$ reported in [1]. The data collapse in the asymptotic regime is not at all satisfying, the data for different waiting times t_w coincide exactly only for $C_q = 0.45$. For this reason we tried another aging scenario, proposed in the context of spin glasses by Fisher and Huse [2], which we call the *activated dynamics:*

$$C_q(t + t_w, t_w) \sim \tilde{C}\{\ln[(t + t_w)/\tau]/\ln(t_w/\tau)\}, \qquad (3)$$

where τ is a fit parameter and plays the role of an effective microscopic time scale. Figure 1 shows the scaling plot for such a scenario, which gives a much better data collapse in the asymptotic regime $t \geq t_w$.

The origin of such an activated dynamics scaling in spin glass phenomenology [2] is simply a logarithmically slow coarsening process $\xi(t) \sim \ln(t)^a$, where $\xi(t)$ is a time dependent spatial correlation length and a is some exponent. This plus the observation that in coarsening dynamics the two-time correlation function $C_q(t + t_w, t_w)$ should depend on the ratio of the two length scales $\xi(t_w)/\xi(t + t_w)$ alone yields the aging behavior (3).

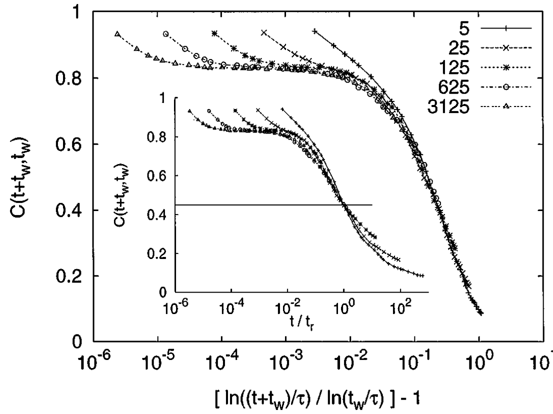

FIG. 1. Activated dynamics scaling plot according to Eq. (3) with $\tau = 0.005$. We shifted the scaling variable by one to the left to have a better resolution of the crossover region. The inset shows a scaling plot of our data according to the scenario proposed by Kob and Barrat [1] [see Eq. (2)]; the full line corresponds to $C_q = 0.45$. The relaxation times are $t_r = 14.5$, 106, 700, 6000, and 30 000 for $t_w = 5$, 25, 125, 625, and 3125, roughly a dependence $t_r \propto t_w^{1.1}$. All times are in LJ units.

Three things are worth being noted: (i) In the context, in which Eq. (3) was first suggested, namely, the 3D Edwards-Anderson (EA) spin glass model, this form does not seem to work [3]. (ii) Only very recently a growing length scale has been observed in the very same model we are considering here [4]. (iii) An even better data collapse can be obtained by plotting $C_q(t + t_w, t_w)$ versus $\ln(t)/\ln(t_r)$, with a relaxation time t_r individually chosen for each waiting time t_w. Here it turns out that $t_r(t_w)$ grows faster than a power law.

In conclusion, we have shown that the aging behavior of a Lennard-Jones glass is more appropriately described by an activated dynamics scaling rather than simple aging, as claimed by Kob and Barrat in Ref. [1].

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[1] W. Kob and J.-L. Barrat, Phys. Rev. Lett. **78**, 4581 (1997).
[2] D. S. Fisher and D. A. Huse, Phys. Rev. B **38**, 386 (1988).
[3] J. Kisker, L. Santen, M. Schreckenberg, and H. Rieger, Phys. Rev. B **53**, 6418 (1996).
[4] D. Lancaster and G. Parisi, J. Phys. A **30**, 5911 (1997); G. Parisi, cond-mat/9801034.

