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

In a recent Letter Kob and Barrat 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 1) they find aging in this glassy systems and 2) that 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.

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 ($32768 = 32^3$ particles) and similar times ($2 \cdot 10^6$ time steps, 1 time step corresponding to 0.01 LJ-units). The aging properties of the system manifest themselves in the two-time autocorrelation function

$$C_q(t+t_w, t_w) = \frac{1}{N} \sum_i e^{-q |r_i(t+t_w)-r_i(t_w)|},$$

(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 choose 100 randomly distributed vectors and averaged $C_q$ over these vectors. The function (1) was evaluated after every 10 time steps and 5$^a$ 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

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

(2)

with a relaxation time $t_r \propto t_w^a$. 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 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, which we call the activated dynamics:

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

(3)

where $\tau$ is a fit-parameter and plays the role of an effective microscopic time scale. Fig.1 we show 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 is simply a logarithmically slow coarsening process $\xi(t) \sim \ln(t)^a$, where $\xi(t)$ is a time dependent spatial correlation length and $a$ 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 scale $\xi(t_w)/\xi(t+t_w)$ alone yields the aging behavior (3).

Three things are worth being noted: 1) In the context, in which (3) was first suggested, namely the 3d EA spin glass, this form does not seem to work. 2) Only very recently a growing length scale has been observed in the very same model we are considering here. 3) 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 with a power law.

To conclude 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 [1].

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Date: 18 February 1998

PACS numbers: 61.43.Fs, 02.70.Ns, 61.20.Lc, 64.70.Pf

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