We have carried out molecular dynamics simulations to understand the dynamics of a *tagged pair of atoms* in a strongly non-ideal glass-forming binary Lennard-Jones mixture. Here atom B is smaller than atom A ($\sigma_{BB} = 0.88\sigma_{AA}$, where $\sigma_{AA}$ is the molecular diameter of the A particles) and the AB interaction is stronger than that given by Lorentz-Berthelot mixing rule ($\epsilon_{AB} = 1.5\epsilon_{AA}$, where $\epsilon_{AA}$ is the interaction energy strength between the A particles). The generalized time-dependent pair distribution function is calculated separately for the three pairs (AA, BB and AB). The three pairs are found to behave differently. The relative diffusion constants are found to vary in the order $D_{BB}^R > D_{AB}^R > D_{AA}^R$, with $D_{BB}^R \approx 2D_{AA}^R$, showing the importance of the hopping process (B hops much more than A). We introduce a *non-Gaussian parameter* ($\alpha_P^2(t)$) to monitor the relative motion of a pair of atoms, and evaluate it for all the three pairs, with initial separations chosen to be at the first peak of the corresponding partial radial distribution functions. At intermediate times, significant deviation from the Gaussian behavior of the pair distribution functions is observed, with different degree for the three pairs. A simple mean-field (MF) model, proposed originally by Haan [Phys. Rev. A 20, 2516 (1979)] for one component liquid, is applied to the case of binary mixture, and compared with the simulation results. While the MF model successfully describe the dynamics of the AA and AB pair, the *agreement for the BB pair is less satisfactory*. This is attributed to the large scale anharmonic motions of the B particles in a weak effective potential. Dynamics of next nearest neighbor pairs are also investigated.
\[ \sigma_{AA}^{3} g_{2,\text{rad}}(r_{o},r;t) \]

- (a) \( t = 4\tau \)
- (b) \( t = 20\tau \)
- (c) \( t = 100\tau \)
- (d) \( t = 300\tau \)
\[ \sigma_{AA}^3 g_{2,\text{rad}}(r_0, r; t) \]

- (a) \( t = 4\tau \)
- (b) \( t = 20\tau \)
- (c) \( t = 100\tau \)
- (d) \( t = 300\tau \)

Graphs showing the distribution of \( \sigma_{AA}^3 g_{2,\text{rad}}(r_0, r; t) \) for different times. Each graph is labeled with the corresponding time in units of \( \tau \).
$g_{2,\text{ang}}(r_o, \theta; t)$
Figure 1: MSRD (inverse 1norm) of AA pair (a) as a function of time (t).
AB pair (b)
MSRD

BB pair (c)

time (t)
The graph shows the function $\alpha_2(t)$ over time (t). The solid line represents curve A, while the dashed line represents curve B. The x-axis represents time in units of 10 to the power of the number on the axis, and the y-axis represents the value of $\alpha_2(t)$ ranging from 0 to 1.
\[ \alpha_2(t) \]

Graph showing the behavior of \( \alpha_2(t) \) over time. The graph has a logarithmic scale on the x-axis for time (t) and a linear scale on the y-axis for \( \alpha_2(t) \). The graph includes three curves labeled AA, AB, and BB.
\( \sigma_{AA}^3 g_{2,\text{rad}}(r_0, r, t) \)

(a) \( t = 10\tau \)

(b) \( t = 50\tau \)

(c) \( t = 100\tau \)
\[ \sigma_{AA}^3 g_{2,rad}(r_o, r, t) \]

(a) \[ t = 10\tau \]

(b) \[ t = 50\tau \]

(c) \[ t = 100\tau \]
$\sigma_{AA}^3 g_{2,\text{rad}}(r_o, r, t)$

(a) $t = 10\tau$

(b) $t = 50\tau$

(c) $t = 100\tau$
\[ \sigma_{AA}^3 g_{2,\text{rad}}(r_0, r, t) \]

(a) \( t = 10\tau \)

(b) \( t = 100\tau \)
\( \sigma_{AA}^3 g_{2, \text{rad}}(r_0, r; t) \)

- **(a)** \( t = 10\tau \)
- **(b)** \( t = 50\tau \)
- **(c)** \( t = 100\tau \)
- **(d)** \( t = 300\tau \)
$\Delta L^{XY}$

time (in $\tau$)
$\sigma_{AA}^{3} g_{2,\text{rad}}(r_{o}, r; t)$

(a) $t = 10\tau$

(b) $t = 50\tau$

(c) $t = 100\tau$

(d) $t = 300\tau$
\[ \frac{r}{\sigma_{AA}} \]

(a) \( t = 4\tau \)

(b) \( t = 20\tau \)

(c) \( t = 100\tau \)

(d) \( t = 300\tau \)

\[ \sigma_{AA}^3 g_{2,\text{rad}}(r_0, r, t) \]