The effect of size-ratio on the rheology of plastic deformation in two-component supercooled system

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2種粒子を混合した過冷却系に対して分子動力学 (MD) シミュレーションを行い、粒子サイズ比の増大に伴って結晶化が起こりにくくなる様子を観察した。局所的結晶配向を表すパラメータを定義することで、共通の結晶軸方向を持った領域が、粒子サイズ比の増大とともに縮小する様子を可視化した。同時に、局所的な配向の乱れを示すパラメータも導入され、格子欠陥や系の不規則性が定量化された。さらに、系にshear流動を課すシミュレーションを行い、大きなストレステンソルを伴った粒子が直線上に分布する"stress chain" の出現を観測した。stress chain の長さと結晶性との関係についても報告する。

1 Introduction

In two-component systems under super-cooled conditions, particle-size asymmetry drastically influences rheology and dynamics of glass transitions. Here, we perform systematic molecular dynamics (MD) simulations of two-dimensional supercooled systems to investigate the transition between glassy and crystalline states. We also perform non-equilibrium simulations under shear flow. For rather small particle-size asymmetry, we observe the long "stress chain", the chain of particles with significantly large values of local stress tensor.

2 Local crystalline order

MD simulations are performed for a system containing $N = N_1 + N_2$ particles interacting via Lennard-Jones potentials, with $N_1 = N_2 = 500$. We assume that the size-ratio σ_1/σ_2 and the mass-ratio m_1/m_2 satisfies $m_1/m_2 = (\sigma_1/\sigma_2)^2$.

We define a complex number, $z_{jk} = x_{jk} + i\, y_{jk}$, with the displacement vector $\mathbf{r}_{jk}$ between jth particles and kth, $\mathbf{r}_{jk} = \mathbf{r}_k - \mathbf{r}_j = x_{jk}\hat{\mathbf{e}}_x + y_{jk}\hat{\mathbf{e}}_y$. We then introduce a parameter Φ_j as

$$\Phi_j = \sum_{k \in bond} \phi_{jk} \tag{1}$$

where $\phi_{jk} = z_{jk}^6/|z_{jk}^6|$, and "bond" means all the nearest-neighbour partiles of particle j. This parameter represents the direction of local crystal axis at the position of particle j, and display the domain in which particles have the common direction of crystal axis. For instance, in pure crystal, where this crystal has triangular lattice, and the direction of crystal axis has the angle α, we write $z_{jk} = re^{i(\frac{2\pi}{6}n+\alpha)}$. Then Φ_j becomes $6e^{6i\alpha}$. Φ_j is consist with 6-th rotational symmetry, and indicates the direction of local crystal axis, α.

Next, we caluculate the differnce $\delta\Phi_{jk} = \Phi_k - \Phi_j$, and define R_j as

$$R_j = \sqrt{\sum_{k \in bond} |\delta\Phi_{jk}|^2}. \tag{2}$$

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It represents the "irregularity", such as the defects in crystal, the grain boundary in poly-crystal, and so on. This is because $R_j = 0$ in pure crystal, while R_j takes on non-zero values when the particle is located near the "irregularity". In glassy state, R_j is finite for almost all j's. The parameter R_j thus represents the degree of local disorder around jth partcle, and the average $< R_j >$ represents the disorder of the whole system. Figure 1 displays snapshots of Φ_j and R_j with various size-ratios, and Figure 2 shows $< R_j >$. We observe that the local crystal domain becomes smaller as the size ratio is increased, indicating prevention of crystallization.

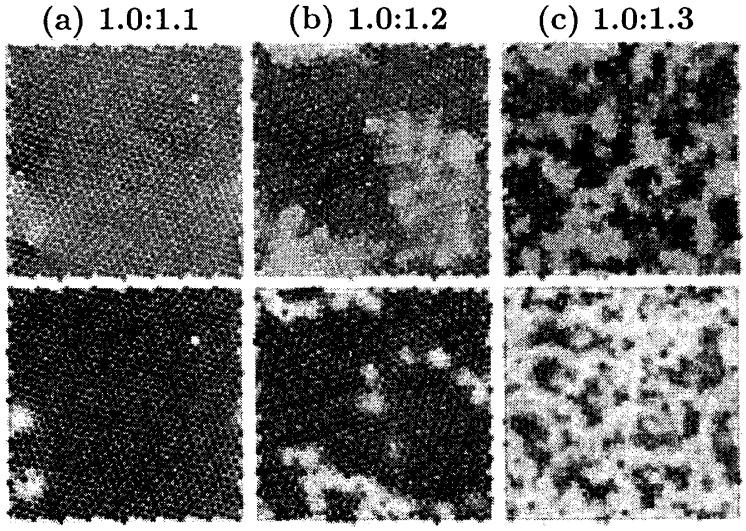

Figure 1: Snapshots of Φ_j and R_j

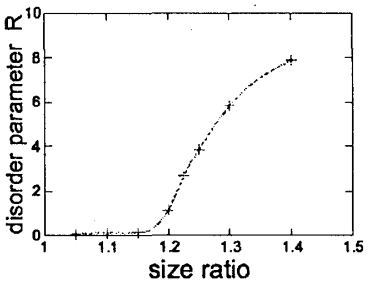

Figure 2: degree of disorder

3 Non-equilibrium simulations under shear flow

We impose constant shear flow on the above system using the Lee-Edwards boundary condition, and caluculate the stress tensor for each particle. The long "stress chain" is observed, when the size-ratio is comparatively small. Figure 3 are snapshots of local stress tensor with various values of size-ratio.

We are also performing simulations which impose desired stress by the "real-wall" boundary condition, in which vertically non-periodic and walls are made by restricted particles. In this simulation, we expect that the stress chain would appear more clearly.

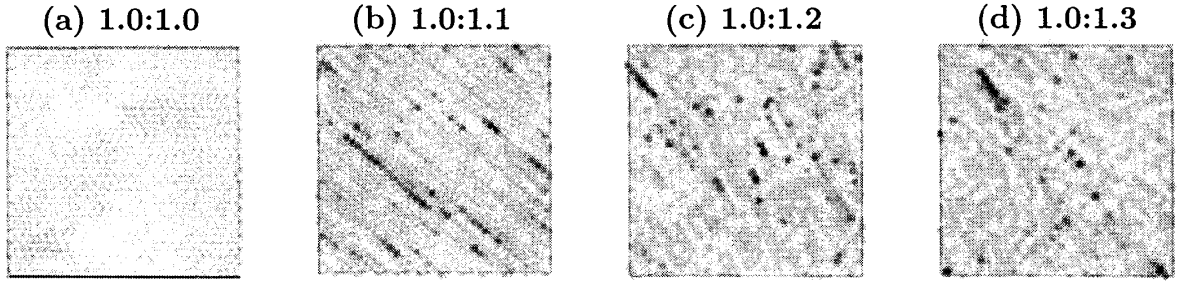

Figure 3: Snapshots of local stress. The shear field is applied horizontally: (a)(pure crystal) is already ruptured.