Identification of the Glass Transition Using Voronoi Encoding

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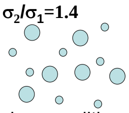
❖ Amorphous solids and "glassy" materials are becoming extremely common in technological applications, due to their very special mechanical properties. Understanding of the mechanical properties of glasses remains elusive since the glass transition itself is not fully understood, even in well studied examples of glass formers in two dimensional.

❖ The system of binary mixture of discs, interacting via a soft repulsion, is simulated by Monte Carlo and Molecular Dynamics under slow cooling regime. Structural features are visualized by Voronoi Diagram. We observe a new clan of defects, "liquid-like" defects (cells). These cells play crucial role in the evolution of the glass transition. It is shown that i) the glass transition is identified with the disappearance of liquid-like regions and ii) liquid-like regions appear in the glass state under mechanical strain.

Glass Former Explored

❖ A *2D* equimolar mixture of two kind of particles with diameter ratio σ_2/σ_1=1.4

❖ Repulsion via a soft core potential



$$u_{ab}=\varepsilon(\sigma_{ab}/r)^{12},\ a,b=1,2\quad \sigma_{aa}=\sigma_a,\quad \sigma_{ab}=(\sigma_a+\sigma_b)/2$$

❖ N=1024 particles were enclosed in a square box with periodic boundary conditions

❖ Methods used for equilibration at a given temperature :

Monte Carlo & Molecular Dynamics

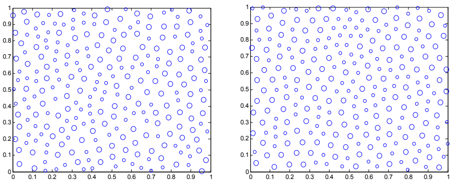
❖ Previous results: liquid-like behavior ➔ T>0.5

dynamical relaxation slows down considerably ➔ T<0.5

❖ In previous studies a precise glass transition was not identified.

No structural differences between liquid and solid states

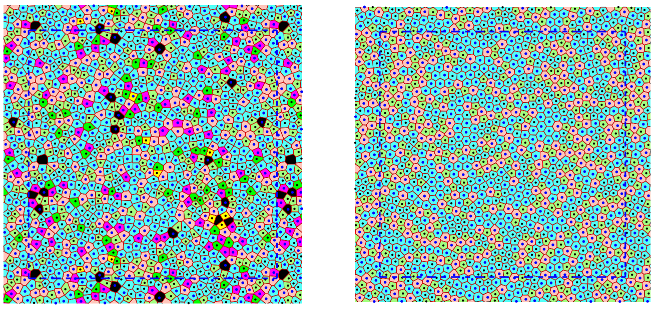
Liquid; T=3.0. Glassy state; T=0.1.



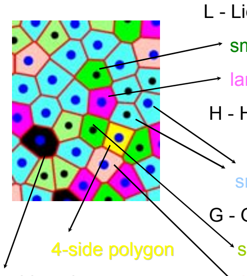
Solution:

Voronoi Diagram

T=3.0, T>T_g T=0.1, T<T_g



Tree classes of Voronoi cells:



L - Liquid-like cells – appear in the liquid phase

small in 7 side polygon,

large in 5 side polygon .

H - Hexagonal cells – appear in the crystalline ground state and also in the glassy phase

small or large in 6 side polygon.

G - Glass-like cells – appear in the glassy phase

small in 5 side polygon,

large in 7 side polygon.

4-side polygon

8-side polygons

Glossary

❖ The polygon of Voronoi Diagram associated with any particle contains all points closest to that particle than to any other. The edges of such a polygon are the perpendicular bisectors of the vectors joining the central particles.

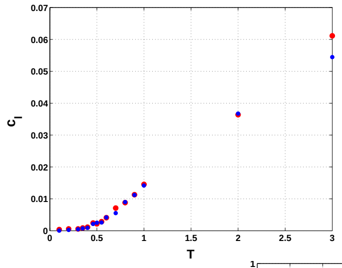
❖Liquid-like cell is defined for particle, which occupies inappropriate volume, e.g. small particle in heptagons or large particle in pentagons.

❖ Glass-like cell is defined for small particle in pentagons and large particle in heptagons.

Concentrations of Liquid-like cells

The concentration c_ℓ of these liquid-like defects becomes so small in the glass phase that we cannot distinguish it from zero.

For temperatures larger than 0.8 the concentration follows closely to exponential fit

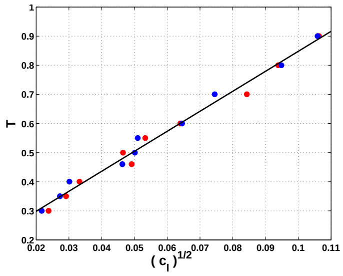


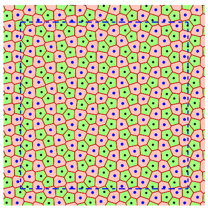
$$c_l = A\exp-(\Delta U/T),$$
$$A\approx 0.094, \Delta U\approx 1.90$$

Concentration of liquid-like cells c_l under slow cooling: large particles in pentagons (red dots) and small particles in heptagons (blue dots).

For temperatures in the range 0.3<T<0.8 we find a fit to

$$c_l = B(T-T_g)^2,$$
$$B\approx 0.02, T_g = 0.16\pm 0.02$$





Low Temperature Phase

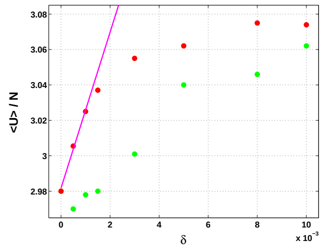
With Only Glass-Like Cells

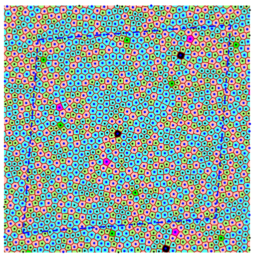
Behavior of Glass Under Shear

A linear shear transformation which conserves area

$$\begin{pmatrix}x'\\ y'\end{pmatrix}=\begin{pmatrix}1+\delta & \sqrt{(1+\delta)^2-1}\\ \sqrt{(1+\delta)^2-1} & 1+\delta\end{pmatrix}\begin{pmatrix}x\\ y\end{pmatrix}$$

The response of the system to shear is first elastic and then becomes plastic ➡ Liquid-like cells are formed





The measured energy <U>/N of the system after the shear is shown in red dots. The rhombic box is then returned to square box, energy at the end is shown in green dots. When the δ exceeds 10^{-3} the linear dependence is lost due to a plastic response.

Summary.

❖ A novel view of the glass transition is presented, identifying the transition as associated with the disappearance of newly identified liquid-like cells.

❖ It is shown that these liquid-like cells appear in the glass state when mechanical strain is applied.