Formation of orientational glass, strain glass, and ferroelectric glass in anisotropic particle systems: Structural heterogeneity and large response

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Nonspherical molecules such as KCN can form a crystal without long-range orientational order for mild molecular anisotropy, while liquid crystal phases can appear for large molecular anisotropy. Such crystals are called plastic crystals in a rotator phase. They undergo an orientational phase transition as the temperature T is further lowered, where the crystal structure is cubic at high T and non-cubic at low T. With inclusion of impurities in such solids, the so-called orientational glass has been realized. Around the transitions, a peak in the specific heat and softening of the shear modulus have been observed. In real systems, the molecules often have dipolar moments, yielding dielectric anomaly. As a similar example, metallic ferroelectric glass, called relaxor, has been studied extensively.

We propose a microscopic model of molecular dynamics simulation to study orientational glass in three dimensions. We present simulation results for mixtures of mildly anisotropic particles and spherical impurities. We also include the dipolar interaction to study ferroelectric glass with anomalously large dielectric constant.

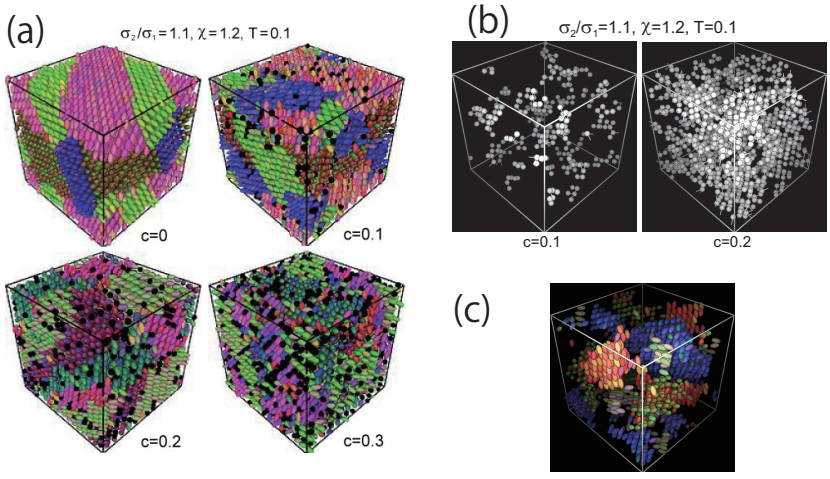

FIG. 1: (a) Frozen domain structures composed of four rhombohedral variants. With increasing the composition c of the impurities (black points), the orientational disorder increases, leading to a decrease in the domain size. (b) Snapshots of impurities composing clusters for $c = 0.1$ (left) and for $c = 0.2$ (right) with mesoscopic heterogeneities. (c) Snapshot of anisotropic particles forming ordered domains embedded in a disordered matrix.