# GLASS TRANSITION IN THE GAUSSIAN CORE MODEL

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The Gaussian core model[1] has a simple pairwise repulsive potential of the form $\exp(-r_{ij}^2)$. This model exhibits many interesting properties in three dimensions, including two stable crystal structures: a low-density fcc phase and a high-density bcc phase. In addition, "waterlike" anomalies such as a negative melting volume are also observed. The particular potential form also produces striking duality relationships[2] between the properties of the high- and low-density crystals.

In a series of molecular dynamics runs, the phase behavior at three different densities[3-5] has been characterized by successive heating and cooling of a system of 432 particles. At reduced density $\rho^* = 1$, no spontaneous crystallization is observed as the temperature is lowered through the melting temperature $T_m^* = 6.0 \times 10^{-4}$ to absolute zero. Examination of the pair correlation functions, even for strongly quenched states, shows that they more closely resemble liquidlike pair correlation functions instead of those for the crystalline state.

At a temperature $T_g^* = 1.7 \times 10^{-4}$, which we identify as the glass transition temperature at this density, the self-diffusion constant as measured by the mean-squared particle displacement versus time goes to zero. Another measure of the glass transition dynamics is afforded by the anharmonic energy as a function of temperature. Upon heating a defect-free bcc crystal, the anharmonic part of the lattice energy rises slowly. However, for the glass, the anharmonic energy increases much more rapidly as the glass transition temperature is approached from below.

Another signature of the glass transition is given by the ratio of values of the pair correlation function at the second minimum and the first maximum.[6-7] It has been observed in computer simulations of other systems, and our work confirms this result, that this ratio is 0.14 at $T_g$. A splitting of the second peak of the pair correlation function is commonly used as an indicator of the glass transition temperature. We observe no such splitting for this model at this density.

We stress that we have produced a long-lived glassy state for the three-dimensional Gaussian core model at $\rho^* = 1$. No spontaneous crystallization was ever observed below $T_g^*$ even after the quenching procedure had been arrested above absolute zero.

## REFERENCES

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