Structure of High-Density Amorphous Ices

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The structure of amorphous ice under pressure has been studied by molecular dynamics at 160 K. The starting low-density phase undergoes significant changes as the density increases, and at ?=1.51~g/cm^3 our calculated $g_{OO}(r)$ is in excellent agreement with *in situ* neutron diffraction data obtained at 1.8 GPa and 100 K on very high density amorphous ice (VHDA) made at 150K. As the system is further compressed up to ?=1.90~g/ cm^3, the structural modifications are continuous up to the highest density. The analysis of orientational distributions reveals that dense amorphous ice is characterised by major distortions of the tetrahedral geometry, and that the structural changes on densification can be interpreted as a trend towards a disordered closed packed structure [1]. The onset of the angular distortions is driven by temperature and explains the existence of two high-density forms of amorphous ice, HDA and VHDA [2].

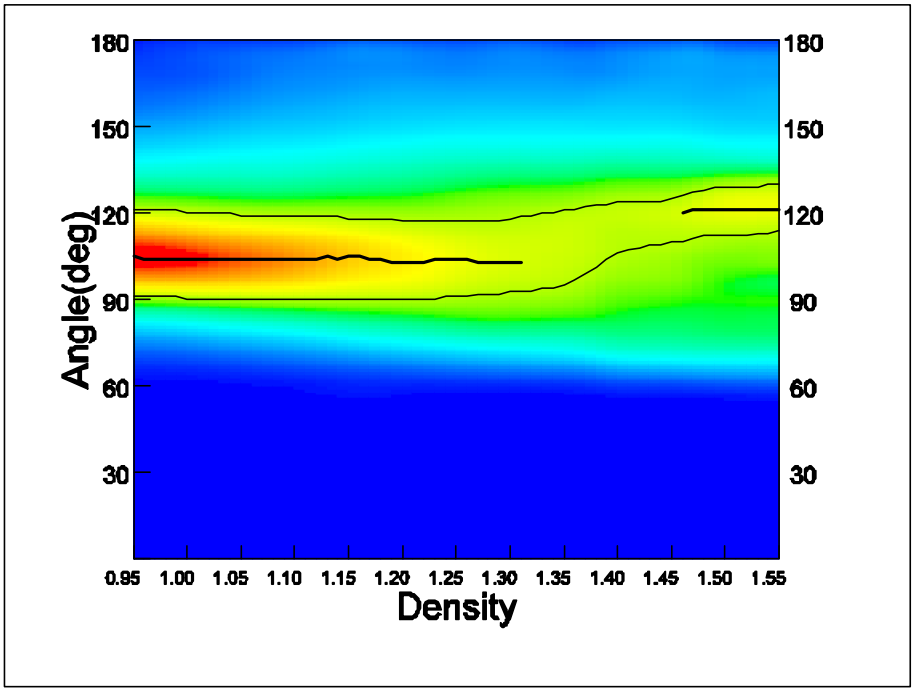

Figure 1: Orientational distribution of the tetrahedral cage as function of density at 160 K.

References

[1] - A.M. Saitta, T. Strässle, G. Rousse, G. Hamel, S. Klotz, R.J. Nelmes, and J.S. Loveday, *submitted for publication.*

[2] - A.M. Saitta, T. Strässle, and S. Klotz, *in preparation.*