Isosbestosis-Distinguishing between Phases and Fictions

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Several recent studies of amorphous ice have reported the growth of one set of spectral or difraction features at the expense of another set. Typically the diffraction or spectroscopic profiles when plotted on top of one another are found to pass through a common point, the so-called “isososbestic” point. The existence of such a point has then been taken to imply the existence or coexistence of two phases of the material in question (for example high density and low density amorphous ice in the present study).

In this talk I explore the nature of such an isosbestic point in the diffraction pattern of amorphous ice. By a series of computer simulations (each involving 4400 water molecules in a cubic box) of the diffraction pattern of amorphous ice at different densities I demonstrate that it is perfectly possible to generate (at least on the computer) a single phase material that proceeds continuously from one form to another, while at the same time exhibiting an isosbestic point in the corresponding diffraction patterns. All this is achieved with a common molecular interaction potential. It will be argued that exactly the same would be true for spectroscopic data from disordered materials if it could be calculated from such a simulation.

This observation throws into question the notion that diffraction and spectroscopic experiments on a disordered material can tell us *anything* about the degree or nature of phase separation in the material being investigated. In other words the observation of an isosbestic point in the diffraction or spectroscopic pattern is a *necessary* condition for phase separation but is not *sufficient* to prove it. In the case of amorphous ice this is leading to much confusion about whether the system can exist in a single or multiple phases simultaneously.

In fact the same simulations also show that amorphous ice can transform rather easily between high density and low density forms at virtually constant pressure, but at no point is there any indication that the simulated system has separated into distinguishable phases. An analysis of the observed structural transition will be presented, to the extent that it is available at the time of the talk.