Abstract No.: ehrl0256

X-Ray Diffraction Studies of Confined Methyl Iodide

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Beamline(s): X18A

Introduction: The study of confinement effects on quantum and classical systems has been of great interest for many years. Studies of many systems have shown that confinement changes thermodynamic and structural properties of the adsorbate drastically. Typically, systems in confinement exhibit an enhancement of the gas-liquid temperature transition, a depression in the liquid –solid temperature transition, and hysteresis upon melting of the adsorbate. The melting point is then found in between the confined freezing and the bulk freezing temperatures[1,2]. Examples of this behavior have been seen in many types of confining media Vycor glass, sol gel and cement[3-5] to name a few, and the adsorbates vary greatly, quantum systems such as H_2 and helium, classical systems O_2, complex systems H_2O, rare gases argon and krypton and metals such as mercury and indium[6-15].

Methods and Materials: Methyl iodide (CH_3I) confined in porous GelTech glass (200Å pores) x-rays diffraction and neutron scattering.

Results: Methyl iodide (CH_3I) confined in porous GelTech glass with a pore diameter of 200Å has been studied both with x-rays and neutrons. The x-ray scattering studies performed on beamline X18A at the NSLS clearly show the appearance of a crystalline phase at 168 K, well below the bulk solid transition. The structure of the confined crystalline phase is consistent with the known structure for the bulk solid. Companion neutron studies of the EISF and Debye Waller factor also observed a transition for the confined Methyl Iodide. This transition, however, was located at 205 K – just slightly below the bulk freezing temperature. Detailed X-ray scattering studies near the melting temperature provided insight into the discrepancy between the x-ray and neutron studies. The x-ray scattering studies revealed that confined methyl iodide exhibits two transitions, the first is a transition from a liquid to a glassy solid at 203K apparent due to the change in the high Q scattering and the second transition is from a glassy solid to a crystalline solid. Figure 1 shows the three phases of confined methyl iodide.

Conclusions: More studies of the diffusivity of this sample need to be undertaken.

Acknowledgments: Beamline X18A at the NSLS, the High flux Backscattering Spectrometer at NCNR, NIST, and the NSF Scattering Studies Grant

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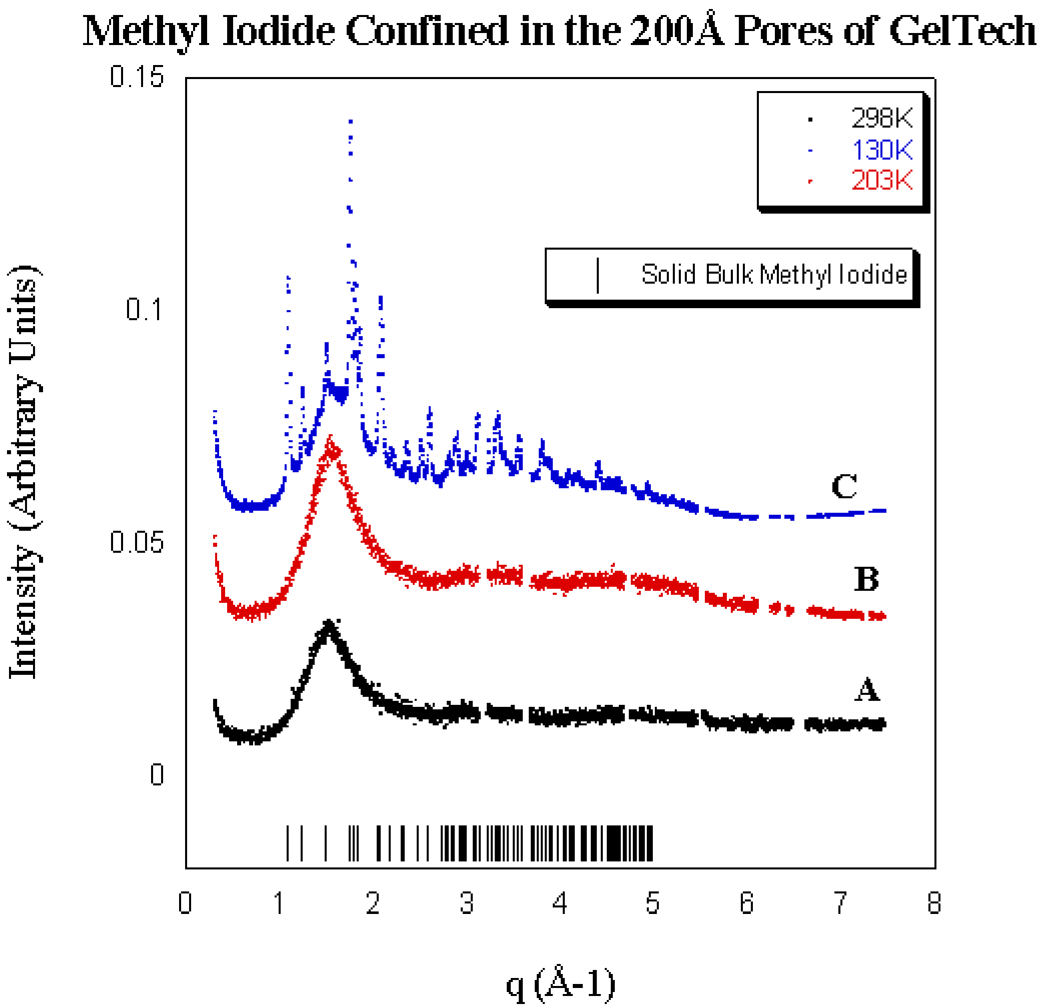

Figure 1: Diffraction data of methyl iodide confined to the 200Å pores of a GelTech monolith at 3 different temperatures. A) Is the liquid pattern at 298K. B) The pattern of the glassy phase at 203K and C) At 130K Brag peaks corresponding to bulk methyl iodide with a board underlying amorphous component. The slits at the bottom are the known diffraction peaks for solid bulk methyl iodide. Beryllium peaks masked out.