Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Neon Hydrate at High Pressure: an in-situ Neutron Diffraction Study XIAOHUI YU, Los Alamos Natioanl Lab — Clathrate hydrates are a group of ice-like, crystalline inclusion compounds which form through the combination of water and suitably sized "guest" molecules. There are mainly three crystallographic structures of the hydrate clathrate: SI, SII and SH, which are determined by the shape and size of the included gas molecular. However, when the neon gas pressure got increased to 0.48 GPa, we found that the neon gas could be enclathrate in the ice II frameworks which is totally different structure from the traditional cubic clathrate. Through the in-situ neutron diffraction study, the detail structure of Ne hydrate, including the atom positions, can be derived using the Rietveld refinements. The Ne atoms are just in the middle of H_2O channels and sandwiches by two H_2O rings The thermal equation of state was calculated and compared with pure ice II. We found that inclusion of Ne atoms could enlarge the ice II H_2O hexagonal rings, however, shortened the H_2O channels. Although the Ne atoms crystallized in ice II frameworks, the thermal vibration is significant compared to the host atoms. The distribution of Ne atoms are presented by MD simulations.

Xiaohui Yu
Los Alamos Natioanl Lab

Date submitted: 02 Nov 2012 Electronic form version 1.4