Abstract Submitted for the MAR09 Meeting of The American Physical Society

Heterogeneity of nitrogen multilayers adsorbed on graphite M. GOLEBIOWSKA, L. FIRLEJ, University of Missouri Columbia, Department of Physics and Astronomy; LCVN, Université Montpellier, B. KUCHTA, University of Missouri Columbia, Department of Physics and Astronomy; Laboratoire Chimie Provence, M.W. ROTH, University of Northern Iowa — The low temperature structures and phase transitions in nitrogen multilayers physisorbed on graphite are analyzed using Monte Carlo simulations. The systems that differ in number of layers and their relative packing (hexagonal or cubic) are analyzed. The nitrogen molecules are simulated as rigid, interacting via site-site potential (Etters model). The interaction with graphite includes atomic corrugation (Steele's potential). We show that the temperature and the mechanism of both orientational and melting phase transitions vary with the surface coverage and change from layer to layer. In particular, melting of the bilayer is preceded by compression of the first layer, which has not been observed before. The results are compared with simulations of two similar systems: (i) three nitrogen layers confined in slit graphite pore, and (ii) an adsorbed incommensurate structure that mimics low temperature alpha phase of bulk nitrogen.

Michael Roth

Date submitted: 08 Dec 2008

Electronic form version 1.4