Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Pt surface structure in presence of an oxygen atmosphere TIMO JACOB, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Faradayweg 4-6, D-14195 Berlin, Germany — Nowadays Platinum is used to catalyze a whole variety of different reactions. Expecially for electrocatalytic processes (such as in fuel cells) Pt is still one of the most sufficient materials providing a high rate for oxygen reduction at the cathode. However, this reaction occurs in a multi-component environment and under conditions of finite temperature, pressure, and electrode potential ($p = 1\,\mathrm{bar}$, $T = 80 - 100\,\mathrm{C}$, $\phi \neq 0\,\mathrm{V}$). Thus, the model of an pure and perfect Pt(111) surface, which is often used to study this reaction, is clearly incomplete. Therefore, to study the cathode reaction mechanism our first investigations aim on the realistic Pt(111) surface structure, which then will be the basis of further studies. Using density functional theory (DFT) in combination with a modified *ab inito* atomistic thermodynamics (capable to treat the electrode potential), we started with the $V = 0$ case and calculated the corresponding p/T-phase diagram, which led to interesting surface-oxide structures.

Timo Jacob
Fritz-Haber-Institut der MPG, Faradayweg 4-6, D-14195 Berlin, Germany

Date submitted: 23 Nov 2004 Electronic form version 1.4