Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Nitrogen Adsorption, Solubility and Transport within Group V Metals PANITHITA ROCHANA, EKIN OZDOGAN, JENNIFER WILCOX, Department of Energy Resources Engineering, Stanford University — It is well known that Group V metals have strong-binding characteristics to diatomic molecule, e.g. N_2, O_2, H_2, and CO. Within this study, N_2 has been investigated to determine the mechanism of surface adsorption, dissociation and subsequent atomic diffusion into the bulk crystal structure of vanadium(V). Alloys of ruthenium(Ru)-V have been examined indicating that Ru can be used to tune the electronic structure of the bulk to enhance atomic diffusion. Electronic structure calculations based on density functional theory have been studied on the investigation of N_2 adsorption on 3 low-index surfaces, (110), (100) and (111). Preliminary investigations indicate that the V(111) surface binds N_2 the strongest at fcc site (E_{ads} = 1.4eV). To determine bulk solubility, binding energy calculations are carried out as a function of N concentration. N was found to be stable primarily at O-sites within the bulk V lattice. Bader charge and density of states analyses are analyzed to investigate the mechanism of bulk absorption and solubility phenomena. Results will be presented on the adsorption, bulk solubility, and transport of N in V and V-based alloys. The application to this study is toward the design of an N_2-selective dense membrane in which atomic N may be produced on the permeate side with hydrogen as a sweep gas for the ammonia synthesis process.

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Date submitted: 16 Nov 2010 Electronic form version 1.4