Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Mechanical and Tribological Properties of Amorphous Carbon Films J. DAVID SCHALL, GUANGTU GAO, KEVIN VAN WORKUM, JUDITH A. HARRISON, United States Naval Academy, Department of Chemistry — Incorporation of silicon into hydrogenated amorphous carbon films has been shown to reduce film stress, make the friction coefficient less sensitive to moisture, and increase thermal stability while maintaining high hardness, low wear, and small friction coefficient. Molecular dynamics simulations utilizing the reactive empirical bond-order potential (REBO) have been used to examine the temperature dependence of the material and tribological properties of hydrogenated amorphous carbon films containing silicon. The REBO potential is one of the few potential energy functions capable of modeling chemical reactions likely to accompany sliding. Existing models for the C-Si-H potential are based on the original REBO potential developed by Brenner in 1990. These models do not calculate elastic modulus accurately. A new parameterization for the inclusion of Si into the second generation REBO potential has been developed. Calculations of elastic modulus from the second generation Brenner potential are in much better agreement with experimental values. Initial studies have shown that the inclusion of Si in amorphous carbon films increases the amount of sp^3 bonding in the film while decreasing the graphitic sp^2 content, making the films more diamond-like.

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Date submitted: 09 Jan 2006 Electronic form version 1.4