Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Studies of Thermally Annealed Graphitic Amorphous Carbon Resulting in a Decrease of Quasi-Stone-Wales Defects and Increase in Bandgap J.R. DENNISON, T.E. DOYLE, JODIE CORBRIDGE, Utah State University, STERLING SMITH, Princeton University, NEAL NICKLES, Ball Aerospace — We used a novel vibrational dynamics model for planar disordered materials (the embedded ring approach) to determine the structural evolution of thermally annealed graphitic amorphous carbon (g-C). The vibrational model assumes that constituent atoms of a material are arranged in n-membered planar rings embedded in the effective medium, a continuous random network of atoms. Standard structural models of g-C-a ubiquitous form of disordered carbon present in the production of diamond films, fullerenes, graphenes, nanotubes, and graphite-suppose that g-C is composed primarily of a structural distribution of such carbon rings with 4 to 8 atoms. We have calculated the in-plane normal modes and frequencies for embedded carbon rings and used these frequencies to fit Raman spectra of g-C annealed to temperatures ranging from 22 $^\circ$C to 1050 $^\circ$C. From the relative intensities of the different frequency peaks, our procedures provide quantitative ring statistics for the structure of g-C. In particular, we have found that unannealed g-C can have many 5- and 7-membered rings, but that the fraction of 6-membered rings increases with annealing temperature consistent with the known result that g-C evolves to nanocrystalline graphite under high T annealing.

J.R. Dennison
Utah State University

Date submitted: 07 Dec 2004 Electronic form version 1.4