Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Microscopic Origin of Infrared Activity in Graphite GUN SANG JEON, GERALD MAHAN, Pennsylvania State University — We investigate the phonon dispersion of the graphite within a generalized bond-charge model with emphasis on the microscopic origin of the infrared active mode. The resulting dispersion is in good agreement with those obtained by the experiments which include the full optical spectra obtained by the recent x-ray scattering. The computed strengths of the infrared peak are found to be comparable to the experimental values. We show that the dipole moment responsible for the infrared activity is induced by the interlayer Coulomb interaction between π- bond electrons.

Gun Sang Jeon
Pennsylvania State University

Date submitted: 29 Nov 2004 Electronic form version 1.4