Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Deformation of sp^2 graphitic nanostructure by irradiation with highly charged ion[1] YOSHIYUKI MIYAMOTO, Fundamental and Environmental Research Laboratories, NEC — I will discuss possibility of structural deformation of graphitic sp^2 network by irradiation of highly charged ions. Meguro *et al.*, [Appl. Phys. Lett..**79**, 3866 (2001)] reported indication of nano-diamond formation on graphite surface when it is irradiated by Ar^{+8} ions with incident kinetic energy of 400 eV. The nano-diamond structure was suggested from STS and IR spectrum taken after irradiation showing energy gap of 6 eV and C-C stretching with the frequency of 1360 cm^{-1}. This structural change was considered to be induced by injection of holes from highly charged ion (Ar^{+8}) while role the kinetic energy of Ar ion was thought to be marginal. Electron-ion dynamics simulation combined to the time-dependent density functional theory [O. Sugino, Y. Miyamoto. Phys Rev B**59**, 2579 (1999), *ibid*, Phys. Rev. B**66**, 088901(E) (2002)] has been performed to examine the mechanisms of the structural change. This simulation has found that the role of incident kinetic energy of Ar^{+8} and subsequent cooling mechanisms also play crucial role in determining the structural change. More details will be presented and discussed in my talk.

[1]All calculations were performed by using the Earth Simulator.

Yoshiyuki Miyamoto
Fundamental and Environmental Research Laboratories, NEC

Date submitted: 12 Nov 2006 Electronic form version 1.4