Determination of crystallite size L_a in nanocarbon materials by Raman spectroscopy: an open question

Katz E.A.*, Shames A.I.*, Zeiri L.*, Makarova T.L.**

*Ben-Gurion University of the Negev, Be'er-Sheva 84105, Israel
**Umea University, 90187 Umea, Sweden

Raman spectroscopy is widely used for structural characterization of nanocarbon materials. The band at about 1580 cm^{-1} (*G*-band) corresponds to the E_{2g} mode in the graphite structure. Ideal single-crystalline graphite should reveal only the *G*-band in the spectral range from 1200 to 1700 cm^{-1}. However, any disorder of the graphitic sp^2 regions resulting in the decrease of in-plane domain size (L_a) leads to the appearance of so-called *D*-band at about 1340 cm^{-1}. Accordingly, the relative intensity of the *D*- to *G*-bands (I_D/I_G) is widely used for a qualitative representation of L_a.

This work presents a systematic study of the I_D/I_G ratio and other *D*- and *G*-band parameters as a function of the excitation laser energy for a variety of nanocarbon samples: large and small polyhedral onions, glassy carbon, ball-milled nanographite, nanodiamonds. Our results clearly demonstrate that the dependence of I_D/I_G ratio on excitation energy varies considerably for different materials. Correct determination of L_a in various nanocarbon systems by Raman spectroscopy remains an open question so far and should constitute stuff for a future experimental and theoretical study.