

# Resonant multiwavelength Raman spectroscopy and structural features of polymerized three-dimensional C<sub>60</sub>

Khorobrykh F S<sup>1,2,@</sup>, Klimin S A<sup>3</sup>, Kulnitskiy B A<sup>1,2</sup>,  
Kvashnin A G<sup>4</sup> and Popov M Yu<sup>1,2</sup>

<sup>1</sup> Technological Institute of Superhard and New Carbon Materials,  
Tsentrlnaya Street 7a, Troitsk, Moscow 108840, Russia

<sup>2</sup> Moscow Institute of Physics and Technology, Institutskiy Pereulok 9,  
Dolgoprudny, Moscow Region 141701, Russia

<sup>3</sup> Institute of Spectroscopy of the Russian Academy of Sciences, Troitsk,  
Moscow region, Russia

<sup>4</sup> Skolkovo Institute of Science and Technology, Skolkovo Innovation Center  
Bldg 3, Moscow 143026, Russia

@ fedor.khorobrykh@phystech.edu

We studied resonance effects and structure of ultrahard fullerite under high pressure (up to 90 GPa). The studies were carried out using resonant multiwavelength Raman spectroscopy (257–1064 nm) and piezospectroscopy, high resolution transmission electron microscopy and density functional theory calculations [1]. We have revealed that resonant excitation of modes (inactive at other wavelengths) takes place at a wavelength of 1064 nm in ultrahard fullerite synthesized at 25 GPa with the application of shear deformations and in nanodiamonds in a size range of 2–5 nm. According to calculations, the phonon density of states of ultrahard fullerite spreads from zero to 1700 cm<sup>-1</sup>. We studied of ultrahard fullerite up to 90 GPa and indicated that the three-dimensional C<sub>60</sub> structure consists of at least two types of clusters formed by covalent bonds with a different set of force constants [2]. The intensity of Raman scattering depends on the wavelength of the exciting radiation (resonance effect) and a set of force constants at 532 and 405 nm excitation, the clusters with bulk moduli of 580 and 730 GPa accordingly are formed.

[1] Chernozatonskii L A, Serebryanaya N R and Mavrin B N 2000 *Chem. Phys. Lett.* **316** 199–204

[2] Khorobrykh F, Kulnitskiy B, Churkin V *et al* 2022 *Diamond Relat. Mater.* **124** 108911