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A Phenomenological Model for the D-Band in Disordered Carbon Materials

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Abstract – We describe and implement a phenomenological model for the Raman spectrum in disordered graphene. The model describes well the intensity ratio between the D-band and the G-band for a variety of disordered configurations.

Graphene, is a prototype for studying π electrons, and disorder in graphene is currently one of the frontier themes in both condensed matter physics and relativistic quantum electrodynamics [1]. Ion bombardment is a method for modifying (near) surface properties of materials, largely used to study effects related to disorder, leading to either desirable or undesirable alterations in the materials properties. Using this technique, combined with scanning tunneling microscopy and Raman spectroscopy, it is possible to obtain a disorder quantification in graphene trough the so called D band and G band intensity ratio (I_D/I_G).

In this work, we describe a phenomenological model for the I_D/I_G ratio and its implementation using a stochastic simulation of bombarded graphene and we compare our theoretical results with experimental data. Our model considers that a single impact of an Ar ion on the graphene sheet causes modifications in two length scales measured from the impact point (see Figure 1). Within the shorter radius r_S structural damage from the impact occurs, possibly causing vacancy formation, breaking and reconstruction of bonds, which causes destruction of hexagonal carbon rings. We call this the “structurally-damaged” or S-region (red circle). For distances larger than r_S but shorter than r_A, the lattice structure is preserved, but the proximity to a defect causes mixing of Bloch states near the K and K' valleys and breaking of selection rules, leading to an enhancement of the D band. We call this the “activated” or A-region (green circle). In qualitative terms, an electron-hole excitation will only be able to “see” the structural defect if it is created sufficiently close to it and if it lives long enough to probe the defective region. If the Raman scattering process occurs at distances larger than r_A-r_S from the defective region, the wavevector k emerges as a good quantum number for analyzing scattering selection rules and those regions will only contribute to the G band. This simple phenomenological model produces the full red line in Figure 2, which fits the I_D/I_G experimental data, as a function of the average distance L_D between defects, almost perfectly.

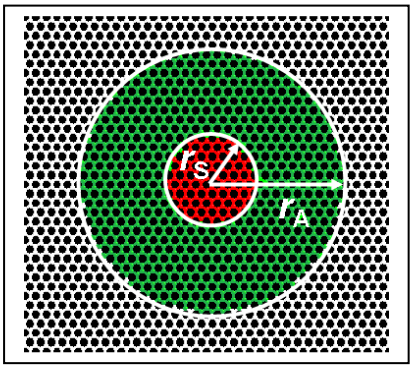

Figure 1: Activated (green) and structurally-damaged (red) regions, resulting from an impact of a single Ar ion in the graphene sheet..

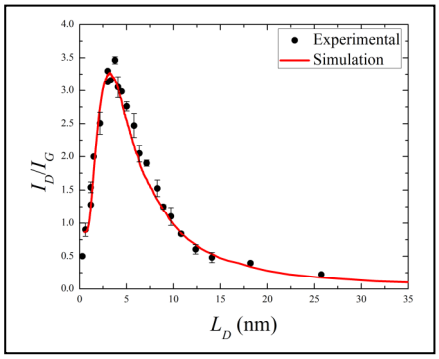

Figure 2: Experimental (dots) and theoretical (red line) values for the I_D/I_G ratio as a function of the average distance between defects.

References

[1] Geim, A. K. & Novoselov, K. S., The rise of graphene. *Nat. Mat.* **6**, 183-191 (2007).