Microstructure Analysis of Graphene by Wide Angle X-ray Scattering

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Carbon occurs in many forms, of which diamond (made up of sp^3 hybridized carbon) and graphite (made up of sp^2 hybridized carbon) are the most common ones. As another and most recently discovered form of carbon, Graphene, an extraordinary material has fascinating properties like an extremely high tensile strength and electric conductivity. For important applications such as supercapacitors quite large quantities of graphene in the form of dispersions and bulk materials are needed, which need to be prepared by chemical synthesis. One prominent method generates graphene flakes by the mechanical exfoliation of pristine graphite in a liquid environment [1] (fig. 1). Yet, such treatment under partially harsh conditions might result in a structural alteration of the ideal graphene structure. Furthermore, the layers might form stacks of graphenes stacked on top of each.
The main structural dimensions of these graphene stacks, constituting "non-graphitic carbons", i.e. the "microstructure" is generally described by the average lateral extension L_a and the stack height L_c, respectively [2]. Further important and relevant parameters are respectively the C-C bond length l_{CC}, the average distance a_3 between the layers and parameters quantifying the substantial degree of disorder in the stacking and the layers themselves. By acquiring Wide Angle X-ray/Neutron Scattering (WAXS/WANS) data (fig. 2) and the use of an advanced approach of analysis for the carbon microstructure (method of Ruland & Smarsly [3]), the microstructure could be determined. This will allow to quantify the number of graphenes per stack as well as the disorder in the stacking as well as the extension and the intrinsic order of a single graphene plane. These approach of the microstructure analysis of graphene will answer several questions like the number of graphene layers per stack or the layer extension as well as the disorder of both.

References

[1] R. Patton et al., Nat. Mater., 13 (2014) 624-630
[2] Warren, B. E., Phys. Rev., 59 (1941) 693–698
[3] Ruland W. & Smarsly, B. M., J. Appl. Cryst. 35 (2002) 624–633
[4] M. Zheng. et al., Synth. Met., 258 (2019) 116201

Figures

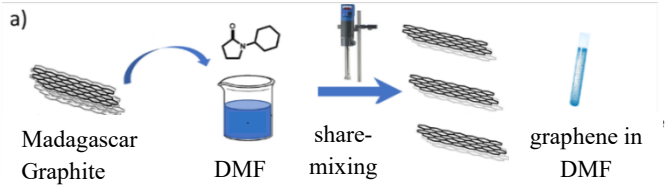

Figure 1: Procedure to produce liquid-exfoliated graphene flakes (EXG 3000 ink) [4].

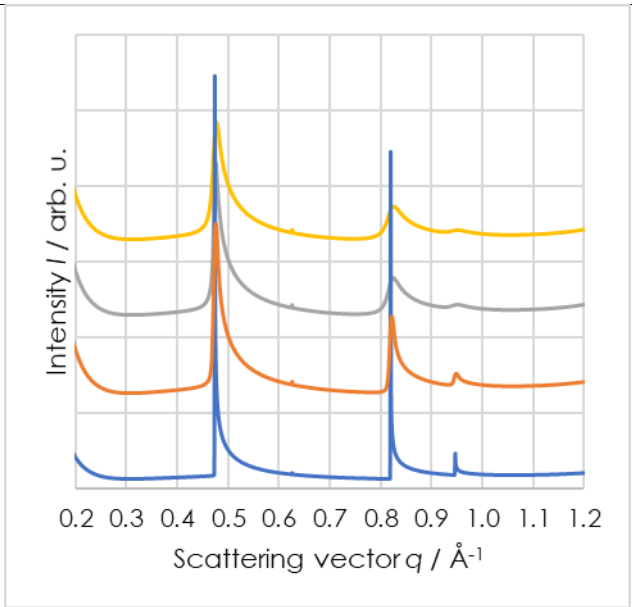

Figure 2 (right): Simulated Wide Angle X-ray Scattering (WAXS) data of different big and ordered graphene planes.

Blue: big (L_a = 1 µm) ordered (0.5 x scaled)
Orange: small (L_a = 10 nm) ordered
Grey: big disordered
Yellow: small disordered