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Supporting information for article:

Modelling of glass-like carbon structure and its experimental verification by neutron and X-ray diffraction

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In order to estimate reliably the goodness of agreement between the modelling results and the experimental data it is important to quantify possible inaccuracies resulting from both statistical and systematic errors. The statistical and systematic errors attributed to inadequacies in the diffraction data measurements and processing were estimated as discrepancies between the structure factors and the pair distribution functions determined experimentally and computed for polycrystalline nickel and silicon powder standards for the neutron and X-ray measurements, respectively. The deviations between the experimental and simulated structure factors and pair distribution functions for the glassy carbons were compared with the deviations computed for the standards for the neutron and X-ray measurements. The figures of the functions together with the discrepancies are presented in Figs. S1 and S2. As it can be seen from the comparison, the discrepancies between the experimental and computed diffraction functions for the standard samples are much smaller than that which are observed between experimental and simulated functions for the glassy carbons.

Moreover, the level of the errors due to the counting statistics in the diffraction experiments were estimated as the standard deviations of the mean from 40 or 6 sets of 1 hour or 20 minutes, for X-ray and neutron experiments respectively. The determined standard deviations of the mean for each point of the collected intensity function versus the scattering angle for X-ray and neutron diffraction experiments are very low and oscillate around 0.01%

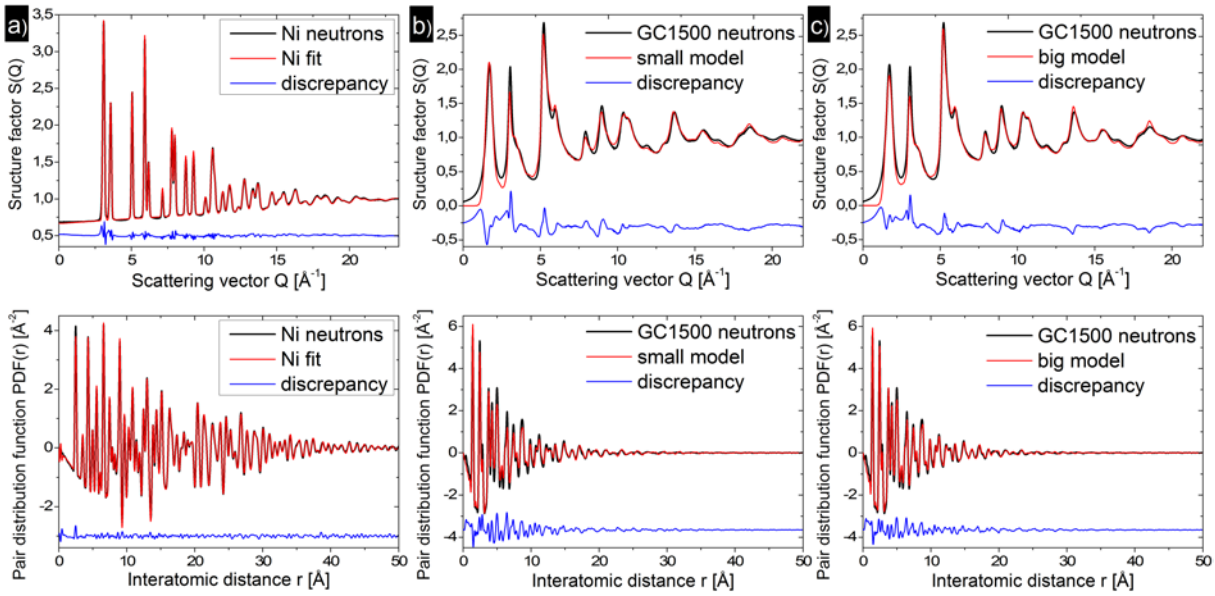

Figure S1

Comparison of the discrepancies between the structure factors and the pair distribution functions determined experimentally and computed for polycrystalline nickel standard for the neutron diffraction measurements (a) with the discrepancies between experimental functions for the glassy carbon heat-treated at 1500ºC and simulated functions for the proposed "small" model of the structure (b) and for the proposed "big" model of the structure (c).

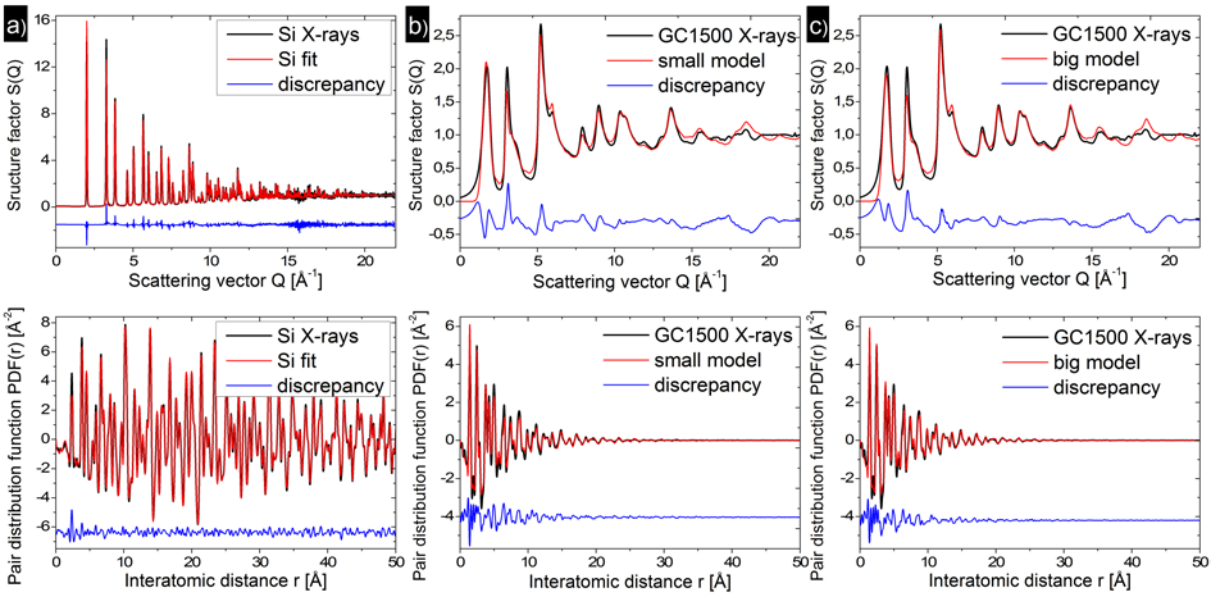

Figure S2

Comparison of the discrepancies between the structure factors and the pair distribution functions determined experimentally and computed for polycrystalline silicon standard for the X-ray diffraction measurements (a) with the discrepancies between experimental functions for the glassy carbon heat-treated at 1500ºC and simulated functions for the proposed "small" model of the structure (b) and for the proposed "big" model of the structure (c).