THE COMPARISON OF DIFFERENT DECONVOLUTION AND ANALYSIS APPROACHES OF THE RAMAN SPECTRA OF CARBIDE-DERIVED CARBONS

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Raman spectra of 31 different carbide-derived carbons (CDC) synthesized at temperatures (T_{syn}) ranging from 500 to 1100 °C have been measured. The corresponding spectra have been deconvoluted with three different approaches. The correlation between the width of the G-band and the T_{syn} of CDC was established, when 3-peak deconvolution approach was applied. The relation of the width of the D-band to the T_{syn} was only apparent with the 4-function deconvolution approaches. The crystallite sizes (L_a) of carbons have been calculated from Raman spectrum according to recently proposed equations [1–2] and from XRD data. The L_a values calculated from Raman spectra were significantly larger from the L_a values calculated from the XRD data, which might be due to the typical structure of CDC. However, it is difficult to attribute a physical meaning of the crystallite size L_a for CDCs. Thus, it is suggested to report the width of the D-band (while applying a 4-band deconvolution), the width of the G-band (while applying a 3-band deconvolution) directly, without calculating a definite numerical value (L_a).

References

1. J. Ribeiro-Soares, M.E. Oliveros, C. Garin, M.V. David, L.G.P. Martins, C.A. Almeida, E.H. Martins-Ferreira, K. Takai, T. Enoki, R. Magalhães-Paniago, A. Malachias, A. Jorio, B.S. Archanjo, C.A. Achete, L.G. Cançado, 2015, *Carbon*, 95, 646–652.
2. P. Mallet-Ladeira, P. Puech, C. Toulouse, M. Cazayous, N. Ratel-Ramond, P. Weisbecker, G.L. Vignoles, M. Monthioux, 2014, *Carbon*, 80, 629–639.

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