Application Note B-XRD1107

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B-XRD1107 - Material characterization by PDF and RDF analysis

Introduction

Pair Distribution Function (PDF) and Radial Distribution Function (RDF) analyses can derive atomic distances and atomic coordinates from an X-ray diffuse scattering pattern regardless of the crystallinity of the materials. Therefore, it is possible to perform the analysis for amorphous materials and nanomaterials that present broad peaks called halos.

Measurements and results

The X-ray scattering pattern from amorphous materials like amorphous carbon has much broader peaks compared to those of crystalline materials (Figure 1). These peaks are caused by the X-ray diffuse scattering corresponding to the various C-C distances. Hence, real space information, such as atomic distances and atomic coordination numbers, can be obtained from the inverse Fourier transformation of the X-ray diffuse scattering. Figure 2 shows an RDF profile, where the horizontal axis is the atomic distance and the vertical axis is the atomic coordination number. Peak positions and integrated intensities correspond to atomic distances and the atomic coordination number of carbon in the structure shown in Figure 3.

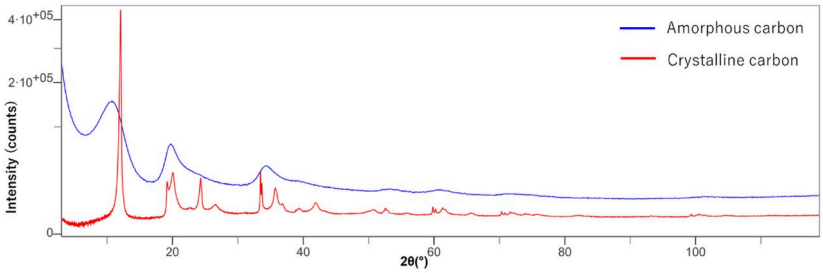

Figure 1: X-ray scattering pattern

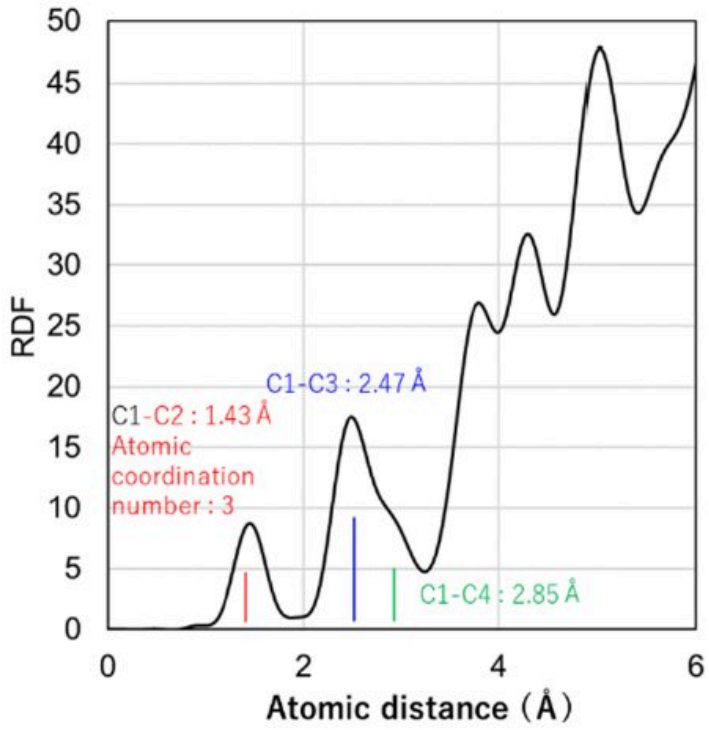

Figure 2: RDF profile from amorphous carbon

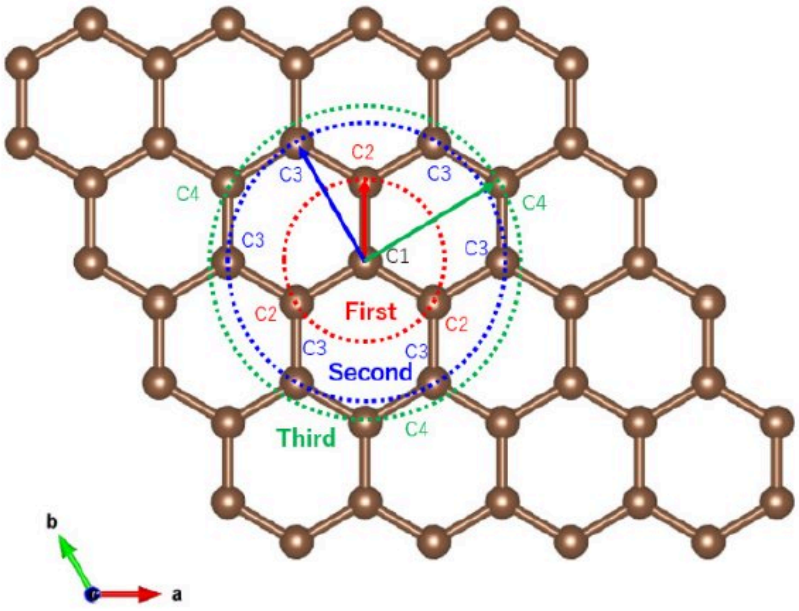

Figure 3: Crystal structure of carbon

Related products

HyPix-3000

Compact photon counting x-ray detector

SmartLab

Advanced state-of-the-art high-resolution XRD system powe red by Guidance expert system software

SmartLab Studio II

Windows-based software suite for Rigaku's X-ray diffractom eters