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Using neutrons for the study of amorphous materials: PDF analysis and titanium glasses

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The atomic-scale structure of liquids and glasses is crucial for understanding their material properties. However, amorphous materials lack of translational periodicity that leads to the Bragg peaks observed in the diffraction pattern for a crystal. Instead, the diffraction pattern is diffuse, and it is a challenge to solve the structure. The understanding of the neutron diffraction patterns measured for structurally disordered materials is achieved by means of Pair Distribution Function (PDF) analysis. This theory allows to obtain real-space structural information in the form of partial pair-distribution functions g(r) [1]. Due to the complexity of glassy and liquid systems, understanding their structures often requires of multiple techniques and PDF analysis on neutron diffraction experiments has efficiently been used in numerous systems [2][3].

One application where this technique is found useful is on the understanding of nucleation, crystal growth and the physical properties of glasses. This is of increasing interest among industry due to the potential versatility of the material's design. For this purpose, PDF analysis proves to be a powerful technique when combined with other techniques such as TEM, x-ray diffraction or NMR. Determining the structure of the systems, although still challenging, becomes possible. This information can lead to the design a priori of new families of glasses without the need of producing and testing many different materials. For example, in titanium glasses the presence of this metal has been observed to play a structural role on: (i) its optical properties (ii) inner crystal growth processes. These systems benefit from the negative neutron scattering length of titanium in contrast with its positive x-ray scattering length. Thus, a quantitative analysis of the short-range structure is possible when these two techniques are combined.

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