Diffraction for industries, businesses and health

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Powder diffraction is widely used at, or requested by, industries. Even more, new regulations are including the use of powder diffraction and even its data treatment by the Rietveld method. Several examples will be provided.

I. The amount of respirable low-solubility dust particles in air in the workplace is undesirable and already subject to regulation(s). A key subgroup is respirable crystalline silica which if inhaled it increases the risk of developing serious silica-related diseases, including: (a) silicosis, (b) lung cancer; (c) chronic obstructive pulmonary disease; and (d) kidney disease [1]. OSHA (Occupational Safety and Health Administration of USA) **Method ID-142** (2015) describes the collection of airborne respirable α-quartz and/or cristobalite in the breathing zone of personnel and the subsequent analysis by X-ray diffraction according to Method **NIOSH-7500**. In Spain there are related regulations: (1) **MTA/MA-014/A11** by Insituto Nacional de Seguridad e Higiene en el Trabajo, INSHT, "Determinación de materia particulada (fracciones inhalable, torácica y respirable) en aire - método gravimétrico"; (2) **MTA/MA-056/A06** by INSHT "Determinación de sílice libre cristalina (cuarzo, cristobalita, tridimita) en aire - Método del filtro de membrana / Difracción de rayos X"; and (3) Guía Técnica – Métodos de determinación de fracción respirable y sílice cristalina respirable" Departamento Técnico. Instituto Nacional de la Silicosis. Some details about our meticulous implementation will be provided but some specific details of our know-how will not be shared.

II. ASTM C1365 test method for cement Rietveld quantitative phase analysis validation procedure uses SRM 2686a reference material from NIST, which is a reference Portland clinker with reported elemental and mineralogical analyses. Laboratories and cement factories can implement ASTM C1365, by using the powder diffraction data of SRM 2686a collected with their X-ray equipments and employing their protocols but the output shall be within the ASTM C1365 limits. We were aware of problems for validating ASTM C1365 by several industries and we have thoroughly studied SRM 2686a using: (1) strictly monochromatic CuKα_1 'flat reflection geometry'; (2) strictly monochromatic MoKα_1 'flat transmission geometry'; and (3) synchrotron radiation 'rotating capillary transmission geometry'. Our results [2] indicate that belite in SRM 2686a is composed of two polymorphs (β- and α'$_H$-) that must be included in the analyses. The use of a unique phase for describing belite and inadequate peak shape modelling explain the problems found for implementing ASTM C1365. Polymorphism matters.

III. ALBA synchrotron and DRX unit of SCAI of University of Malaga have provided powder diffraction analyses for different industries and fields. Some examples will be sketched.

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Data accessibility. SRM 2686a powder diffraction data are deposited at Zenodo and they can be freely downloaded (doi: 10.5281/zenodo.1318500). Many data are confidential (they are subjected to NDA).

[1] https://www.osha.gov/dsg/topics/silicacrystalline/
[2] Garcia-Mate, M.; et al. "Rietveld quantitative phase analysis of SRM 2686a – A standard Portland Clinker" *Cement and Concrete Research*, **2019**, *115*, 361–366.