AVVISO DI SEMINARIO

Giovedì 22/02/2024, h 15.00
Aula M, DiSC, via Marzolo 1

Diffraction Line Profiles and Diffuse Scattering from Nanocrystals

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The traditional analysis of diffraction patterns from polycrystalline materials ignores the diffuse scattering component, usually absorbed into the background. However practical, this approach can interfere with a correct evaluation of structural and microstructural parameters. This is especially true if the diffraction domains are on the nanoscale, since features resulting from the correlation of atomic displacements in the innermost coordination shells and phonon confinement effects modify the thermal diffuse scattering (TDS), which overlaps with the broad peaks of the Bragg component. The diffuse component grows with the atomic mean square displacement (MSD), particularly high in superionic compounds, as well as for most organic materials, and in small nanocrystals for the large fraction of surface atoms. Including diffuse scattering in powder diffraction analysis is a topic not covered in recent years, with existing models dating back several decades, and in any case limited to monatomic systems or by strong approximations. Yet diffuse scattering in powder diffraction contains information on atomic level disorder, with the static and dynamic components of the MSD shared by the Debye-Waller coefficient commonly used to describe the thermal effects on the Bragg peak intensity only. Including diffuse scattering in the modelling of diffraction patterns can therefore provide more information and improve the analysis of thermal and static disorder parameters.
In this contribution, I'll present methods to study domain shape/size and strain in nanocrystalline systems and discuss how to include TDS in a traditional whole pattern analysis by the Rietveld method. The natural comparison of the results shown is with Total Scattering methods, and with atomistic simulations based on DFT and MD, useful tools both for *in silico* tests and to support the interpretation of experimental results.

Prof.ssa Silvia Gross (DiSC)

Il Direttore del Dipartimento di Scienze Chimiche
Prof. Stefano Mammi