

Nome da disciplina: **Métodos Cristalográficos Aplicados a Compostos Policristalinos**

Nº de créditos: **12** Carga horária: **180 horas**

Docente responsável: **Prof. Dr. Carlos de Oliveira Paiva Santos**

Docente colaborador: **não há**

## **EMENTA**

Métodos de mínimos-quadrados aplicado ao método de Rietveld, Estratégias de coleta de dados, determinação e refinamento de estruturas cristalinas com dados de difração por policristais. Análise quantitativa de fases. Determinação de tamanho de cristalito e microdeformação. Indetificação de polimorfos.

## **BIBLIOGRAFIA**

1. "International Tables for X-Ray Crystallography" - vol. A, B e C. Kynoch Press, Inglaterra (1983).
2. Advances in X-ray Analysis. Vol. 40. Proceedings of the 45<sup>th</sup> Annual Conference on Applications of X-ray Analysis. International Centre for Diffraction Data (ICDD). Denver, Colorado, EUA. 3-8 de agosto de 1996.
3. Alastair J. Florence, Norman Shankland, Kenneth Shankland, William I. F. David, Elna Pidcock, Xuelian Xu, Andrea Johnston, Alan R. Kennedy, Philip J. Cox, John S. O. Evans, Gerald Steele, Stephen D. Cosgroveh and Christopher S. Framptoni. Solving molecular crystal structures from laboratory X-ray powder diffraction data with DASH: the state of the art and challenges. *J. Appl. Cryst.* 38, 249–259, 2005.
4. Angeles G. De la Torre, María-Gema Lopez-Olmo, Carmen Alvarez-Rua, Santiago García-Granda, Miguel. A. G. Aranda. Structure and microstructure of gypsum and its relevance to Rietveld quantitative phase analyses. *Powder Diffraction* 19 (3), September 2004.
5. Brian H. Toby, CIF applications. XII. Inspecting Rietveld fits from pdCIF: pdCIFplot. *J. Appl. Cryst.* 36, 1285-1287, 2003.
6. Brian H. Toby, Robert B. Von Dreele and Allen C. Larson. CIF applications. XIV. Reporting of Rietveld results using pdCIF: GSAS2CIF *J. Appl. Cryst.* 36, 1290-1294, 2004.
7. C. O. Paiva-Santos. Aplicações do método de Rietveld. Instituto de Química, UNESP.<http://labcacc.iq.unesp.br/publicacoes/aplic/Aplicacoes do Metodo de Rietveld.pdf>. 2005.
8. D. Balzar, N. Audebrand, M. R. Daymond, A. Fitch, A. Hewat, J. I. Langford, A. Le Bail, D. Louër, O. Masson, C. N. McCowan, N. C. Popa, P. W. Stephens and B. H. Toby. Size-strain line-broadening analysis of the ceria round-robin sample. *J. Appl. Cryst.* 37, 911–924, 2004.
9. G.W. Brindley. The Effect of Grain or Particle Size on X-ray Reflections from Mixed Powders and Alloys, Considered in Relation to the Quantitative. *Philos. Mag.* 36, 347-369, 1945.
10. Gregory A. Stephenson, Applications of X-ray powder diffraction in the pharmaceutical industry. *The Rigaku Journal*. 2-15, Vol. 22, no. 1, 2-15, 2005.

11. H.M. Rietveld. A Profile Refinement Method for Nuclear and Magnetic Structures. *J.Appl. Cryst.* 2, 65-71, 1969.
12. Introduction to X-ray Powder Diffractometry. Ron Jenkins & Robert L. Snyder. John Wiley & Sons, Inc. 1996.
13. J.C. Taylor, C.E. Matulis. Absorption contrast effect in the quantitative XRD analysis of powders by full multiphase profile refinement. *J. Appl. Cryst.* 24, 14-17, 1991.
14. Klug., H.P. and Alexander, L. E. "X-Ray Diffraction Procedures for Polycrystalline and Amorphous Materials", J. Wiley and Sons, New York, USA, 1974.
15. Leonid A. Solovyov. Full-profile refinement by derivative difference minimization. *J. Appl. Cryst.* 37, 743-749, 2004.
16. Sampath S. Iyengar, Neelima V. Phadnis, Raj Suryanarayanan. Quantitative analyses of complex pharmaceutical mixtures by the Rietveld method. *Powder Diffraction* 16 (1), March 2001.
17. The Rietveld Method. IUCr Monographs on Crystallography 5. Edited by R.A. Young. International Union of Crystallography. Oxford University Press, 1993.
18. S. K. Manik and S. K. Pradhan. X-ray microstructure characterization of ball-milled nanocrystalline microwave dielectric CaZrO<sub>3</sub> by Rietveld method. *J. Appl. Cryst.* 38, 291-298, 2005.
19. V. Brodski, R. Peschar and H. Schenk. Organa – a program package for structure determination from powder diffraction data by direct-space methods. *J. Appl. Cryst.* 38, 688–693, 2005.
20. V. H. S. Utuni, A. V. C. Andrade, H. P. S. Correa e C. O. Paiva-Santos. Kcristal: Linux 'live-CD' for powder crystallography. *J. Appl. Cryst.* 38, 706–707, 2005.