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This Week's Citation Classic®

Hosemann R & Bagchi S N. *Direct analysis of diffraction by matter.*
Amsterdam, The Netherlands: North-Holland, 1962. 734 p.
[Fritz-Haber-Inst., Max-Planck-Gesellschaft, Berlin, Federal Republic of Germany and Calcutta Univ., India]

The monograph presents the theory of diffraction established by using "function algebra" for the analysis of data on noncrystalline matter. Preceding it, the theory of paracrystals was published[1] based on a mathematical formulation using the concepts of reciprocal space of P.P. Ewald and the interrelations of the three principal theories of structure: crystals, of (1) Laue and Bragg; and liquids, of (2) Zernike-Prins and of (3) Debye, Guinier, and Warren. A harmonic synthesis was obtained applicable to the quantitative analysis of diffraction data of lattice defects, which for the structure of noncrystalline matter led to the formulation of microparacrystals. [The *SCI*® indicates that this book has been cited in over 775 publications.]

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Lattice Defects and Microparacrystals

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Of importance in the development of theory for three-dimensional structures is the concept of reciprocal space formulated by P.P. Ewald, FRS (perhaps more correctly "Founder of Reciprocal Space"!) with whom I got acquainted in 1937. It is only with the help of the concept of reciprocal space that the mathematical background of noncrystalline matter could be constructed.

Max von Laue invited me in 1950 to give a lecture on our theory of paracrystals before the Physical Society to an audience of illustrious scientists gathered at Göttingen after the war. This was decisive for the new description of semi- and noncrystalline states of condensed matter presented, and with a handshake I was invited by von Laue to Berlin to found the Department of Paracrystal Research. Later, in 1960, he expressed in his book[2] the conviction that the quantitative analysis of lattice defects by diffraction data would open up "eine neue Wissenschaft" der "Zwischenkörper zwischen kristallinem und amorphem Zustand" [Editor's note: a new science of intermediate condition between the crystalline and amorphous states]. The foundation of one-dimensional paracrystals formulated with convolution polynoms and products was presented by him.

The book develops systematically the mathematical basis for the structure of noncrystalline matter based, at that time, on the application of Fraunhofer patterns to models. Their application to real cases came later, demonstrating the way to obtain straightforward information on microparacrystals by quantitatively studying the distorted reflections. In due course the concepts of microparacrystals were applicable not only to polymers but also in general to other noncrystalline matter, for instance, to promoted iron catalysts.[3]

Microparacrystals consist of lattice bricks of different sizes. Each of them has statistically the same *a priori* environment as neighbour bricks. A practical example is the three-dimensional paracrystalline structures of SiO_2 glass[4] published in 1984. We found a new member for the free enthalpy, the "tangential enthalpy," which for microparacrystals of N^3 bricks is proportional to N^4 and determines the equilibrium state of all noncrystalline matter $\sqrt{N}.g = \alpha^* = \ \approx 0.15$. This α^* law, the tangential enthalpy, and the structure of the microparacrystals are the first witness of the conviction of "neue Wissenschaft" of von Laue.

The frequent citation might be indicative of the need for a mathematical basis for the description of noncrystalline matter, which at that time was undertaken for the first time by me as a physicist. Having dedicated some years to studies in radioactivity (with G. v. Hevesy), cosmic radiation (with H. Geiger), and the small angle scattering by acetylcellulose (with R. Glocker), I felt the lack of a mathematical foundation for colloid sciences and undertook its realisation, stimulated by H. Staudinger and P.H. Hermans. Today, the mathematical theory of paracrystals offers the framework for the quantitative description of the various forms of noncrystalline matter such as colloids, polymers, glasses, and other surface active or catalytical solids. As was pointed out by M. Pfender,[5] it took a long time to arrive at this point. Unfortunately, with my retirement in 1980, the paracrystal research at the Max Planck Institut was discontinued, although M. Hentschel, A. Lange, and some others continue work in the establishment of the Bundesanstalt für Materialforschung, Berlin. G. Hinrichsen of the Technical University of Berlin deserves credit for drawing attention to this work.

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1. **Hosemann R.** Der ideale Parakristall und die von ihm gestreute kohärente Röntgenstrahlung (The ideal paracrystal and its diffusion of coherent X-radiation). *Z. Phys.* 128:465-92. 1950. (Cited 120 times.)
2. **von Laue M.** *Röntgenstrahlinterferenzen* (*X-ray interference*). Frankfurt am Main, FRG: Akademische Verlagsgesellschaft, 1960. 476 p. (Cited 180 times.)
3. **Hosemann R, Preisinger A & Vogel W.** Über den α-Fe-$FeAl_2O_4$-Mischkristall in aktivierten Ammoniakkatalysatoren (On the α-Fe-$FeAl_2O_4$-mixed crystal in activated ammoniac catalysis). *Ber. Bunsen. Ges. Phys. Chem.* 70:796-802. 1966. (Cited 40 times.)
4. **Hosemann R, Hentschel M, Lange A & Brückner R.** Dreidimensionale Analyse der Parakristallinen Struktur von Kieselglas (Three-dimensional analysis of the paracrystalline structure of flint glass). *Z. Kristallogr.* 169:13-33. 1984. (Cited 5 times.)
5. **Pfender M.** Parakristallforschung, eine neue Wissenschaft (Paracrystal research, a new science). *Umschau* 18:518. 1983.

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