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This Week's Citation Classic

Rachinger W A. A correction for the $\alpha_1\alpha_2$ doublet in the measurement of widths of X-ray diffraction lines. *J. Sci. Instrum.* **25**:254, 1948.
[Baillieu Laboratory, University of Melbourne, Australia]

An inherent difficulty in the measurement of the widths and profiles of Kα X-ray diffraction lines is their doublet structure. A simple graphical construction allows the separation of overlapping α_1 and α_2 components. [The *SCI*® indicates that this paper has been cited in over 240 publications since 1961, making it the 4th most-cited paper published in this journal.]

W.A. Rachinger
Department of Physics
Monash University
Clayton, Victoria
Australia

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"The year 1947 found me, a raw physics graduate, saturated with studies of atomic and nuclear physics, trying my luck in a new field as a master's candidate in a metallurgy department. My introduction to this world of furnaces, alloys, and phase diagrams was softened by my assignment to a supervisor, W.A. Wood, a physicist himself, sympathetic to the strange and sometimes inadequate ways of young physicists in this environment. His interest was in the mechanism of plastic deformation in metals. The power of the electron microscope had not yet been brought to bear on this problem; the tools of the trade were the light microscope and the X-ray diffraction camera.

"Dislocation tangles and walls were unheard of. Indeed, the word 'dislocation' was usually uttered with a touch of scepticism. Two views of the structure of a cold worked metal were current. One was that the crystal grains were broken down into smaller crystallites, the other that localised strains caused variations in interplanar spacing. X-ray diffraction was seen as the appropriate method to distinguish between these two models. Both would give rise to X-ray line-broadening; crystallite-broadening would be wavelength dependent but the strain-broadening would not.

"X-ray line profiles were measured manually, point-by-point, by comparing film blackening with an optical wedge, involving tedious microscope observation of a Lindemann electrometer—a long way from today's automation. The measurement of line widths was bedevilled by the doublet structure of the X-ray lines, the Kα_1, and its half-size companion, the Kα_2. With large broadening, the doublet components overlapped so that the width of a single component was not directly measurable.

"The methods available[1,2] for dealing with this problem assumed the isolated line profile to be described by particular algebraic functions, sometimes quite unrealistically. An afternoon's 'doodling' with thin and fat doublet pairs showed that profiles of any form could be separated by a simple graphical construction. Line widths could be calculated and quoted with considerable confidence. Interpretation of the results in terms of the specimen structure was far less certain—a situation which continues to the present day! Nevertheless, X-ray line-broadening studies have remained popular, either as a tool in the investigations of ultrastructure or as a necessary evil in situations where accurate line positions are required.[3]

"Although sophisticated algorithms[4] are now available which can be applied to an online computer-controlled diffractometer to produce patterns free of the Kα_2 component, use of the simple method described above continues.

"Why has the paper been cited so frequently? Certainly not because of deep physical significance or underlying sophistication but rather because it provides workers in many areas with a simple tool. In our increasingly complex laboratories many of us retain a yen for simple things. Although this method is readily adaptable to computer use, it requires in its simplest form only a sharp pencil, graph paper, and a good eye."

1. **Brill R.** Teilchengrössenbestimmungen mit Hilfe von Röntgenstrahlen. *Z. Kristallogr.* **68**:387-403, 1928.
2. **Jones F W.** The measurement of particle size by the X-ray method. *Proc. Roy. Soc. A* **166**:16-43, 1938.
3. **Gupta S K & Cullity B D.** Problems associated with K-α doublet in residual stress measurements. (Rhodes J R, Barrett C S, Leyden D E, Newkirk J B, Predecki P K & Ruud C O, eds.) *Advances in X-ray analysis.* New York: Plenum Press, 1980. Vol. 23. p. 333-9.
4. **Ladell J, Zagofsky A & Pearlman S.** Cu K-α_2 elimination algorithm. *J. Appl. Cryst.* **8**:499-506, 1975.