Nanoscience and the Scherrer equation versus the 'Scherrer–Gottingen equation'

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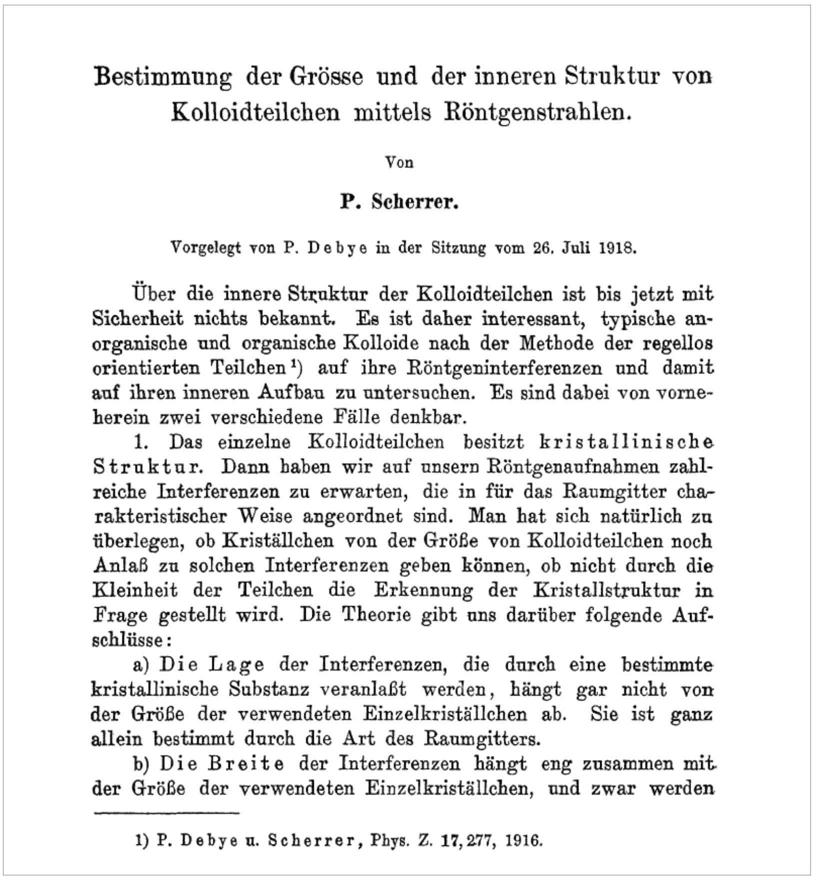
Interest in nanoscience and nanotechnology in South Africa is strong[1] and has received further momentum with the recent launch of the National Nanoscience Postgraduate Teaching and Training Programme. Nanotechnology is generally considered to be a relatively new field and so it may surprise some that the year 1912 has recently been proposed for the birth of modern nanotechnology, to coincide with the invention of the immersion ultramicroscope by Zsigmondy.[2] Although modern microscopes have atomic resolution, the average size of nanoparticles is routinely estimated from the width of X-ray diffraction pattern peaks using a simple equation first published by Scherrer in 1918.[3] In fact, the size of gold nanoparticles determined by Scherrer substantially confirmed the pioneering work of Zsigmondy.[4]

A recent note by Holzwarth and Gibson[5] gives some historical background and motivates why the equation should be associated with Scherrer alone, instead of incorrectly being referred to as the 'Debye–Scherrer equation'. They urge those working in the field to review the basic physics involved, to note the various factors that contribute to the broadening of X-ray diffraction peaks and to cite Scherrer's original paper where appropriate. Therefore it is of interest that a significant and growing number of recent articles attribute the original paper to two authors: P. Scherrer and N.G.W. Gottingen,[6–14] although it is clear from a digitised version of the original article (Figure 1)[15] that Scherrer is the only author. The original paper is in German and a clue to the identity of the enigmatic co-author N.G.W. Gottingen is obtained from the name of the journal, as printed on its title page: 'Nachrichten von der Königlichten Gesellschaft der Wissenschaften zu Göttingen. Mathematisch-physikalische Klasse aus der Jahre 1918'. Confusion regarding the abbreviated journal title has resulted in part of the title being misinterpreted as a second author.


Bestimmung der Grösse und der inneren Struktur von Kolloidteilchen mittels Röntgenstrahlen.

Von

P. Scherrer.

Vorgelegt von P. Debye in der Sitzung vom 26. Juli 1918.

Über die innere Struktur der Kolloidteilchen ist bis jetzt mit Sicherheit nichts bekannt. Es ist daher interessant, typische anorganische und organische Kolloide nach der Methode der regellos orientierten Teilchen 1) auf ihre Röntgeninterferenzen und damit auf ihren inneren Aufbau zu untersuchen. Es sind dabei von vorneherein zwei verschiedene Fälle denkbar.

1. Das einzelne Kolloidteilchen besitzt kristallinische Struktur. Dann haben wir auf unsern Röntgenaufnahmen zahlreiche Interferenzen zu erwarten, die in für das Raumgitter charakteristischer Weise angeordnet sind. Man hat sich natürlich zu überlegen, ob Kriställchen von der Größe von Kolloidteilchen noch Anlaß zu solchen Interferenzen geben können, ob nicht durch die Kleinheit der Teilchen die Erkennung der Kristallstruktur in Frage gestellt wird. Die Theorie gibt uns darüber folgende Aufschlüsse:

a) Die Lage der Interferenzen, die durch eine bestimmte kristallinische Substanz veranlaßt werden, hängt gar nicht von der Größe der verwendeten Einzelkriställchen ab. Sie ist ganz allein bestimmt durch die Art des Raumgitters.

b) Die Breite der Interferenzen hängt eng zusammen mit der Größe der verwendeten Einzelkriställchen, und zwar werden

1) P. Debye u. Scherrer, Phys. Z. **17**, 277, 1916.

Source: Center for Retrospective Digitization, Göttingen[15]; reproduced with the kind permission of the Göttingen State and University Library.

Figure 1: The first page of a digitised version of Scherrer's article, showing Scherrer as the only author.

Having clarified the issue of authorship, to cite correctly the original article one must still consider the most appropriate journal title abbreviation. For the years 1894–1922, during which the journal retained a consistent format, the Scholarly Societies Project website lists 97 variations of the journal's abbreviated name as cited in other journals.[16] Among the data one finds six variations used to cite this particular journal in *Science*, and the abbreviation recently used by Holzwarth and Gibson[7] is different to all of those listed. After deciding on the appropriate journal title abbreviation, one must determine the volume number, which is often given as either 2 or 26.

A volume number could not be found in the journal itself – only the year – which is how the volumes are described on the website from which the paper was downloaded.[15] A number of citations from articles published in the first half of the 20th century also do not give a volume number. Of particular interest is the citation[17] given in the influential Chemistry Abstracts journal *Chemisches Zentralblatt*: 'Nachr. K. Ges. Wiss. Göttingen 1918. 98–100. 26/9. 1918.' Here the volume number and the year are both given as 1918, together with the mysterious numbers 26/9 (from where it is speculated that the incorrect volume number 26 may have originated; possibly the 6 was later truncated to give the incorrect volume 2, as used by Holzwarth and Gibson[5]). The numbers 26/9 can be interpreted as a date (26 September). Consulting the original article, one finds that it was presented by P. Debye in a meeting on 26 July 1918 (Figure 1). This contribution by Debye in the history of the Scherrer equation was not mentioned by Holzwarth and Gibson[5]. The date translates to 26/7 instead of 26/9, but comparing other citations to the journal proves that the date was intended. Finally, although the page numbers are certainly 98–100, the incorrect starting page 96 is used in all but one of the papers cited here.[6-10,12–14]

It is clear that from the outset, Scherrer's paper was cited with errors and these errors were copied from paper to paper. This situation has culminated in the 'birth' of a fictitious co-author – N.G.W. Gottingen. Scientists should show the same attention to detail in reporting their sources as they do in reporting their results, and only cite papers that they have personally consulted. Tracing inaccurate references can be a time-consuming and frustrating, albeit interesting, task.

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