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A new set of charts for two-parameter lattices. By M. ČERNOHORSKÝ, *Czechoslovak Academy of Sciences, Laboratory for the Study of Metals, Brno, Leninova 82, Czechoslovakia*

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A new set of charts for two-parameter lattices has been prepared, the use of which is elucidated by the following example.

Suppose that we have the problem of determining the line distribution in the powder photograph of osmium

with $\text{Cu } K\alpha$ radiation. We first concentrate our attention on the wavelength used and the parameter a (Fig. 1). In the so-called transfer chart, on the wavelength scale we find the value corresponding to $\text{Cu } K\alpha$ radiation. On the corresponding vertical line lattice parameters a

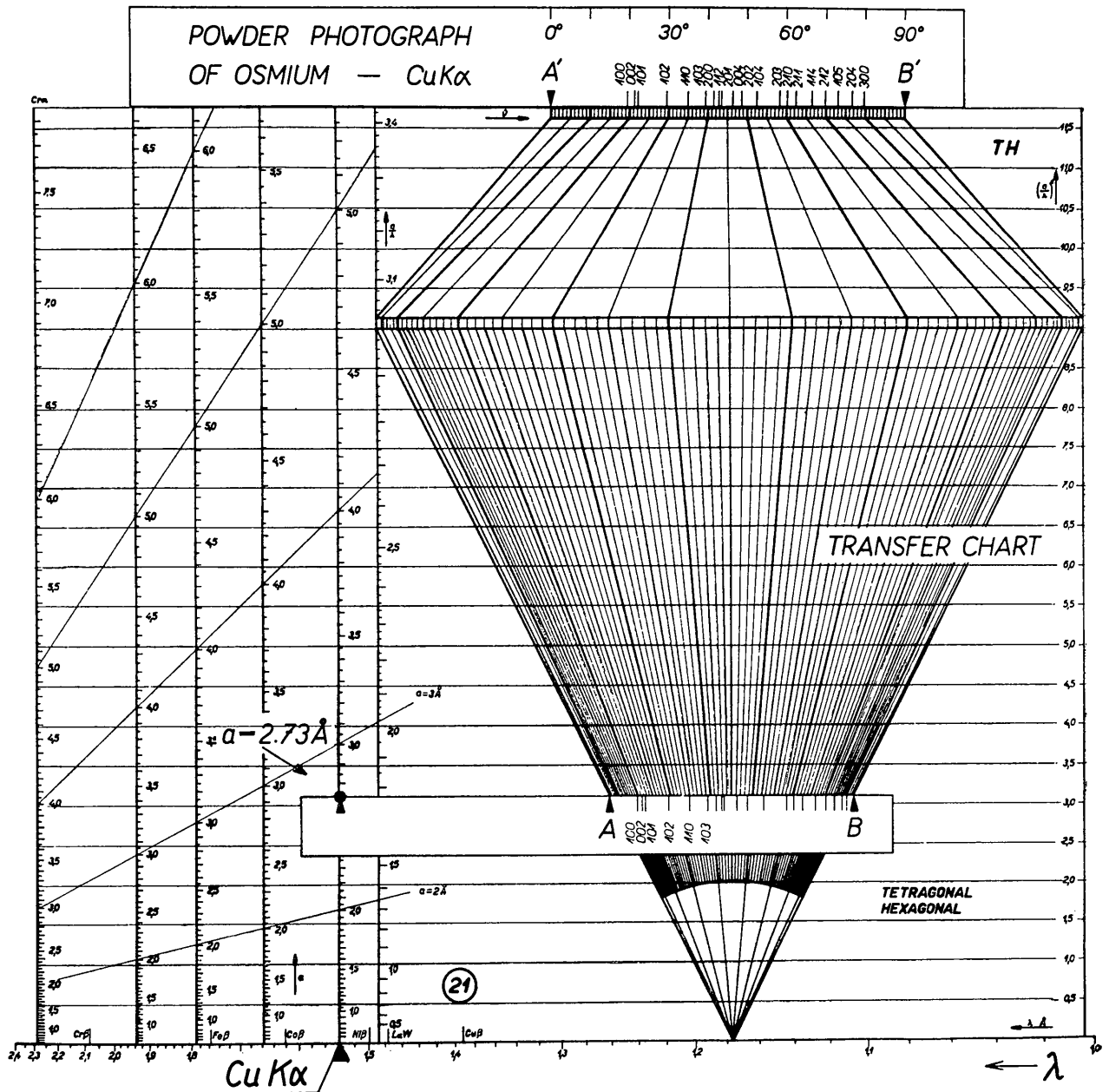


Fig. 1. Illustration of the use of a transfer chart to find the angular positions of lines in the powder photograph of osmium with $\text{Cu } K\alpha$ radiation.

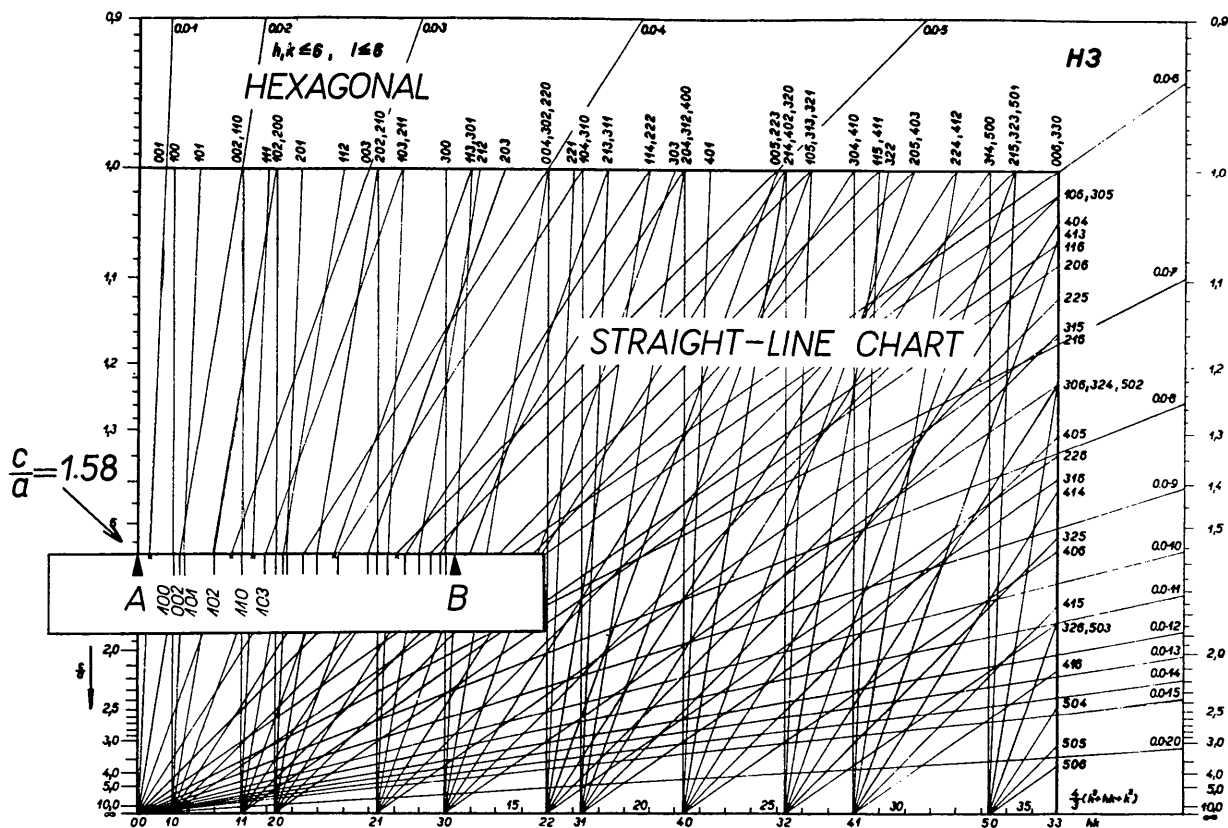


Fig. 2. The use of a straight-line chart to indicate the positions of the hkl reflexions in a powder photograph of osmium.

are plotted. We stop at the value for osmium, i.e. 2.73 \AA . The purpose of this step is to mark the position of the points A and B on a strip of paper. With this strip we pass to the straight-line chart for the respective type of lattice, in this case hexagonal (Fig. 2). The required position for our strip in this straight-line chart is given by the ratio c/a , which is plotted on the vertical axis. For osmium this ratio is 1.58. We can then mark out the points of intersection with the straight lines corresponding to the individual lines hkl . Having finished doing so, let us put our strip in its previous place on the transfer chart (Fig. 1) and transfer the marks with the aid of the auxiliary straight lines to the linear scale of Bragg angles $A'B'$. In this way we obtain the Bragg angle of each diffraction line. The new strip represents a complete scheme of the powder photograph of osmium when $\text{CuK}\alpha$ radiation is used.

It can be seen that the whole procedure of getting a complete diagram of the powder photograph when the lattice parameters and the wavelength are given is very quick. In applying the charts for lattices of other parameters no difficulties can arise, as the charts can be easily extended if necessary. For the simplicity of their construction these features are decisive:

(1) The scale of parameters a is linear in a^2 .

(2) The scale of ratios c/a is linear in $(a/c)^2$.

(3) The slope of the straight line hkl is determined by l only, its point of intersection with the x -axis is given by hk only.

In contrast with the synthesis of powder photographs, the interpretation of powder photographs presents certain difficulties. They consist in our ignorance of the level at which the lines of the powder photograph are to be placed in Fig. 2. In other words it is desirable to know the parameter a , thus making all further steps very easy. For determining the parameter a we use analytical charts in which curves for the diffraction lines of the $hk0$ type only are plotted (Fig. 3). The match of some lines in the powder photograph with these curves enables us to determine the parameter a . Sometimes it is easy to determine the parameter c , too, directly in the analytical chart. Nevertheless, it is best to determine the parameter c in every case with the aid of the straight-line chart.

The detailed description of the charts is given in a publication (Čermohorský, M., Charts for Two-parameter Lattices, Publishing House of the Czechoslovak Academy of Sciences, Prague, 1961, price 12 Kčs) in which a complete set of large-scale charts for cubic, tetragonal and hexagonal lattices is included.

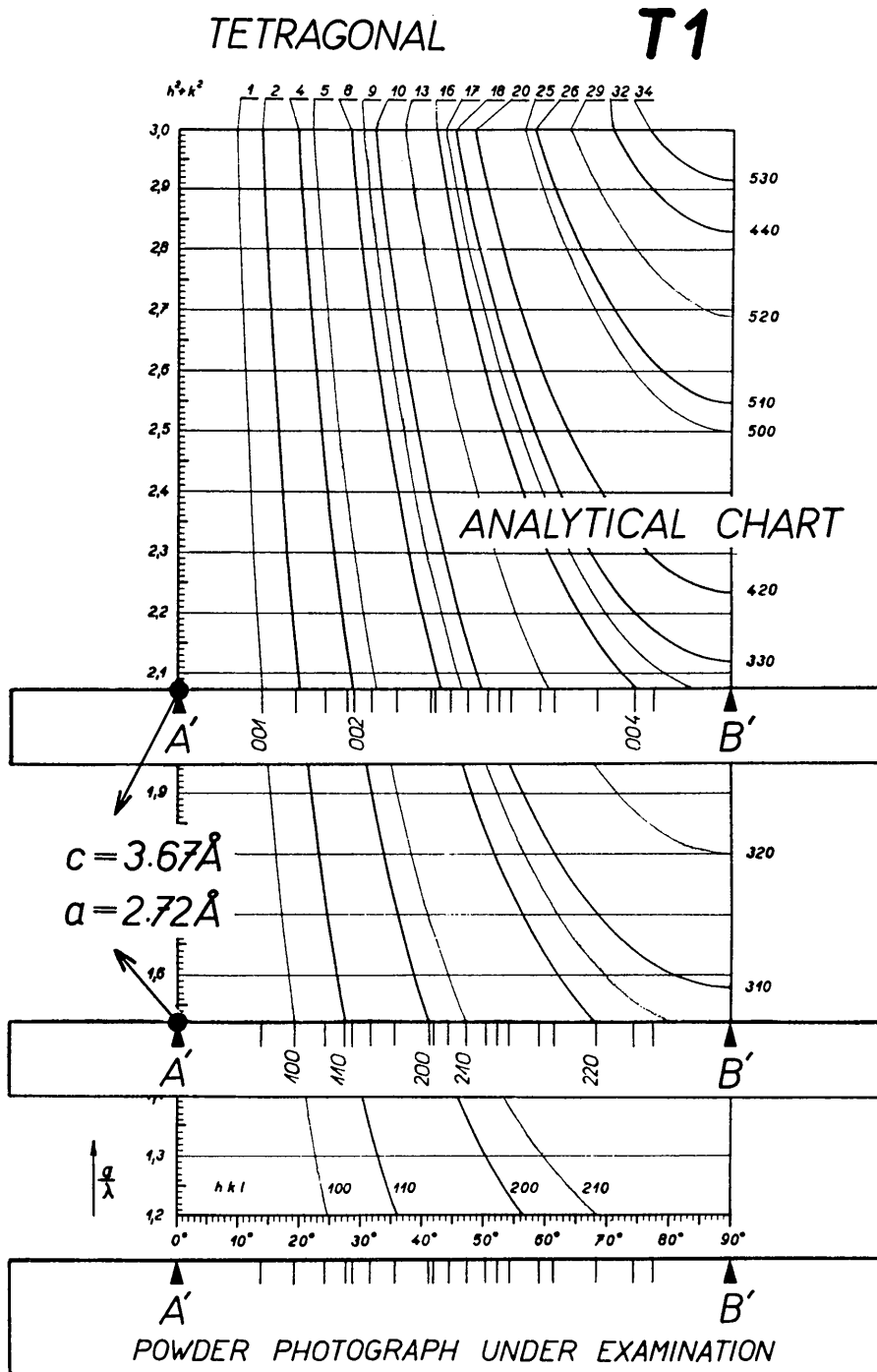


Fig. 3. The use of an analytical chart to find lattice parameters.