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# EXTRATERRESTRIAL APPLICATION OF X-RAY DIFFRACTION

By H. K. HERGLOTZ

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# EXTRATERRESTRIAL APPLICATION OF X-RAY DIFFRACTION

By

H. K. Herglotz

(Presented at Space Science Seminar,
George C. Marshall Space Flight Center,
Huntsville, Alabama, February 23, 1966)

## ABSTRACT

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X-ray diffraction provides information about elemental composition and can identify many compounds and minerals. It is, therefore, a promising candidate for the exploration of surfaces of the moon and earth-like planets if apparatus meeting the requirements of this extraterrestrial application can be developed.

The fundamentals of X-ray diffraction are described and the difficulties connected with their space application are discussed. Hardware, either specifically designed for space exploration or adaptable for this purpose, are reviewed.

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# EXTRATERRESTRIAL APPLICATION OF X-RAY DIFFRACTION

By

H. K. Herglotz *

* E. I. du Pont de Nemours & Co.

SCIENTIFIC PAYLOADS OFFICE
RESEARCH PROJECTS LABORATORY
RESEARCH AND DEVELOPMENT OPERATIONS

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# BIOGRAPHICAL NOTE

Dr. H. K. Herglotz is Research Associate, Engineering Physics Laboratory, E. I. du Pont de Nemours & Co., Wilmington, Delaware. He was graduated with a Masters Degree in Chemical Engineering, Technical University, Prague, Czechoslovakia, 1944. He received his Ph. D. in Physical Chemistry, Mining Academy of Freiberg, Saxonia, 1948. The Technical University, Vienna, Austria, conferred the Dozent-Degree in X-Ray Physics in 1955 and the title Extraordinary Professor in 1962.

While pursuing graduate and post-graduate work, he was an Instructor at the University of Prague and the Mining Academy, and Assistant Professor at the Technical University of Vienna. He was associated with E. I. du Pont de Nemours & Co. as a Physicist in the Pigments Department, 1956 - 59. In 1959 he returned to Austria as Head of Physics Research, Austrian Nitrogen Works, where he remained until 1961.

Dr. Herglotz returned to E. I. du Pont and his present position in 1961. He is the author of more than twenty publications and a member of both the American Physical Society and the Austrian Physical Society.

FIGURE 1. THE FIRST PUBLIC X-RAY DIAGNOSTIC PICTURE (1896)

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# EXTRATERRESTRIAL APPLICATION OF X-RAY DIFFRACTION

## SUMMARY

X-ray diffraction provides information about elemental composition and can identify many compounds and minerals. It is, therefore, a promising candidate for the exploration of surfaces of the moon and earth-like planets if apparatus meeting the requirements of this extraterrestrial application can be developed.

## INTRODUCTION

When people of different backgrounds and different interests hear about X rays, different things invariably come to their minds. Laymen almost automatically think of diagnostic applications in medicine. This, of course, was one of the first and most important applications of X rays, and it still leaves people most impressed.

Figure 1 shows the first public X-ray diagnostic picture; it was taken during the session of the Medico-Physical Society of Würzburg in 1896, in which Professor Röntgen published his new invention. The picture shows the hand of Dr. Kölliker, who was presiding at the session.

Engineers invariably think of the radiographic applications. And Professor Röntgen was also the initiator of radiography. One of the first things he did, being an enthusiastic hunter, was to take a shadowgraph of his shotgun. Figure 2 is the historical picture of the first nondestructive materials testing, which I am sure is applied around the Marshall Space Flight Center quite frequently.

No matter how important these two facets of X ray are, and how much they might occupy the minds of people, from the scientific standpoint information extracted from these two applications is minor in comparison to a third facet, X-ray diffraction. X-ray diffraction gives information about the regular arrangement of atoms, building blocks, molecules, in solid matter. And this is evidenced by the fact that one Nobel prize was issued for the method itself,

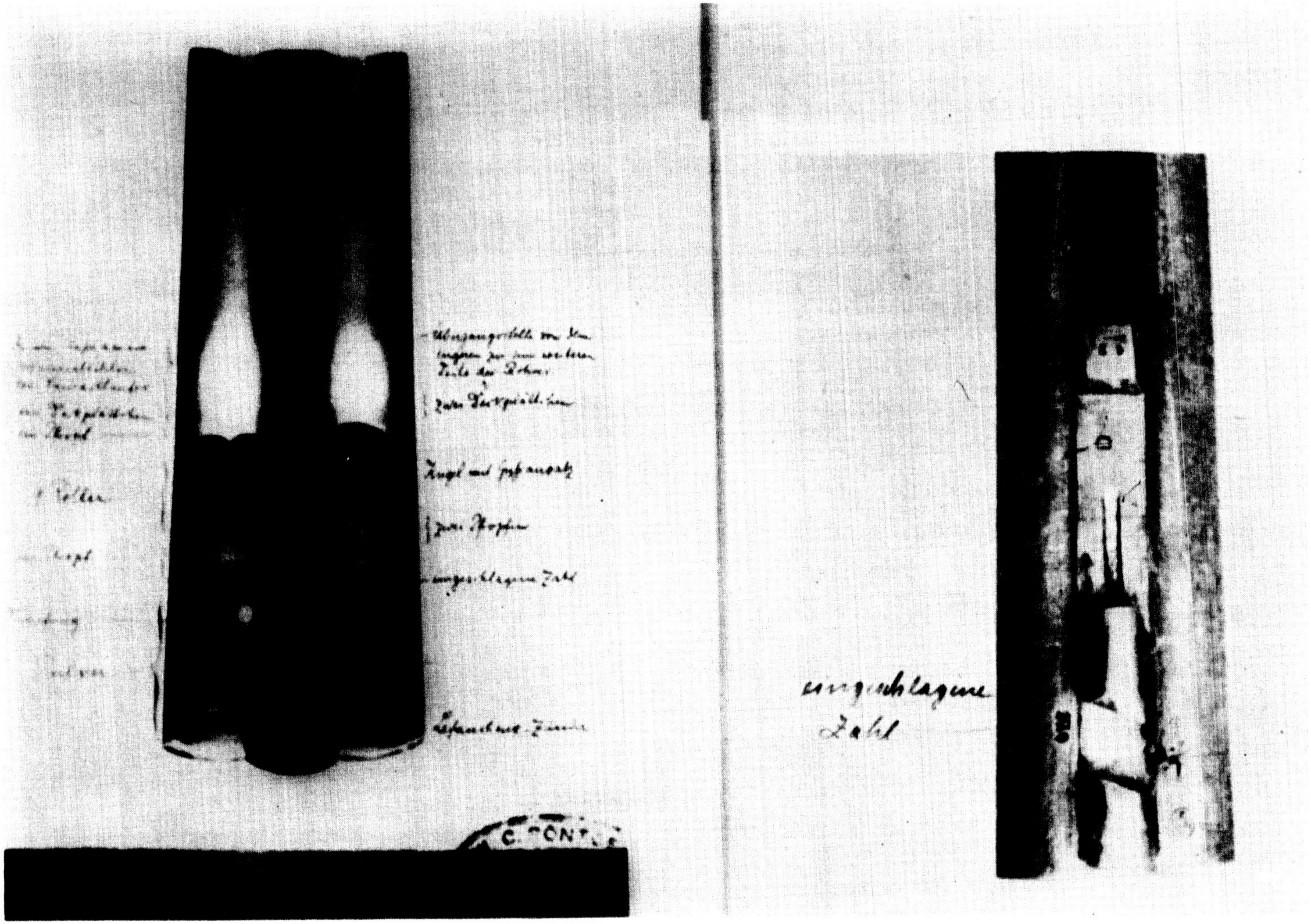


FIGURE 2. THE FIRST NONDESTRUCTIVE MATERIALS TESTING (1896)

to Max von Laue, and shortly after that a Nobel prize was awarded to the two Braggs, and since then for many many tasks that have been performed. Not only the method drew Nobel prizes, but things that were performed by the method and problems that have been solved by the method. Two Nobel prizes were awarded in only the past few years for methods of structural determination.

## ESSENTIALS OF X-RAY DIFFRACTION

To get a little order into the multiplicity of X-ray physics, Figure 3 shows all of X-ray physics; of course it includes materials testing, medicine diagnosis, therapy, and radiography. But today I will deal exclusively with the right-hand side of the picture, the determination of the crystal structure. You might ask what that has to do with extraterrestrial applications. It has a lot to do with them, I think, because the structures of materials, of minerals, and of compounds can be identified by their crystal structure alone. Secondly, the elemental analysis is even more important and applicable, and I will discuss this later.

Now in Figure 4 we have Bragg's equation, which is the most efficient way of plotting all that X-ray diffraction can do in a nutshell. Shown in the figure is the regular arrangement of atoms in a crystal lattice in solid matter. An X-ray wave, represented here by its normal trajectories, impinges on the regular arrangement. Planes are drawn through there. Although these planes do not exist in reality, they are just imaginary, this is a very efficient way to make X-ray diffraction understandable. It connects it with something that is very well known, such as reflection of a mirror; although it has nothing really, or very little, to do with it. A $\lambda$, an X-ray wavelength, a definite wavelength, is reflected by a solid, like a mirror, only at certain angles. And many times these angles are complicated structures; hundreds and thousands of them are representative, both regarding the angle as well as regarding their intensity, for this regular arrangement.

Plotting this equation, $n\lambda = 2d \sin \theta$, d is the distance between two such imaginary planes. The d is, according to the geometry, representative for the arrangement and the intensities representative for the type of atoms that sit on these planes. So with this equation we see that we have three variables. The $\theta$, which we can always measure, is the angle at which the crystal reflects. The intensity is not represented, but the $\theta$ is easily measurable. That's something physicists always like to measure, a length, an angle; and they practically reduce everything to these two measurements.

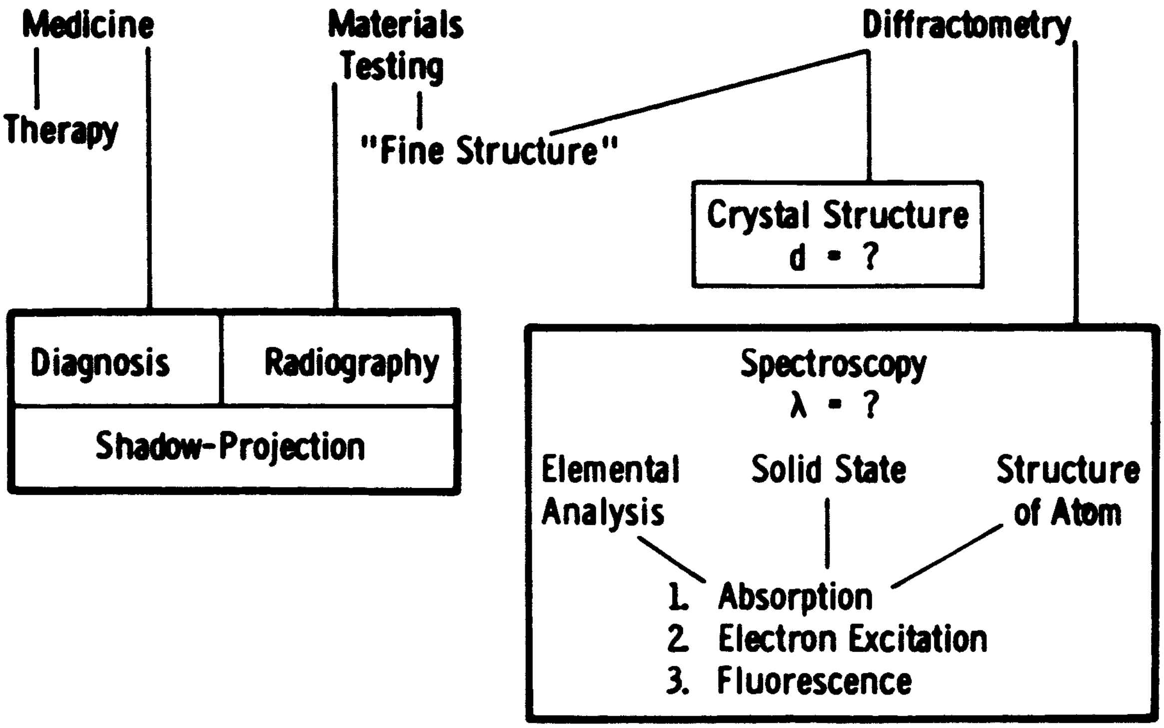
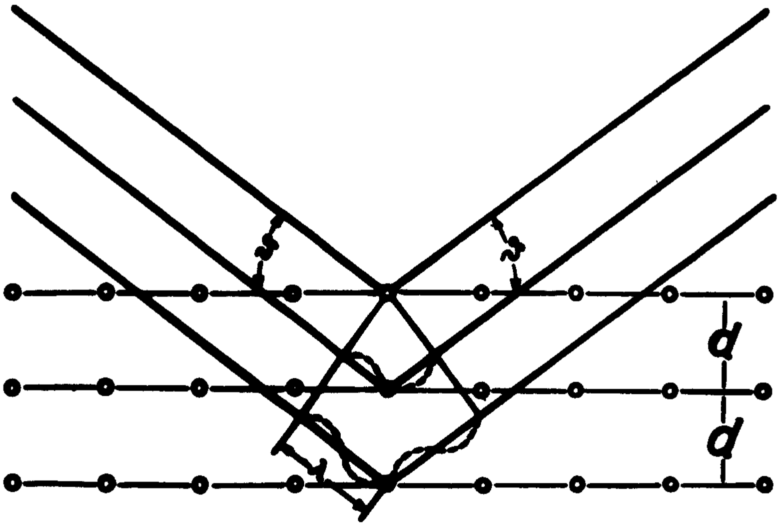


FIGURE 3. X-RAY PHYSICS



$$n\lambda = 2d \sin \vartheta$$

FIGURE 4. THE BRAGG'S EQUATION

If we have λ, a wavelength which is well known, we have a way of finding out the d. And if we have the d, the dimensions, as sometimes in multifine crystal, which we know already, then we have a way of seeing what kind of λ we have.

Both of these tasks are equally important and widely applied. The λ here is representative if it comes from the source. Were the picture larger, I could have brought it a little more down to essentials; we would have depicted the source from which X rays come, which would be a long way out. This source is excited by some means, either X rays themselves or by electron bombardment excited to issue X rays, X rays which are characteristic of the material or the elements in that source. Thus, that λ monochromatic is characteristic for the element from which it comes; we have a way of elemental analysis if we have a crystal that is known. This is one way of applying it, X-ray spectroscopy.

The other way is that we can find out the regular arrangement in solid matter. We use a λ that is well known, for example from a copper standard. We know which wavelength we have and we determine, by measuring angles, many of these d's by simple geometry (that is, straightforward methods that can be very lengthy and today of course done by computers).

These two applications are widely used, all of the analytical chemists, of course, use these tests. There exists no analytical laboratory, I think, without some X-ray spectroscopy for analytical examination of the elements in solid matter. The chemists, the minerologists, the biologists, look for the regular arrangement. And, as I said before, they have had tremendous success demonstrated by the number of Nobel prizes awarded in these fields.

And there are the metallurgists, the polymer chemists, who look again for something else. They look for the arrangement of small regions of various degrees of order and this arrangement in solid matter. They call these regions differently crystallites, or platelets, or lamella, the arrangement of small crystalline particles within the solid.

These two capabilities, elemental analysis and identification of compounds by way of their crystalline structure, going back to the same equation but in a different way, make these methods very eligible for exploration of the moon and earth-like planets. If one can find ways of getting the equipment up there, getting it so simple, so rugged, so resistant to abuse that it survives the tremendous acceleration forces and the impact, and reliable enough that it can work without anybody around, elemental analysis of an extraterrestrial body by X-ray spectroscopy is very attractive.

To make this clear, two spectra are shown in Figure 5. One is an X-ray spectrum of chromium, which I made myself years ago, and you see its utmost simplicity. The other is an optical spectrum of aluminum, only a part of it, a small wavelength range. You see the tremendous complexity in comparison. An element is always easily identified if one can get this X-ray spectrum. The correlation between the wavelength of the characteristic X rays and the atomic number is very simple, so it is practically no problem to identify the element after one has the spectrum.

This correlation was found by Moseley [1] in 1915-16 (Fig. 6), and experiments were done by the two Braggs, W. H. and W. L. Bragg, around the same time, during World War I. Looking at this spectrum one would have thought that the ideal analytical tool had been found. But one didn't hear or see anything about X-ray spectroscopy in analytical laboratories, or in perhaps very few where very selective physicists were working. It did not become a generally accepted tool of analytical chemistry. It was only in the 1950s that the breakthrough came, and the breakthrough came only because of simplification, and X-ray spectroscopy became a tool as soon as the laboratory assistants could switch the equipment on and off and work it as any other device.

Figure 7 is a scheme of an apparatus which does chemical analysis by a so-called fluorescent X-ray spectroscopy, where the X rays in the specimen are excited by more energetic X rays from an X-ray tube. (This can be done by electrons, too, in certain cases, and some of the instruments that will be used in the Surveyor and Voyager programs will work with electron excitation.) The characteristic X rays excited in this specimen are analyzed by an analyzing crystal whose atomic dimensions are well known. Then after they have been dispersed, they are registered, selected according to their wavelength, and caught in a detector that is connected to a recorder. We have an analyzing crystal with dimensions in the order of magnitude of one angstrom unit ($10^{-8}$ centimeters). The wavelength is in the order of magnitude of one angstrom, too. In extraterrestrial applications we have the detector close to the amplifier, and, instead of the little wire that is shown so schematically in the figure, we have a transmission line, which is in the order of magnitude of again one AU (not angstrom unit but astronomical unit, which, instead of $10^{-8}$ centimeters, is $10^{13}$ centimeters). Transmission over such distances has been shown in the pictures returned from Mars. These long transmission lines can be handled, and the recorder can be on earth. The unscrambling of the results can be done on earth leisurely. But whether it can be done outside our own planet needs to be shown.

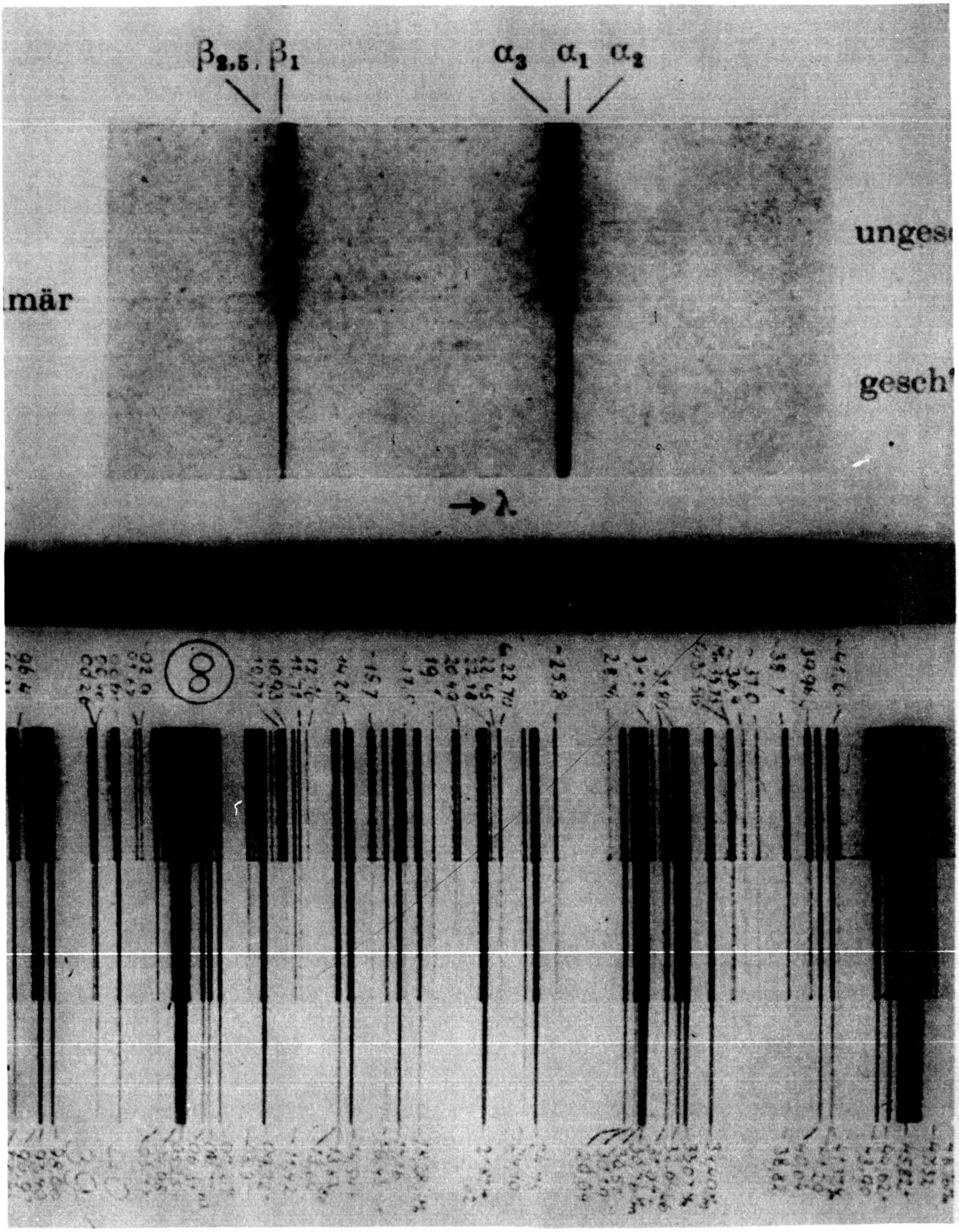


FIGURE 5. THE X-RAY SPECTRUM COMPARED WITH AN OPTICAL SPECTRUM

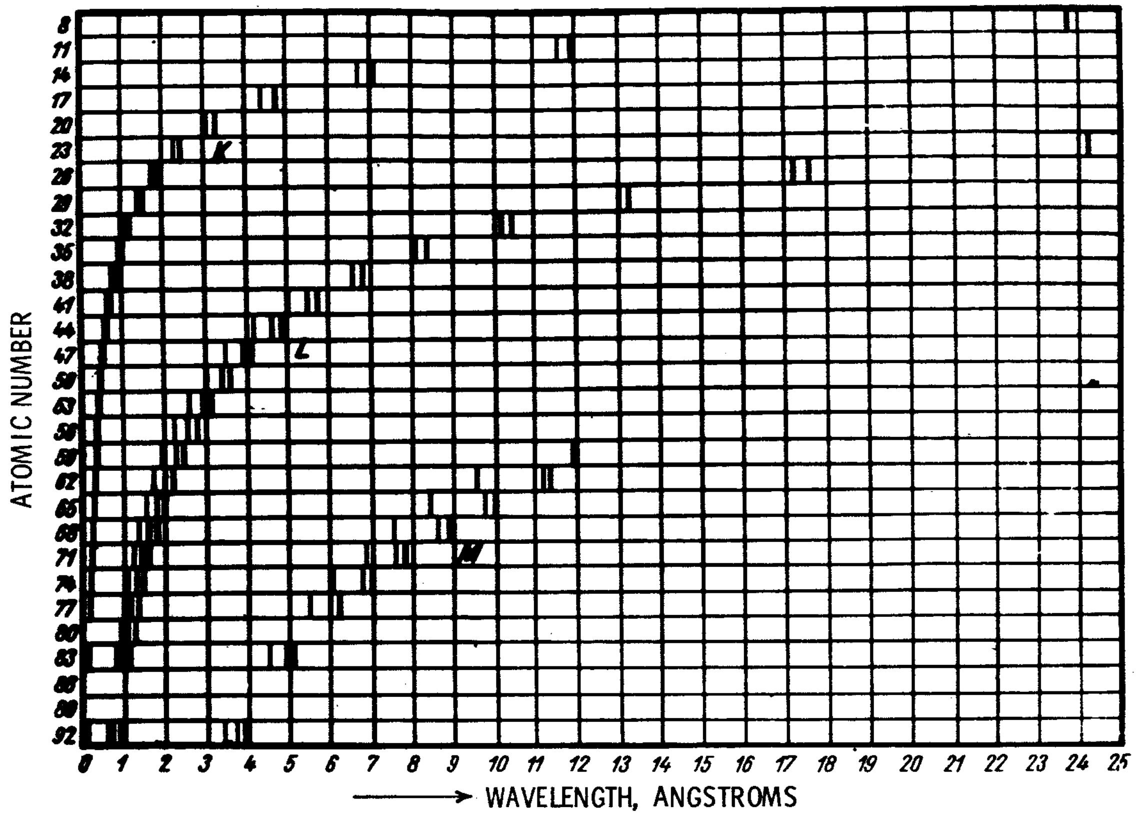


FIGURE 6. MOSELEY'S CORRELATION BETWEEN WAVELENGTH AND ATOMIC NUMBER

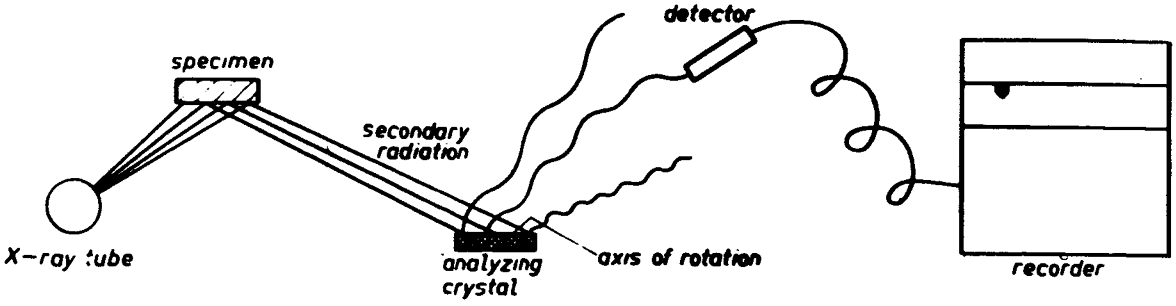


FIGURE 7. OPTICAL ARRANGEMENT OF A MODERN X-RAY SPECTROGRAPH

## EQUIPMENT

The method, as I have said, was known since 1915, and became practical on earth in the 1950s. The difference was the simplicity of the equipment. Another step of simplicity and ruggedness is needed, however, to get the method ready for extraterrestrial applications.

And what are the important things now? A little has changed in the X-ray tubes since Bragg and Moseley. Instead of a gas-filled tube, which is hard to operate, we have very nice X-ray tubes now which can be compact and reliable and current. The voltage can be controlled separately; in the old gas tubes this was impossible. Thus, they have become a lot easier to operate. The analyzing crystals practically haven't changed. They are a little more perfect, easier to get, and we can manufacture them. They would have been ready for space applications in 1950.

It is the detector that has undergone such a development, in sensitivity, simplicity, ruggedness, and reliability, that today one can dare to say that we will lift equipment to the moon and to the earth-like planets a little later. Figure 8 shows the old detector that Bragg used in his experiments; it was an ion chamber. If one looks at it from the standpoint of the picture, the development seems to be very slight. But in reality it was a large, large step, because one of the modern counters still looks very much the same. It is a tube with windows through which the X rays can enter; it is filled by gas; and pictured are an electrode which is on high voltage and one that is connected, in this case, to an electrometer. The X rays entering and being absorbed form ion pairs. This is an amazing thing; no matter what wavelength and no matter what energies these X rays have, 32 electron-volts are necessary to generate one ion pair. In this strong electric field the ion pairs are collected, and they are a measure of the intensity of the X rays.

An electrometer, of course, is a terrible instrument, and I would dare to say that one doesn't use an old electrometer in NASA anymore because it is unreliable. Today we have amplifiers that can amplify very small signals and can get them way above background so that they are ready for this long communication line. But, more important, they are run a little differently, with a higher voltage, so that we get some gas amplification. This is practically what the modern proportional counter is. The voltage is just large enough that each of these ion pairs gets accelerated enough so that it hits other molecules and forms new ion pairs. And here is another amazing thing; over a wide wavelength range there is a constant amplification factor so that the signal is still proportional to the energy of the X-ray quanta and is correctly amplified in the gas.

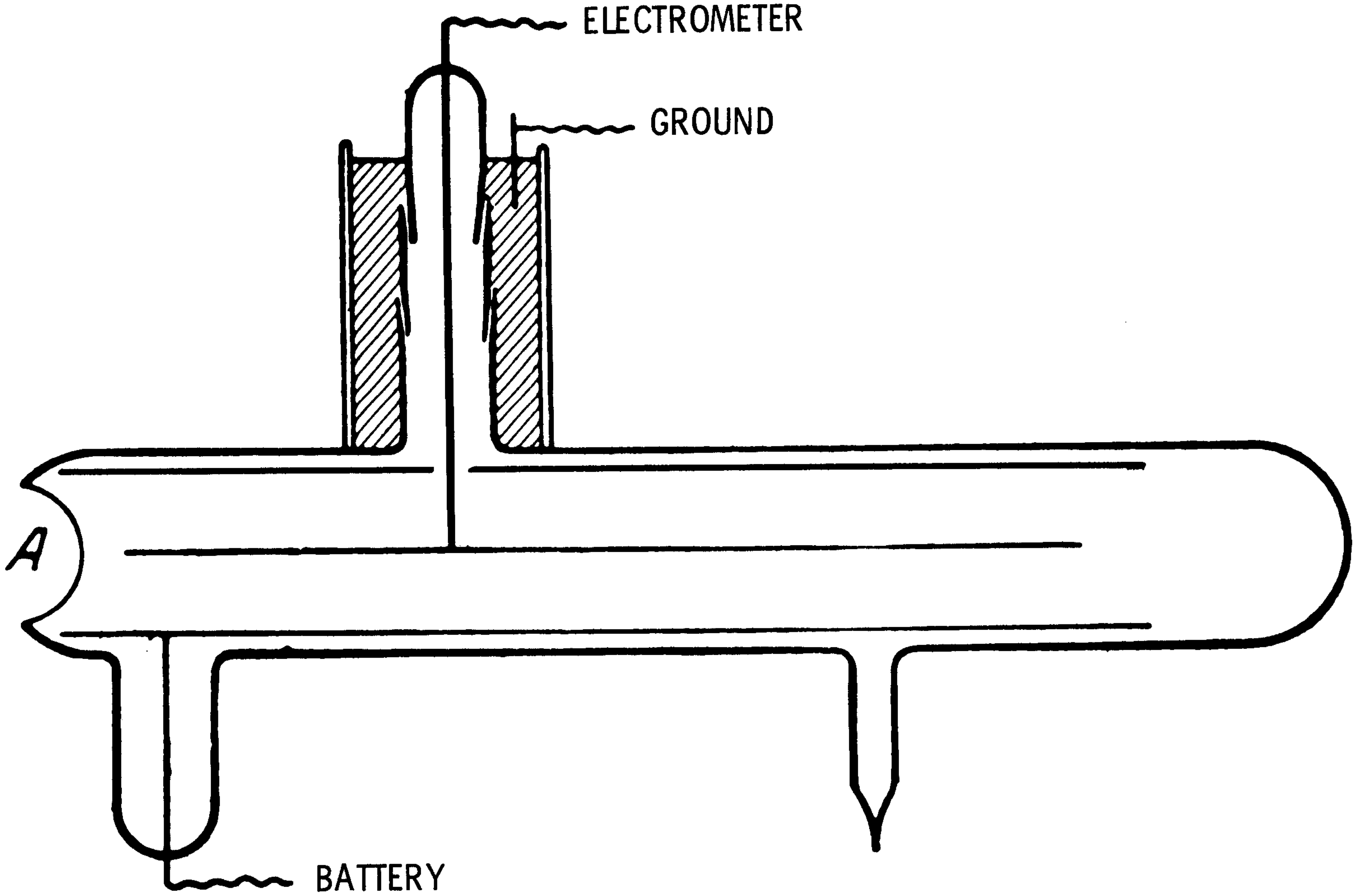


FIGURE 8. BRAGG'S ION CHAMBER

This is a good proportional counter that has tremendous advantages. One of the major advantages, of course, is that one can use pulse-height discrimination, that one can say that so many particles were in this energy range and so many particles were in that energy range. This is even capable, in some cases, of replacing a dispersion device, to replace the crystal, so that one just measures the energy of the quanta entering the proportional counter and gets an idea about the wavelength distribution. Of course this is very crude in comparison to a crystal, but you will see in later applications that we have some non-dispersive devices in some experiments in the Surveyor and Voyager programs.

Now there is a third type of detector, the Geiger-Müller counter. If we make the voltage high enough and if we get the gas discharge breakdown, the signal becomes very large and it is easy to amplify. However, it is no longer proportional to the original energy of the quanta. At the same time the dead time becomes very long since it is a real gas discharge which has to be extinguished first before the next particle can be counted or the next quantum can be counted. Geiger-Müller counters have the advantage that they need very little amplification, that the emitted signal is large, but they have tremendous disadvantages.

There are scintillation counters too. The scintillation counter is shown schematically in Figure 9. Usually a sodium-iodide crystal activates thallium, absorbs the X-ray quantum, and transforms it into a flash of visible light. The visible light penetrates a photoelectron multiplier, which amplifies the signal considerably. I haven't found any real suggestions to use this in extraterrestrial applications; the reason is probably that they are rather delicate, and these dynodes, these single electrodes, have to be kept at a very accurate potential. I mention this only because on earth it is a very common detector.

The next figure shows another detector which is becoming more and more important and will be used widely (Fig. 10). No real suggestions have been made for extraterrestrial applications, but it will be only a matter of time. It is a solid-state detector which practically works the same way as a gas amplifier, that is as a proportional or Geiger-Müller counter. The doped germanium crystal contains a p-n junction and a large lithium compensated region, which is the equivalent of a neutral gas. It is used mostly for real fast particles. It has some great advantages because the absorption of this germanium is so high that it can stop particles of very high energy. The particle it has stopped generates not ion pairs in this case but carrier pairs, and the energy is only about 3 electron-volts for one pair. It acts in the same way as a gas discharge tube. As I said they are more advantageous for heavy particles and for the softer X rays, the X rays of low penetrating power.

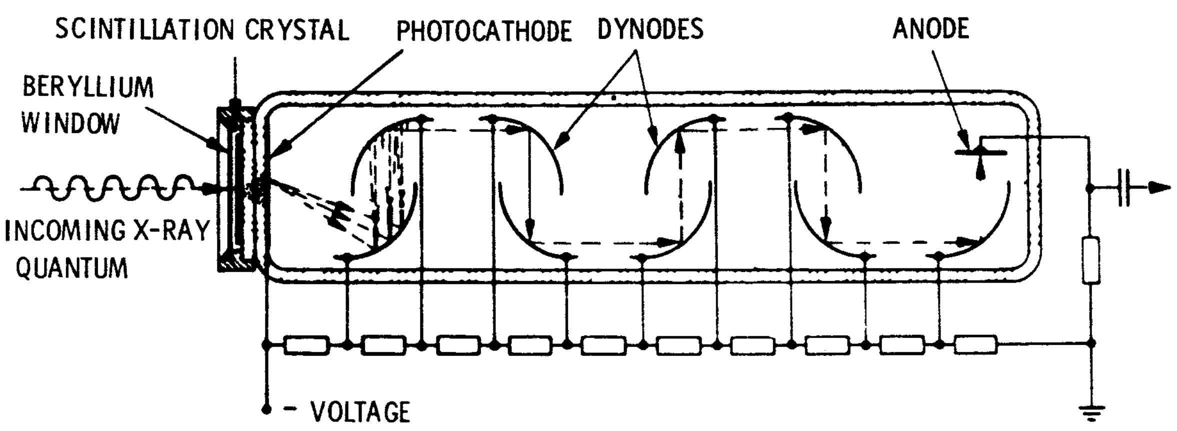


FIGURE 9. SCHEMATIC OF A SCINTILLATION COUNTER

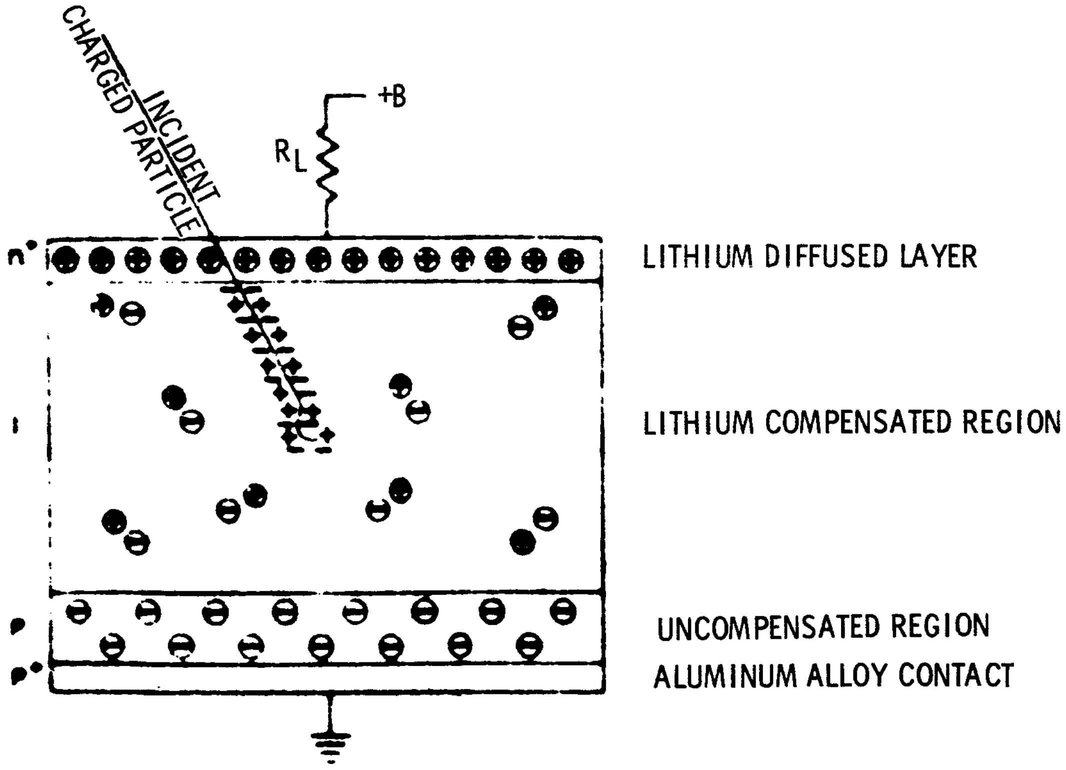


FIGURE 10. SOLID-STATE DETECTOR

The need to condense X-ray equipment before it can go to the moon and planets or into rugged field applications on earth becomes obvious if we look at Figure 11, which shows beautiful and highly developed apparatus for the laboratory.

## PROPOSALS FOR EXTRATERRESTRIAL APPLICATION

Now, I would like to discuss some definite proposals for space exploration. You might ask: why is somebody from industry so interested in extraterrestrial applications? It is not only because I am an amateur astronomer; there is another reason. The necessities for ruggedness and reliability coincide with some of our requirements in industry. The measuring devices we get into plant locations have to work in this rugged environment or they are out. So we pull on the same string, except for one item: our devices have to be cheap. If they are not cheap, we never get them into the plant. If something is very expensive it needs approval from very high levels, and before it gets there usually the problem is not of interest any more. One of our noblest goals is to get our devices cheap and to have the decision and approval made on the lower echelon where there is interest in the result. This, of course, is not so important in space applications. If an X-ray diffraction instrument can be made small enough and rugged enough that it can survive the space environment it wouldn't matter if it costs several thousand dollars more. Figure 12 shows the transportation costs to get payloads outside the earth. In the year of 1966, at the low firing rate, the cost is still about three thousand dollars per kilogram to lift something to a 500-km or 350-mi orbit. Of course it costs a little more to kick it off to get at the escape velocity, but I feel that the difference there will not be significant. Any one of the devices which I will show you later weighs several kilograms; so the transportation costs are still far higher than the cost of some additional components. Here is where the industry and the space people differ in their goal.

### Elemental Analysis

Figure 13 is the X-rays spectrometer scheduled for one of the first Surveyors. It is just my guess, but I feel that pretty soon the astronauts will be capable of bringing back a few rocks in their pockets and we can analyze them on earth instead of sending a complicated X-ray analytical tool up to the moon. I am sure, however, that it will be quite a while before a man could get to Mars to do the job so this will be most useful in the Voyager program. It will need

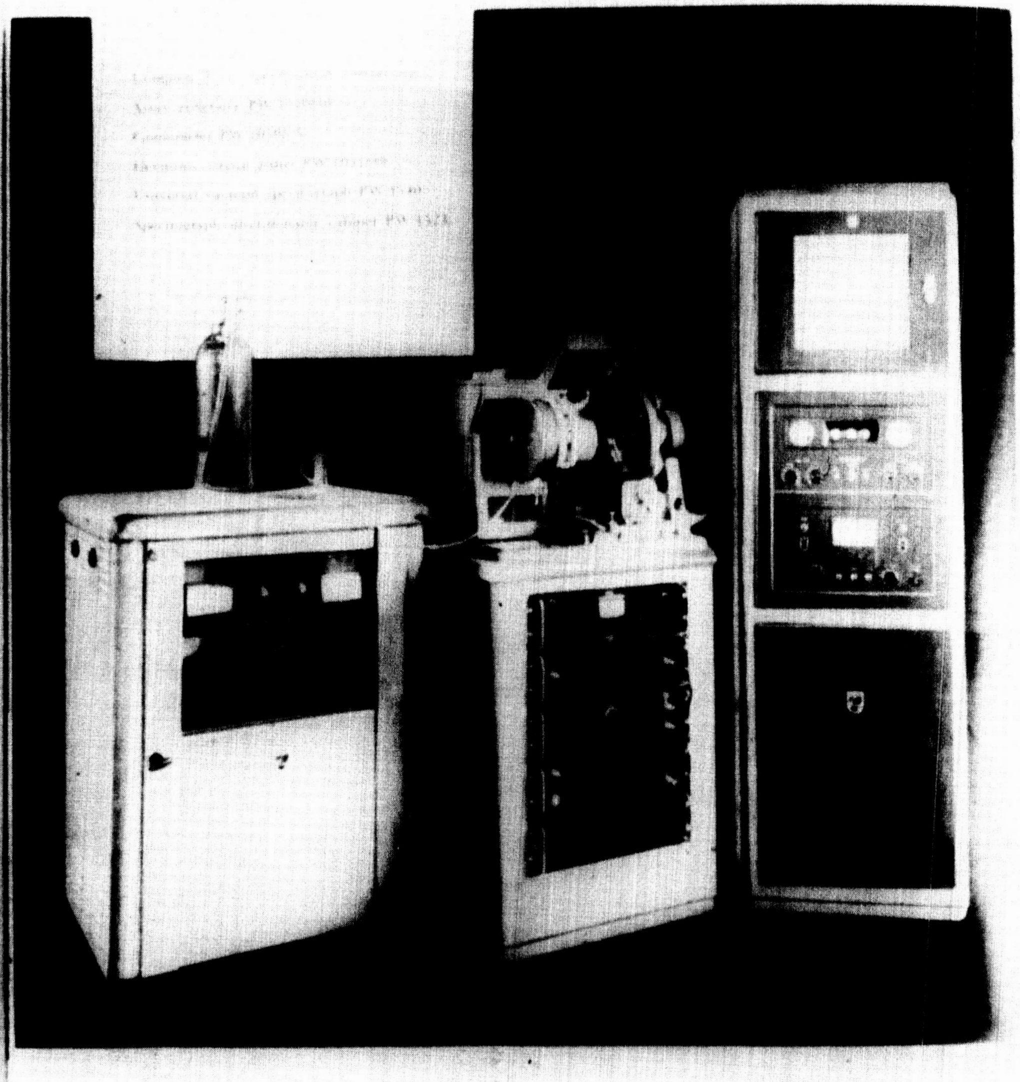


FIGURE 11. LABORATORY APPARATUS

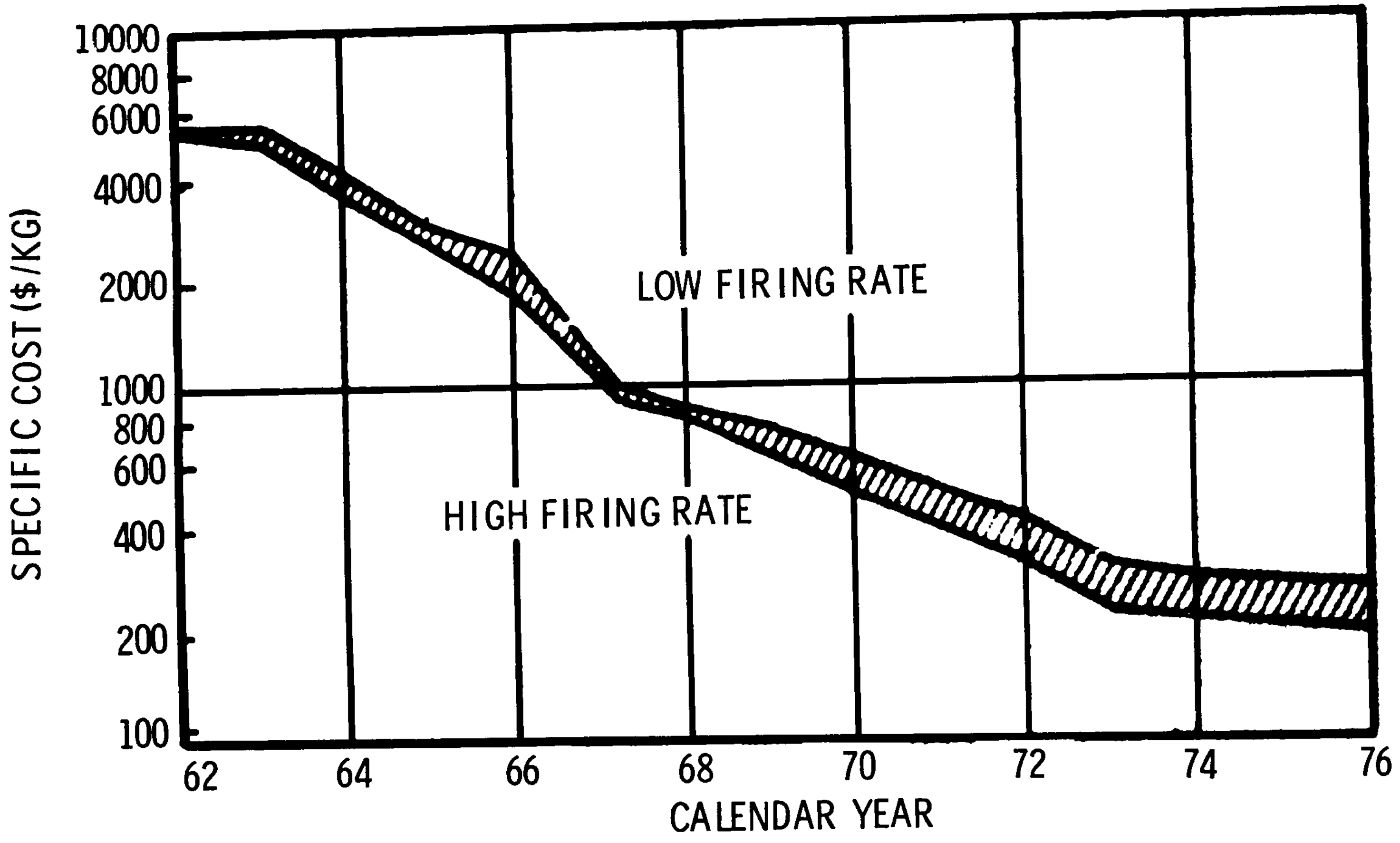


FIGURE 12. TRANSPORTATION-COST TRENDS FOR PAYLOADS IN 500-KM EARTH-SATELLITE ORBITS

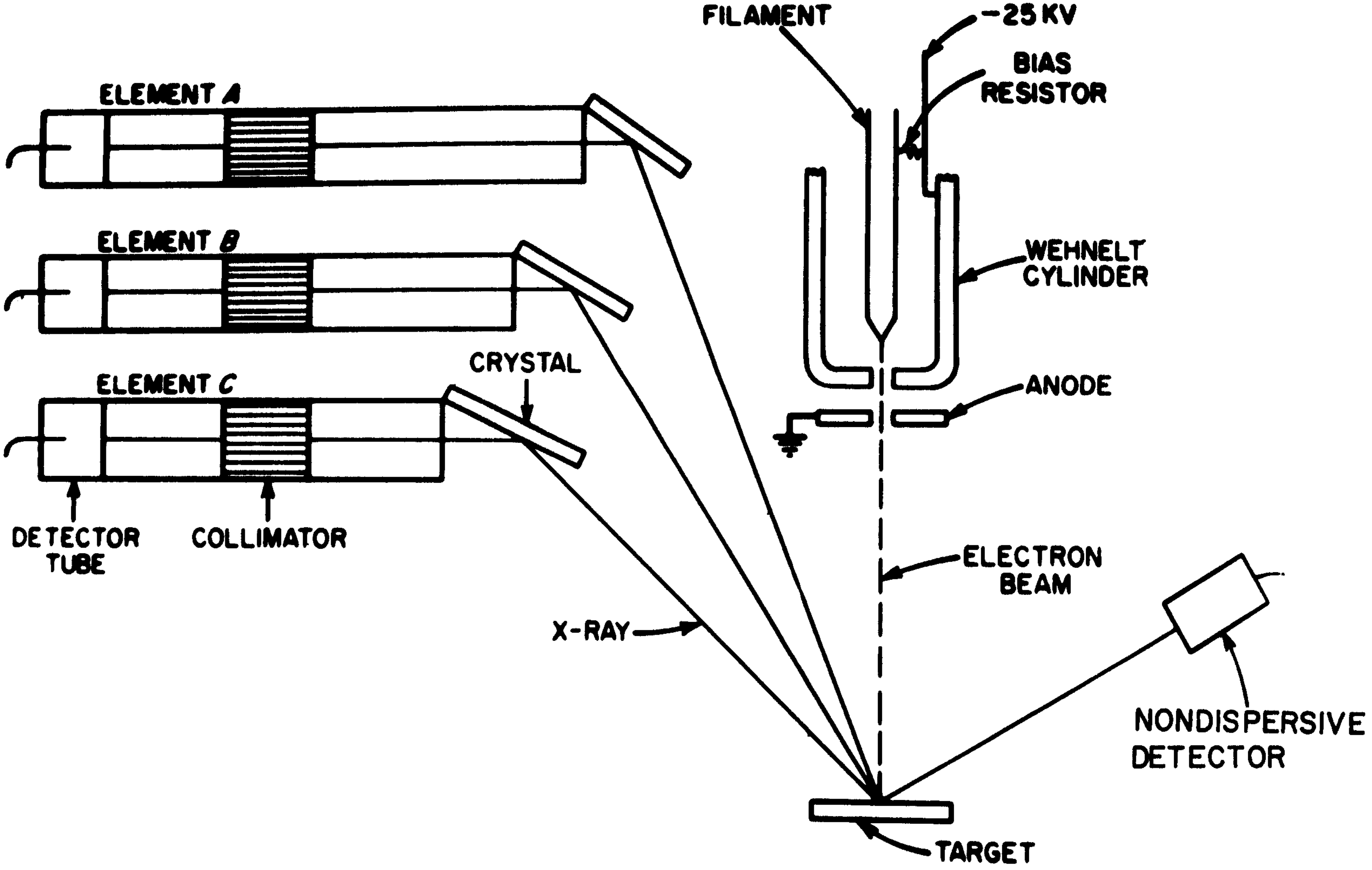


FIGURE 13. SCHEMATIC DRAWING OF THE SURVEYOR X-RAY SPECTROMETER

some alterations, some changes, some improvements. This Surveyor spectrometer works with the lunar vacuum. Please remember that this is an analytical tool; we want to know about the λ's characteristic of the elements on the lunar surface. Thus, we have to rotate the crystal to run through all angles, and, according to the angle, we would know which λ it was and which element it was that emitted the λ. Instead of using the rotating mechanism of the crystal, they decided that it is simpler, easier, and more reliable to use 13 different crystals set at the proper angle and 13 Geiger-Müller tubes made very small. It doesn't need any pulse-height discrimination because the crystal selects the proper wavelength anyway, and it can be made very reliable and with a very large amplification factor.

The X-ray gun emits electrons. This is one of the cases where one uses electrons directly, and the target can be either the moon's surface itself or a sample that has been collected and brought to a window. (Actually, the sample preparation is almost more of a headache than the analysis of the sample.) Electrons are accelerated by a field of 25 kilovolts. They hit the sample, and the sample emits its characteristic X rays. The 13 channels, of which only 3 are shown here schematically, diffract the proper wavelength. There are collimator slots that prevent false signals from getting into the counter so that aluminum, silicon, nickel, chromium, iron, and all of the important elements have one channel.

The next figure shows what the device actually looks like (Fig. 14). Pictured are the electron gun, which is on the other side, the sample window, collimators, and Geiger and proportional counters. Also shown is a nondispersive proportional counter on top of it which can analyze without a crystal. For the Geiger-Müller counter the amplifier electronics can be simple because the signal from the tube is strong enough. This instrument uses 20 watts and weighs 12 kilograms (26 pounds). It is in existence and is planned to be used.

Of course for use in the Voyager program it would have to be modified because in the atmosphere of Mars one couldn't use the vacuum. One would have to carry a vacuum up to Mars. The Surveyor spectrometer was published by A. E. Metzger of the Jet Propulsion Laboratory, which has done most of the work in this field [2].

Figure 15 shows a suggestion for extreme simplification [3, 4]. It is asked: Why take a high-voltage generator and an electron gun and generate X rays by the classical way if one can use a $\beta$ source...and forget about all these radioactive sources which emit electrons of high energy and let this do the job?

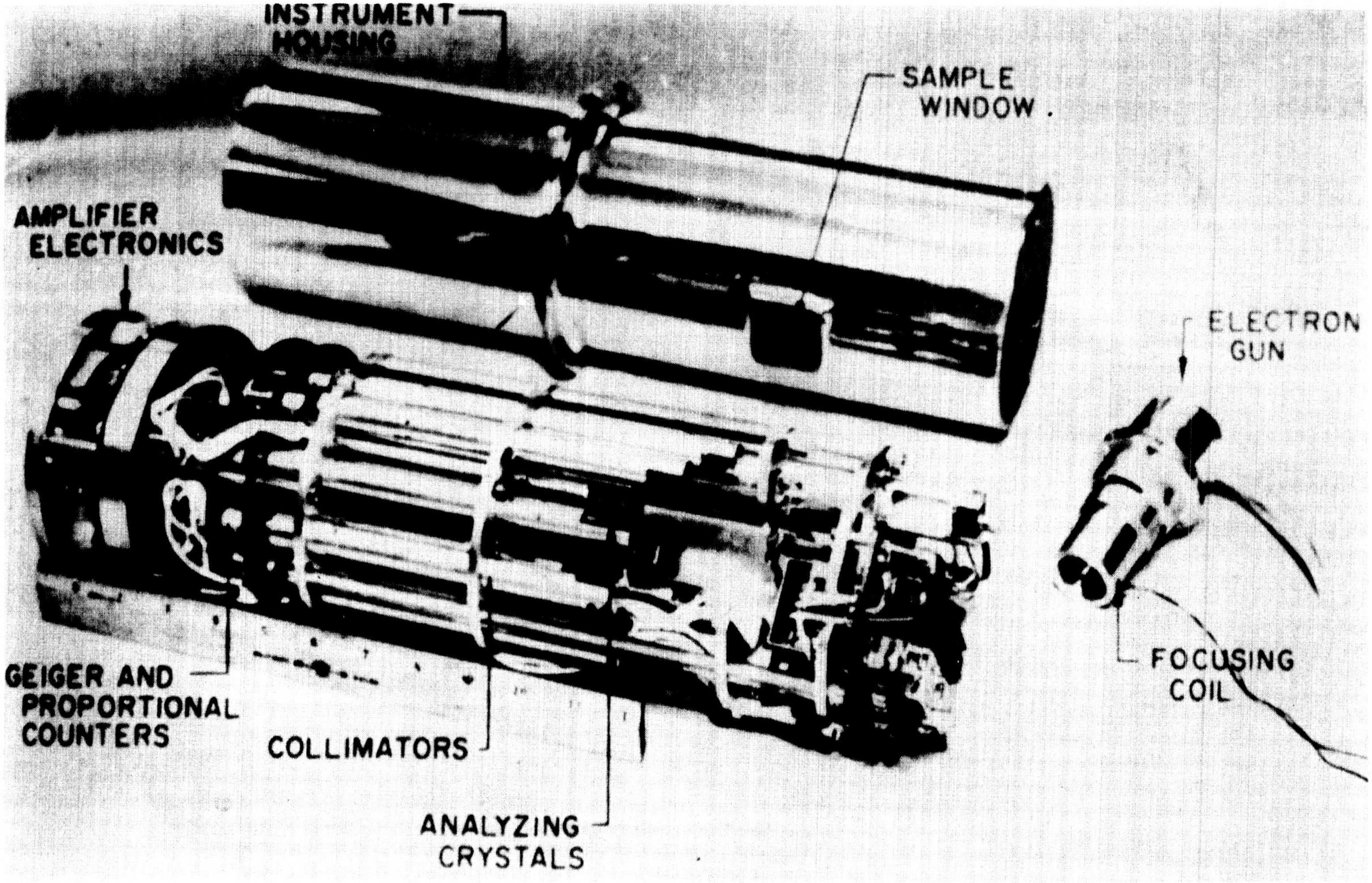


FIGURE 14. PROTOTYPE SURVEYOR X-RAY SPECTROMETER

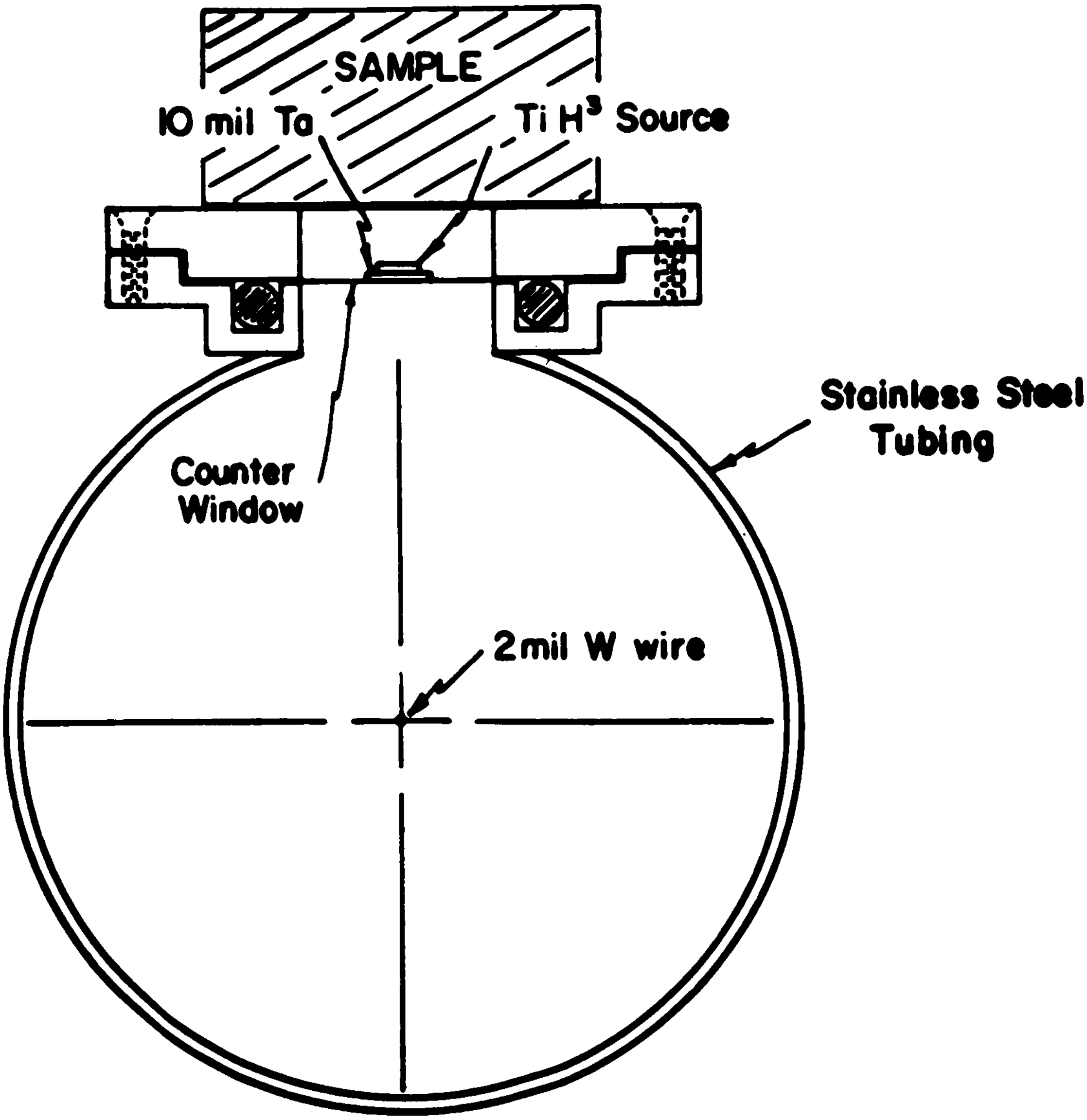


FIGURE 15. END VIEW OF COUNTER

Then the whole device can be stripped down to this (Fig. 15). Pictured is a $\beta$ source, in this case it is tritium, which is a $\beta$ emitter, with 18 kiloelectron-volts peak. It rests on a tantalum sheet; tantalum is a heavy absorber so no direct radiation gets into the counter, only by the feedthrough over the sample. The characteristic radiation of the sample comes in. The counter tube extends perpendicularly to the plane of the picture.

This suggestion has been abandoned for several reasons, the major reason having to do with the source needed just to get a reasonable current and a reasonable signal. The previous Surveyor spectrograph worked with 25 kilovolts and roughly 1 milliampere. Of course this 1 milliampere is in a particular direction, i.e., toward the sample. In this device let's say the source is one curie. One curie means roughly $10^{10}$ decompositions per second; in other words, $10^{10}$ electrons emitted in $4\pi$ and $10^{10}$ times the elementary charge, which is $10^{-19}$ ampere seconds. You get a current of $10^{-9}$ only, and, what is worse, $10^{-9}$ amperes is far too much when you don't need it, and when you do need it, it is far too little. In other words you can't switch it on and off as you need it. The weakness of the signal then calls for more amplification and more complicated amplification. So the device has not materialized, although it looks so extremely simple and so promising.

In this connection I should mention another suggestion which had more luck. It is for the analysis of the low number atomic elements. When I talk about X-ray spectroscopy, I always do so as if all the elements could be analyzed; but this is not true. The low atomic number elements, which are also very important, are still eliminated. We are at a stage now where on earth one can barely do something down to the atomic number of four. This has been the general state of X-ray spectroscopy since the 1920s, and the process is still vero complicated. One can barely do it on earth, and there is no hope yet to shoot it up to the moon or the planets.

And here is something that falls in very nicely. It is a suggestion from A. Turkevich from the University of Chicago [5]. His experiment deals with the backscattering of monoenergetic $\alpha$ particles from a source of curium 242. The backscattering of these is characteristic in the case of light elements. It becomes very uniform with heavy elements. So here one has a means, a very simple means, of analyzing for low atomic number elements. This is scheduled for one of the Surveyor flights in addition to the X-ray spectroscopical analysis which will cover the elements beginning with about sodium upward.

## Mineral Identification

You will remember that in Bragg's equation, $n\lambda = 2d \sin \theta$, the $\lambda$ was the thing to shoot for; the d, the dimension of the crystal, was known; and the $\theta$ was the angle that was measured. Equally important and even more ambitious is the task to identify some compounds, minerals, on the surface of the moon and earth-like planets by way of their crystal structure. This is done on a routine basis on the earth, even for the most complicated materials. Equipment has to be stripped to the bare minimum and simplified beyond recognition for extraterrestrial applications.

Figure 16 shows one very old method, which again comes from the 1920s, from Seemann-Bohlin [6]. It is an old slide from my lectures of Vienna. Now remember, the sample, the unknown, diffracts. The wavelength coming from an X-ray tube is the known variable now. The X ray comes from an X-ray target into a point of divergence and hits the sample. The sample is now a powder with the crystals having all possible directions with respect to the impinging X-ray direction. One doesn't need any rotation; they have all possible angles already. The planes in this sample have all possible directions, and those that have the proper angle for a reflection are selected. The detector in this case was film.

So now the sample can be stationary; the recorder just has to be rotated and turned through all these angles. What makes it so attractive is that the divergent beam, in spite of the angle of selectivity of X-ray diffraction, can be made convergent, and all the energy from the sample can be squeezed into the detector at the right place. It is a so-called power focusing method. People used to say focusing, but it is focusing only in this principal plane. We have to remember that it is three dimensional and the rays coming out of the plane are not really focused.

In Figure 17 again the same geometry of the Seemann-Bohlin method is used, this time for the Surveyor program [7]. In this case the X-ray tube is the divergence point, and it lies on the circle of focusing. We see that the Geiger tube detector now rotates throughout all the angles and the specimen in the holder has the proper curvature.

The curvature of the sample is not very simple. The sample has to be prepared by an automat on the extraterrestrial planet's surface, and plane geometry would be preferrable. There exists an old method from the 1940s that uses about the same geometry but symmetrical (Fig. 18). I bring this up particularly because it is the method published by my former teacher in Vienna,

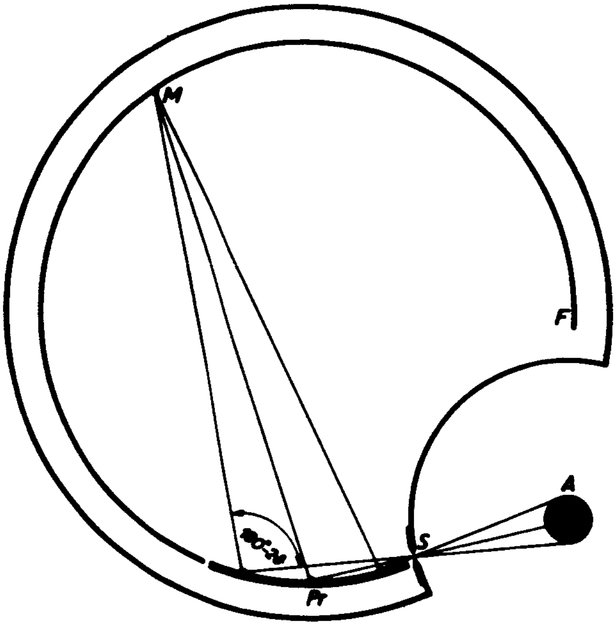


FIGURE 16. THE SEEMANN-BOHLIN METHOD

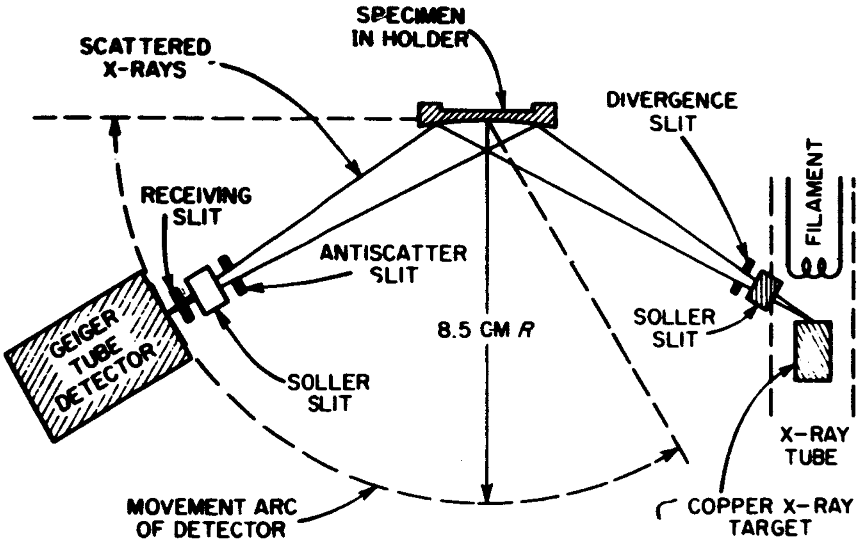


FIGURE 17. SCHEMATIC DRAWING OF SURVEYOR X-RAY DIFFRACTOMETER

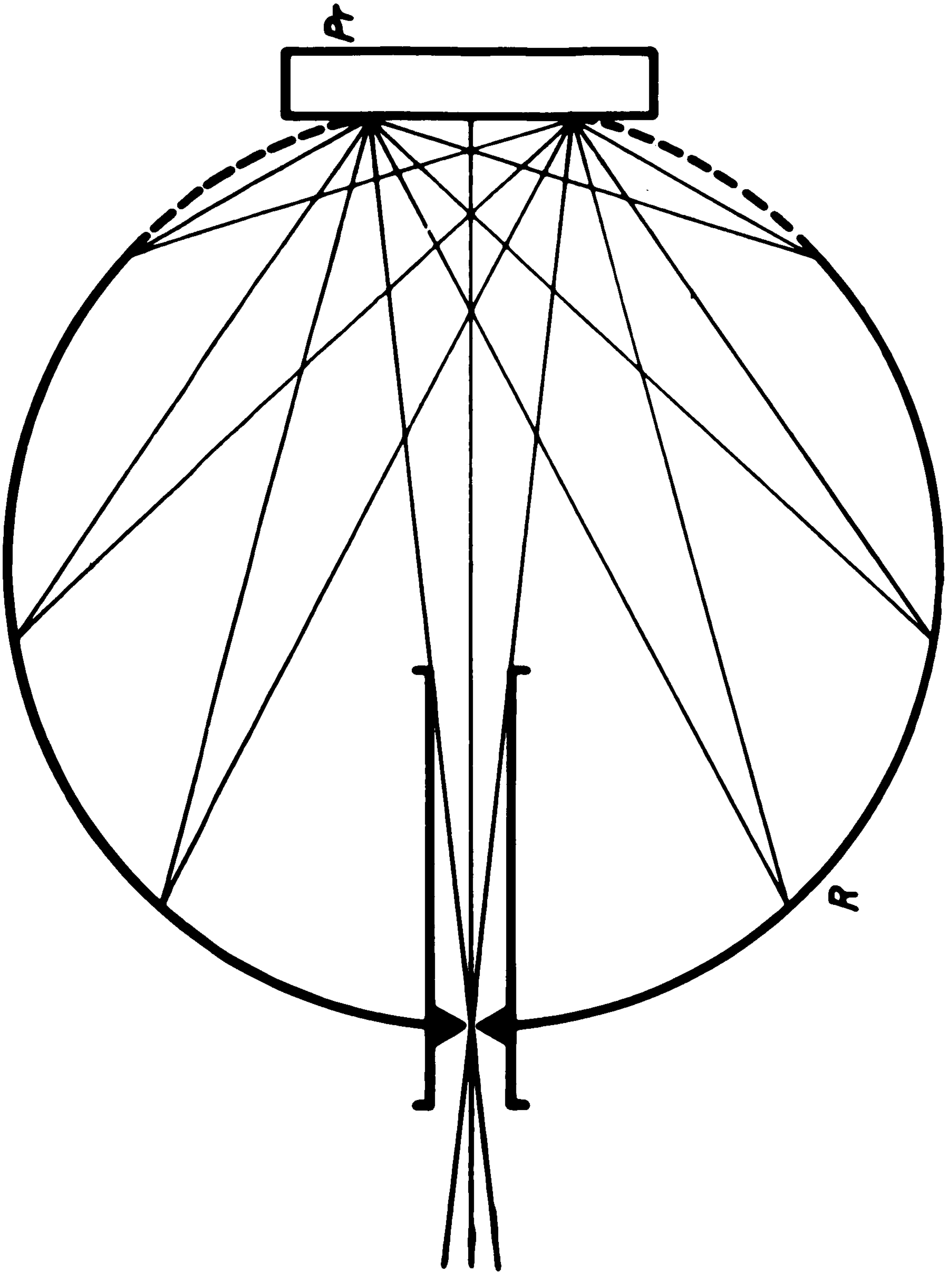


FIGURE 18. REGLAR'S SYMMETRICAL METHOD

Professor Reglar [8]. The perpendicular incidence and the symmetrical arrangements would have certain advantages.

Figure 19 shows the suggestion for a combined spectrometer-diffractometer, a condensed gadget that is supposed to do both elemental analysis and identification of the structure by X-ray diffraction. In this case the sample is again pressed against the focusing sorter. The device needs two sources. One is an electron source for elemental analysis. The electrons impinging on the samples can be switched on. A crystal and a detector are also shown. The second is an X-ray source; the same sample can be investigated for its X-ray diffraction pattern.

Figure 20 is a picture of a spectrometer that was built and only very scantily published two years ago. It is from W. Parrish from the Phillip's Laboratories. The figure shows a gadget with the high voltage supply and the diffractometer with the motor that rotates the crystal [9]. The whole apparatus is built for 25 kilovolts, 1 milliampere; the drive motor again has 56 watts. The whole gadget takes 0.0252 cubic meters (0.9 cubic feet) and weighs 8.1648 kilograms (18 pounds). The performance is surprisingly good and almost matches the one of regular units.

Figure 21 shows some results that this Phillips apparatus gained on earth of minerals that one assumes will be found on the moon. Included are, of course, all silicates, quartz, sanidine, which is the $Si_3O_8$ silicate, and glass. The glasses give, instead of the sharp peaks of high order in crystalline matter, a very broad peak only. The location of this peak is representative for the content of $SiO_2$. Thus, even this furnishes some way of identification by way of the $SiO_2$ content. Mixtures will be very complicated, but, since this can be done on earth by the help of computers, it will not be too difficult to unscramble these data and identify what minerals make up the dust layer, if any, and the bedrock on the moon.

As I mentioned previously, getting the proper sample is far more difficult, and a whole group has published several papers on this subject. There has been some work with a drill which drills 25 centimeters into the bedrock below the surface of the moon and brings up some of the dust from the bit. These are put into a cup, which is transported to the window of the diffractometer. In this case the cup is covered by beryllium foil. Beryllium is very transparent to X rays; it does not interfere with the sample but it furnishes a reference to the 002 interference to beryllium. I am not up to date on the latest data on the performance of this drill, but I know that there have been considerable difficulties to overcome, as one can imagine.

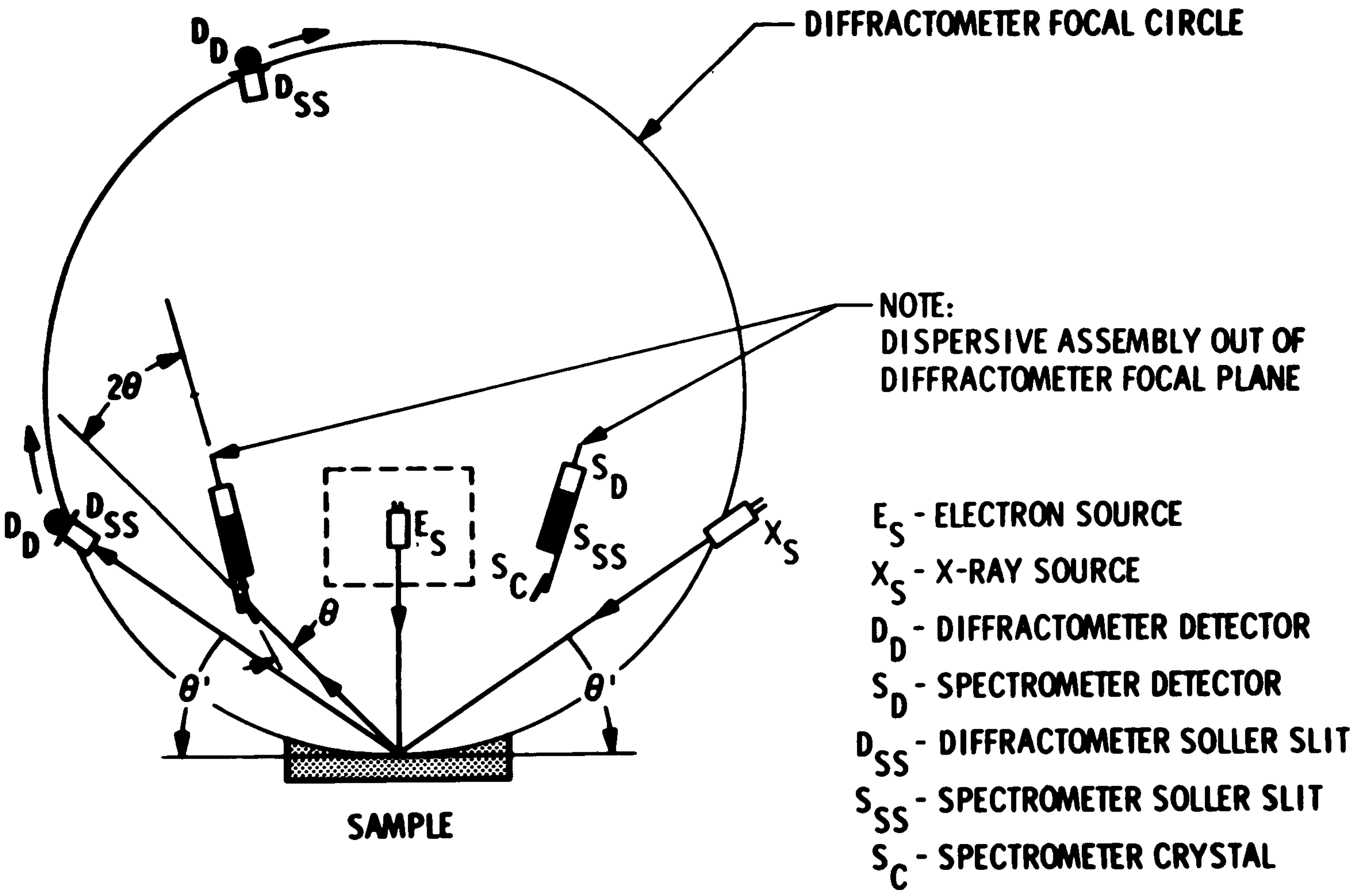


FIGURE 19. SUGGESTED SPECTROMETER-DIFFRACTOMETER

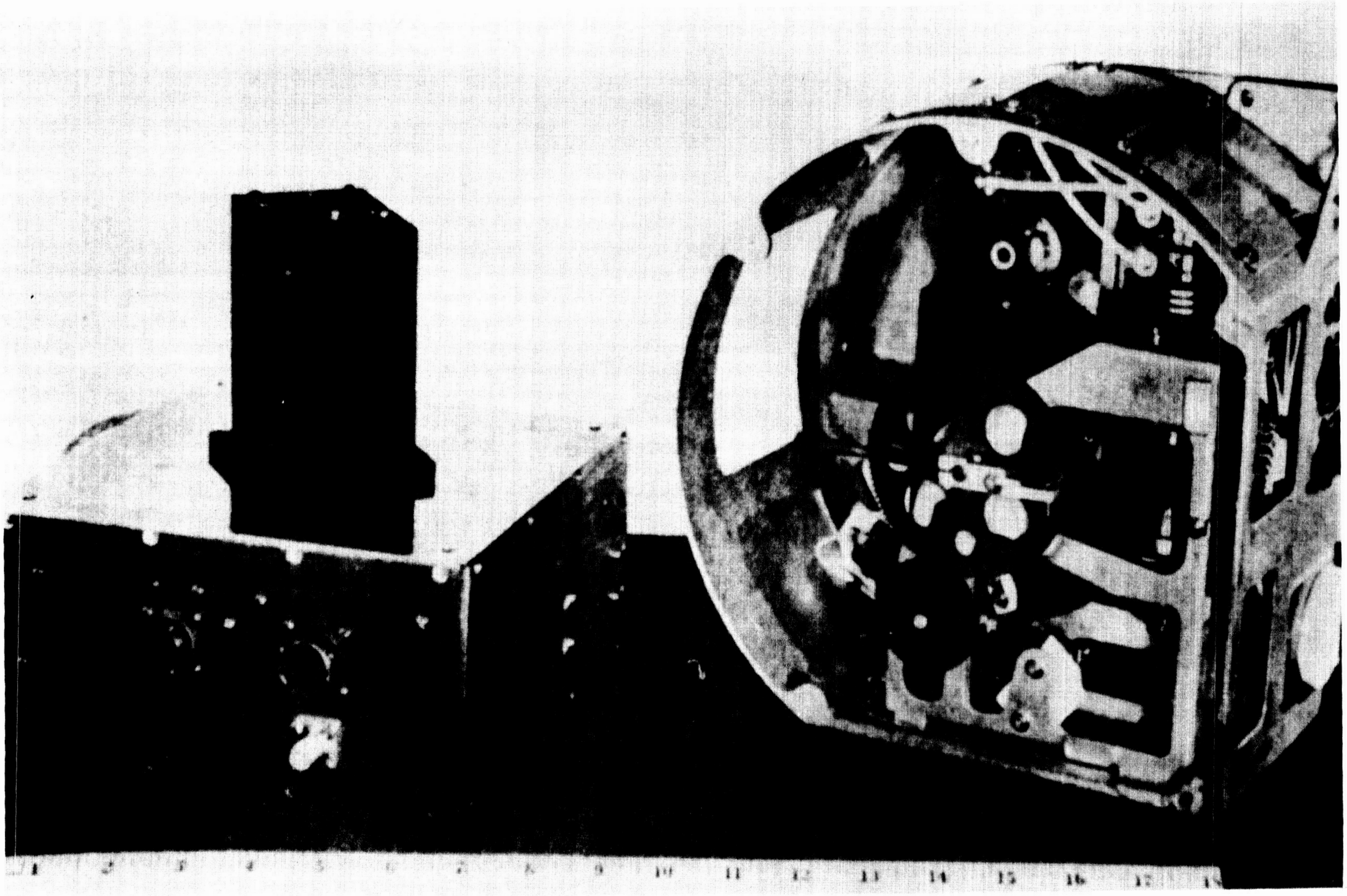


FIGURE 20. EXTERNAL VIEW OF PHILLIPS DIFFRACTOMETER

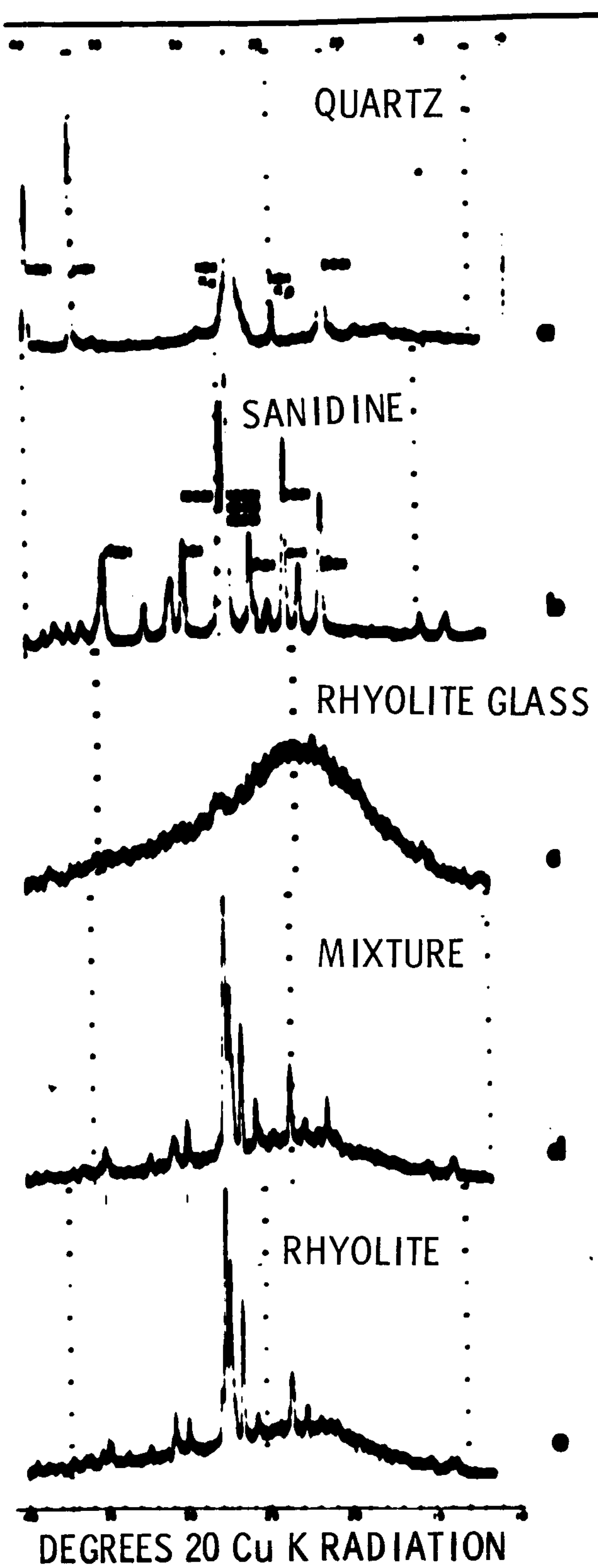


FIGURE 21. RESULTS FROM PHILLIPS DIFFRACTOMETER

## CONCLUSION AND GOALS

I have mentioned several times that the goals here are utmost simplicity, reliability, and ruggedness. Although the motives are quite different, these are the same as we have in industry. There was a time during my work in Austria that the motive was quite different. It was right after the war when to do research in Austria meant that one had to do it with utmost simplicity or it couldn't be done at all. Out of this motivation came an X-ray spectrograph published by H. Herglotz in 1954 [10].

Because of the poor research conditions at that time, this X-ray spectrograph was made with utmost simplicity (Fig. 22). If you look at it, it bears some striking resemblance to some of the X-ray spectrographs of today, the main difference being that it has a film. If the film had been replaced by a detector it would have done relatively well. There was an X-ray tube with an end window, which in this case was pumped continuously. The generated X rays came out of the window directly. Because it was nondestructive, one could bring the X-ray tube very close to a large sample. The X rays impinged on the sample, generating the characteristic X rays. These characteristic X rays were caught in the tiny spectrograph, which was the size of a matchbox and is shown in Figure 23. Again this was Seemann-Bohlin geometry, in the symmetrical case.

Although that example from Austria is very modest in comparison to the quarry of space exploration, it demonstrates the goal of simplification. One talks so much these days about all the money spent on space exploration. Who knows what we will find there? I am convinced anyway, whether there is spin-off or no spin-off, that one will find things that will start a new age just as Columbus' voyage to this hemisphere started a new age. One major spin-off is the flexibility in the space program, which I admire so much. The space industry does not shy away from spending billions on large rockets, because they represent the minimum means to carry measuring devices to extraterrestrial bodies. At the same time, the equipment must be extremely simplified, trimmed of all fat, and still perform and bring back the data. This flexibility, and the ability of the engineers to concentrate on the task and not on the gadget, is remarkable. I am sure it introduces a new aspect into education, the courage to do things the simple way. To get equipment that can do the job, regardless of how simple it is, is a major step forward which is already becoming apparent.

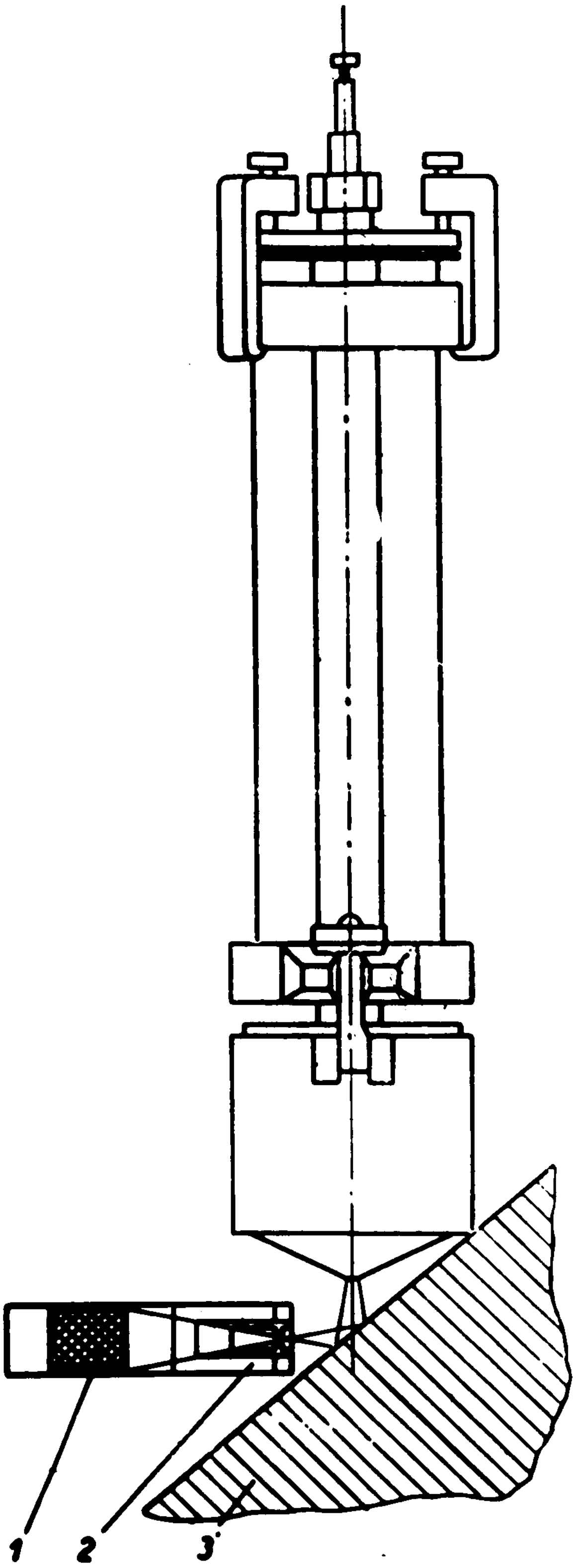


FIGURE 22. EARLY X-RAY SPECTROGRAPH

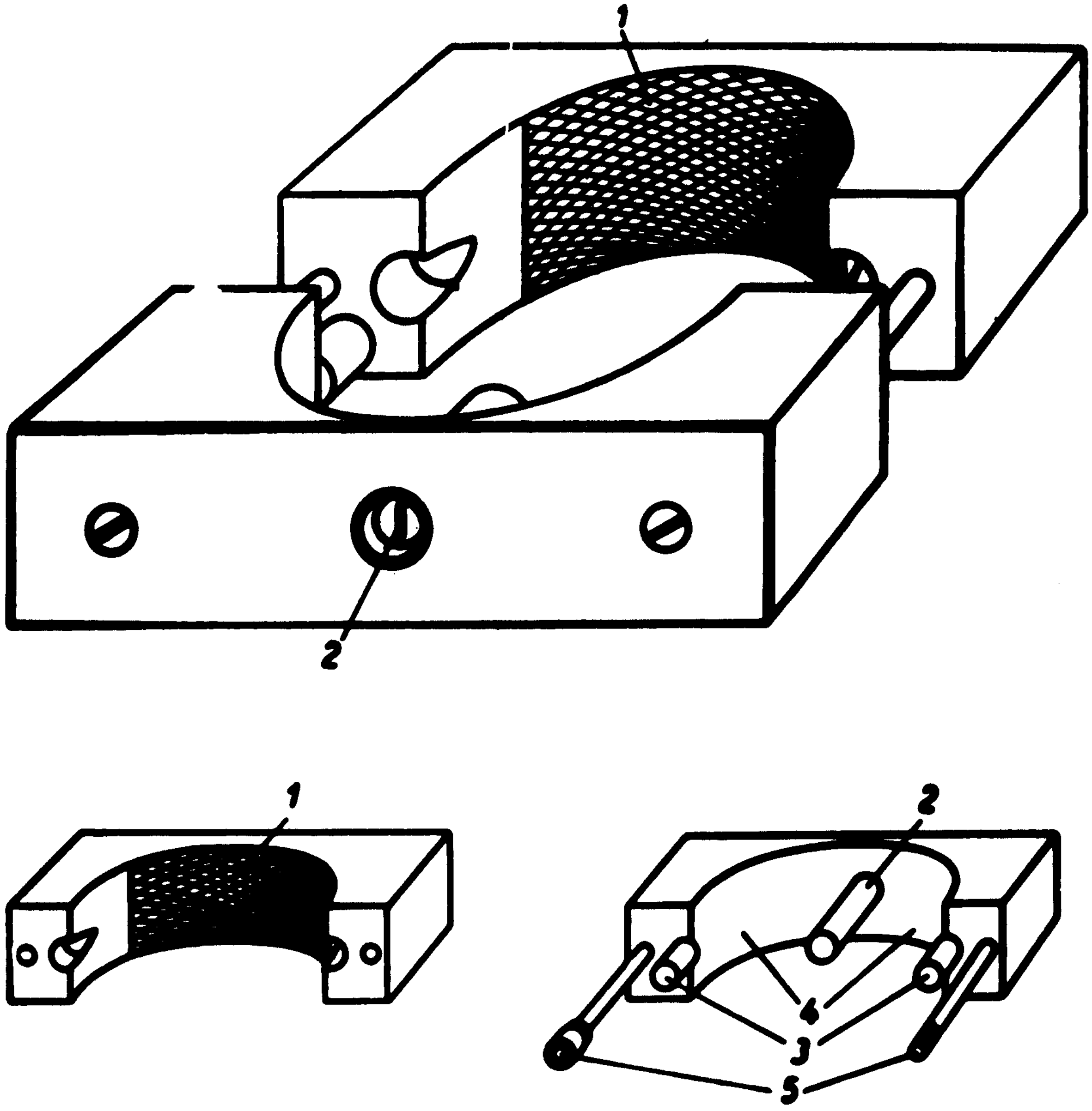


FIGURE 23. PARAFOCUSING CAMERA

# APPENDIX. DISCUSSION

Question: How feasible do you think it is for the exploring astronauts to haul one of these 25 pound X-ray spectrometers around the countryside to take representative analyses?

Answer: Well it certainly is within possibility. But the decision has to be made as to which is simpler, cheaper, and more reliable: to bring the samples back to earth or to do it on the spot.

Question: It has been stated by geologists, and very definitely by astronomers, that perhaps the most important thing that the astronaut can do is bring back 100 pounds worth of samples. He can't bring back, say, several tons, but he might be able to, in addition to the solid chunks, get some analyses of the area within a mile or two of his landing craft. How feasible is it to have a small hand-held spectrometer?

Answer: Thoroughly within the possibilities of today's technology. I guess the consideration really has to be raised whether it would be better to collect these small samples. To carry a hundred pounds of rock would be necessary as long as elaborate samples are needed for the job or for some of the other experiments the geologists certainly will have planned, but for elemental analysis by X ray, the amount of sample needed is very small. Collection of smaller samples on the moon might be the more economical way. Of course I am in no position to decide this.

Question: Is there any objection to calling your focusing circle a rolling circle?

Answer: It is not quite the same as a rolling circle but of course it has definite similarities. I mentioned at the beginning that there is the selectivity of X-ray reflection. With the rolling circle, of course, you have reflection at any angle, while here you have the selectivity right from the beginning. But it certainly is not a great mistake to call it a rolling circle.

Question: I would like to mention something in connection with Dr. Parrish. I had a discussion with Dr. Parrish about two years ago about the same Phillips instrument. He was very disgusted about the results. He submitted to two samples, and, of course, he never got any feedback. He said that this was probably because people don't understand it. They don't believe that by such simple means such a task can be performed or solved. He could not reveal all the details, and since they didn't get all the details they just...

Answer: I'm glad you brought it up. This is always a problem, no matter what one comes up with one has to overcome the inertia of people who think that the best way is the way it has been done, the way that they have learned, and the way that it has been available for a long time. To overcome that, no matter where you are, is always a problem; I guess it is true for any invention and innovation. I think it was Faraday who said that any invention goes through three stages. First it is ridiculed, second it is fought, and third it is declared trivial. It is true for large inventions and small inventions. "Why do you want to do it this way, why should you try to change it; we have this apparatus and it has been performing fine." I am sure Dr. Parrish is disgusted by it because it is a very nice gadget and there is really no reason why it should be restricted to the moon, Mars, and Venus. It could do a good job here on earth.

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# EXTRATERRESTRIAL APPLICATION OF X-RAY DIFFRACTION

By H. K. Herglotz

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