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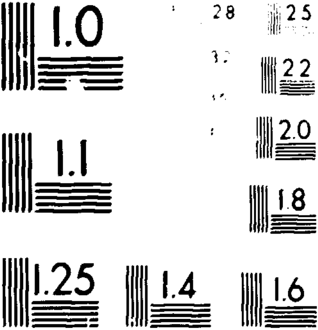

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GUIDELINES ON APPLICATION OF MICROCOMPUTERS IN MINERAL PROCESSING LABORATORY:

TECHNICAL DATA FOR DETERMINING THE FAIR PRICE OF ORES IN DEVELOPING COUNTRIES*

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SUMMARY

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Nature: Study shows that microcomputers can serve, in various ways, the mineral industry and among these in the laboratory they play an important role in determining chemical composition. Case studies demonstrate these statements.

Title: Guidelines on Application of Microcomputers in Mineral Processing Laboratory: Technical Data for Determining the Fair Price of Ores in Developing Countries

Author: P. GADO (HUNGALU Engineering and Developing Centre, Budapest, Hungary), as consultant to UNIDO Technology Programme, Division for Industrial Studies.

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Scope: Powerful, easy to operate, compact and inexpensive microcomputers can replace human labour and intelligence in a great part of laboratory work. This can help developing countries to make a considerable leap towards high level materials research with only a few well trained specialists and a few assistants. The data collected and processed by a microcomputer which is linked to several instruments may assure thorough and complex information for exploring geologists, mining and sales engineers in the mineral industry about ore reserves, quality and other parameters.

Conclusions: Because developing countries supply a major part of the raw materials input to the world economy, and import in return advanced products of higher technology from industrialized countries, the definite aim of imports should be the strengthening of their national capabilities, the updating and upgrading of means available for independent activities in the fields of production as well as in R and D. Abundant investment costs should be devoted to the foundation of microcomputer controlled laboratories in developing countries. This system is promising in finding technical data to determine the best way of marketing and fixing the fair price of ores.

Abbreviations

AMIS	Automated Minerals Information System
APCOM	Application of Computer and Mathematics in the Mineral Industries
BS	Backscattered Electrons
CPU	Central Processing Unit
DMA	Direct Memory Access
DSC	Differential Scanning Calorimetry
DTA	Derivate Thermogravimetric Analysis
EDS	Energy Dispersive X-ray Spectrometer
IMMAGE	Information on Mining, Metallurgy and Geological Exploration
PC	Personal Computer
PC	Professional Computer
RAM	Random Access Memory
ROM	Read Only Memory
SE	Secondary Electrons
SEM	Scanning Electron Microscope
TA	Thermal Analysis
TGA	Thermal Analysis System

Glossary

of some terms relevant to the topic of these guidelines

Algorithm: A finite set of well-defined rules for the solution of a problem in a finite number of steps

Analysis: Chemical or physical procedure by which the components and their parameters are determined in a complex material system qualitatively and/or quantitatively

Architecture: The fundamental design of a computer's hardware

Atomic absorption: Method of chemical analysis based on the fact that atoms absorb selectively definite wavelength of light

BASIC: Beginner's All-purpose Symbolic Instruction Code. A 'conversational' high level computer language for ease of use and ability to perform calculating machine tasks. Usually implemented on general purpose machine

Code: A system of symbols and rules for their use in representing data or instructions

Command: A unit of information understandable to the computer, which, when presented, causes the hardware to execute a particular operation

Compatibility: The ability of two different machines to use the same electrical signals /in hardware/, or the ability of two different computers to use the same program for solution of a particular problem and to produce the same results /in software/

Computer: A functional programmable unit that consists of one or more associated processing units and peripheral equipment that is controlled by internally stored programs, and that can perform substantial computations and control operations of attached equipment without human intervention

Conversational: Pertaining to a mode of operation involving step-by-step interaction between the user and computer by means of a keyboard and display. Each entry on the terminal evokes an immediate response from the computer.

Control: Ability of a machine /or human person/ to intervene in the operation of another equipment in order to accomplish a particular task under predetermined conditions.

Crystal structure: Regular spatial arrangement of atoms or ions and their bonds

Data: A representation of facts, concepts or instructions in a formalized manner suitable for communication, interpretation or processing by human or automatic means

Data base: A structured collection of data treated as an entity

Data set: A collection of data records with a logical relation to each other

Diffraction: Cooperative scattering of radiation from a crystal

Disk: A storage device in which binary information is stored by selective magnetization of portions of the magnetic surface coating on one or both sides of a rotating disk

Evaluation: Defining with degrees of accuracy the many parameters of a mineral deposit with the goal to judge and establish the value of the material included

Floppy disk: A moving head disk storage device whose magnetic surface is removable and flexible, in size and appearance like a small grammophone record in its sleeve

FORTRAN: FORmula TRANsformation. A high level computer language designed mainly for scientific and engineering applications. Has various dialects and extensions

Hard copy: Computer output in permanent, legible form on paper
Hardware: Physical equipment used in data acquisition, storage and processing as opposed to computer programs, procedures, rules and associated documentation
High level language: A generalized method of writing a computer program which allows the programmer to express problems in forms similar to mathematical expressions or natural /English/ language
Infra red absorption: Method for the analysis of mineralogical composition and bond structure of ores
Memory: Device or medium used to store information in a form capable of being retrieved or processed
Microcomputer: Relatively inexpensive, easy to use general purpose computer
Microprocessor: A single large scale integrated circuit which has capabilities for performing arithmetic and logical functions, which can execute these functions by decoding control statements from a stored programme, and which can communicate results to specific devices
Minerals: Naturally occurring, usually inorganic and crystalline substances
Ore: a mixture of minerals which can serve as raw material in the commercial recovery of a metal
PASCAL: A high level language containing many important data structuring and file handling constructs. Formalized in a report in 1973
Procedure: A portion of a computer program which is named and which performs a specific task
Program: The set of instructions which tell the computer what has to be done and in which sequence
RS-232-C: The EIA number of a standard serial interface for connection of diverse equipment to a computer
Scanning electron microscopy: Method for the analysis of three dimensional shape and size of tiny particles based on electron-material interaction
Software: Computer programs, procedures, rules and associated documentation and data pertaining to the operation of a computer system
Specification: A concise statement of a set of requirements to be satisfied by a product or material
Thermal analysis: Method for the mineralogical analysis of ores based on heat induced changes occurring in materials
Utility: Of 'standard' programs, those written to assist in the preparation and testing of user defined codes
X-ray diffraction: Method for the analysis of crystal structure and the mineralogical composition of ores
X-ray fluorescence: Method of chemical analysis based on the knowledge of the characteristic wavelengths emitted by the elements when irradiated by x-rays

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SUMMARY

Powerful, easy to operate, compact and inexpensive microcomputers can replace human labour and intelligence in a great part of laboratory work. This circumstance can help developing countries to make a considerable leap towards high level materials research with only a few well trained specialists and a few assistants. Microprocessor controlled instruments yield reliable and accurate data in almost unattended round-the-clock operation, provided that representative, adaquately prepared samples are available. The data collected and processed by a microcomputer which is linked to several instruments may assure thorough and complex information for exploring geologists, mining- and sales-engineers in the mineral industry about ore reserves, quality and other parameters related to the real value of the product to be marketed. The well founded awareness gained in this way may be helpful to achieve optimum revenues from national resources.

Microcomputers can serve in various ways the mineral industry and among these in the laboratory they are able to play an important role in determining chemical composition by X-ray fluorescence analysis and atomic absorption spectrometry as well as in

determining quantitatively crystallographic phases in multicomponent mixtures by X-ray diffraction measurements, infrared spectroscopy and thermal analysis and microstructural characteristics by computer aided scanning electronmicroscopy.

These statements are demonstrated by case studies. Although a rapid change in the technical performance of the relevant instruments and microcomputer systems is witnessed in our time, a tentative definition is given of their main characteristics and recommendations for the installation of microcomputer controlled laboratory systems.

INTRODUCTION

As a matter of fact developing countries are in general fairly rich in mineral resources. Studying publications like the Mineral Resources Handbook prepared by the US Geological Survey in 1981 or successive issues of the Mining Annual Review, it is easy to recognize that Guinea, Brazil, Guyana, Jamaica and Surinam are among the major bauxite possessing and mining countries; Botswana in one of the leading diamond producers in the world, well on target for an annual national output of 9.5 million carats by 1985. A substantial producer of tungsten and molybdenium ores is China and the arguments could be continued for copper, nickel, lead, zinc, etc. even if energy minerals are not concerned because in the present context they are not interesting. The mining of minerals can provide employment for masses of labour force and contribute singnificantly to the export potential of any country, forming an evident source of revenue. Since it is highly desirable for each economy to benefit as much as possible from natural resources, the availability of certain raw materials may justify the foundation of domestic industries with advantages that need not be explained.

The mining industry in several economies suffered during the early 1980's from serious difficulties. World recession decreased the demand for certain raw materials and the international companies are in doubt about future investments. Weak commodity prices and falling demand coupled with high real interest rates and energy prices have posed serious financing problems for many less developed countries. In some cases political, communications and other disturbances prevalent in the newly independent countries contributed to the decline.

The stringent economic conditions urge all nations more than ever before to find optimum exploitation of their natural resources.

In order to accomplish this goal in respect of minerals, governments and agencies should possess firm information about the size and location of reserves. Decision concerning exploitation of the resources can be based only on such data. The acquisition of reliable data on the other hand requires investment, however, in most cases this pays back rapidly.

The real value of a deposit depends on several factors, some of which are geographical-structural while others are rather technical.

As examples for the former one could mention the proximity of cheap transportation ways like large rivers and oceans, feasibility of local processing because of the availability of the necessary infrastructure, energy or auxiliary materials and appropriate manpower.

Among the technical characteristics of an ore body are the geological features highly influential in determining the mining costs and the parameters desribing quality.

In general the pricing of ores is based almost exclusively on effective mining costs modified by differences in quality. This principle is only partially valid if by political or other reasons fiscal policies are introduced. In the context of the present guidelines we focus on the role of quality as an important ingredient of pricing practice and neglect other kinds of manipulations. The attribute "quality" may have several components, too. The one of main influence on price is the percentage of the metal intended to recover. Another important chemical aspect is the presence of elements which are disadvantageous or harmful from the point of view of processing by usual technologies. E.g. in the case of bauxite, the raw material of the alumina/aluminium industry, the price is the higher the more Al_2O_3 and the less reactive silica can be found in the ore used for processing in a Bayer cycle. The recommendation of the International Bauxite Association /IBA/ to express this preference in the market price is reproduced in Table 1. 1/

Table 1. IBA recommendation for bauxite pricing in dependence from quality

Base grade bauxite	Recommended bonus/penalty calculation	
Available Al_2O_3 = 45 %	Al_2O_3 available 1/45 the price of base grade bauxite	for each percentage point above or below base grade
SiO_2 reactive = 4 %	SiO_2 reactive \$ 1.50/t	

In a closer approach, however, processing costs of a bauxite are influenced considerably by its mineral composition: whether the aluminium is present in the form of trihydrate or monohydrate and other more detailed crystallographic characteristics which can be revealed only by more or less sophisticated materials research and technological tests. Awareness about these characteristics, dependable data in the hands of the negotiator might be therefore strong arguments when time arrives to fix the price of a given bauxite.

The situation seems to be not widely different for other ores. Once a mineral deposit has been discovered there appears a natural desire to develop it as rapidly as possible in order to gain a source of wealth. Yet the mere existence of a mineral deposit is only one element in a successful mining enterprise, its grade, physical and chemical characteristics give other important dimensions of its economic viability. Development of new mines of low grade minerals may result in much lower national returns than expected. Reckoning with the potential of co- and by-products may change the situation of a venture. The growing market for these products became very important in the recent period. Many mineral products were mined as by-products of major metals such as copper, lead and zinc. The rising prices of these by-products enabled base metal mines to remain profitable even in the face of increasing costs. During the late 1970s improved recovery of by- and co-products like gold, silver, gallium, vanadium and molybdenium had been accomplished. In some cases such metals had initially been regarded as a source of small extra benefit in the started mining activity, however, later some of them yielded almost equal profit to the base metal itself. Thus the accurate analysis of the minor constituents may also be crucial to find the real value of an ore before marketing it.

If a few tenths of percentages of a rare metal can decide the profitability of a mining project because as a recovered by-product it adds enough to the income side to turn the balance from loss to gain, then it is clear that the corresponding analyses must be accurate at least to the same extent. The premium price achievable in the bargain based on measurement results good enough to withstand any control from the side of the buying party, might compensate for the efforts invested in acquiring the inevitably large amount of data.

Developing countries in the past often had been handicapped by the lack of appropriate laboratories and instrumentation necessary for determining the quality of their mineral products. Also, recruiting of well trained engineers and technicians might have been a problem. Recently, the hardship seems to be shifted in many countries to another field. Now intelligent instruments can be purchased to relieve the burden of carrying out routine measurements, data logging and evaluation, however, there is a shortage of engineers who understand the principles of materials technology and the manner in which computers may be used to improve the effectivity of laboratory work and the accuracy of results.

Cost-effectiveness in the developed economics have been achieved in the past few years partially by the intensive use of computers. In the mining industry computational techniques had been introduced at least in five main fields. These are:

i/ data acquisition and processing
ii/ process control
iii/ modelling of operations
iv/ development of data bases
v/ market analysis and financial calculations

The trends can be well followed from the proceedings of the eighteen APCOM / = Application of Computers and Mathematics in the Mineral Industries / meetings held between 1961 and 1984. Those willing to respond to the challenge and deepen their knowledge in this have a substantial advantage as compared to those in remote computer centres. The mineral industries are able to draw on these advances in the rapidly developing fields of information technology and data processing.

MAIN COMPUTER APPLICATIONS IN THE MINERAL INDUSTRY

Coming back to the five main fields, as mentioned, of computer applications let us briefly elucidate and define them one by one:

i/ Data acquisition and processing is widely used in the mining industry both in exploration and production. In exploration the computer is utilized to reduce the field data of geochemical and geophysical survey to meaningful anomalies, plot them on maps and further analyse the significance of these anomalies in terms of exploration targets. Thus the computer's role is extended to the interpretation phase and leads to reserve estimation and analysis. As a fast calculator it can help to perform grade interpolation and create a mineral inventory model. The interpolation techniques like inverse distance weighting, the polygonal method or Kriging are all implemented on computers in order to obtain easily accurate information on geologic reserves taking into account duly cut-off grades.

In production the volume of data is so immense and the requirements so immediate that the demand on the computer is even more pronounced. Here not only the material of drill holes but also that of blast holes and toe sampling is used to model the ore body and verify the interpretation technique and the mine plans based upon it.

ii/ Process and production control by computer techniques can be implemented at several levels ranging from simple stabilization control to advanced optimizing control. Successful combination of instrumentation, computer hardware and control strategies may result in 5 to 10 percent increase of the throughput of a mineral processing plant or the productivity of a mine. A process control system is based on first defining the objectives to be achieved, defining the controllable variables in a unit operation, available sensors that may be used to detect changes in the circuit-operation and techniques for controlling the process variables in order to compensate for disturbances in operation. The need for primary sensors to measure accurately and reliably the changes in controlled process variables cannot be overstressed.

Besides dynamically compensating for mechanical, equipment maintenance and inventory perturbations such a system also stores and edits maintenance related information about parts, components and equipment, provides past history on equipment and predicts failures, uses a model of optimum operation to decide interventions. As the level of control becomes more advanced, greater process efficiency can be achieved but greater process knowledge and more instruments are required to obtain the benefits. Although engineers strive to control in a process as many variables as possible to realize continuous optimum production, at the present control seems to be feasible only upto a certain approximation for a number of reasons, some of which are: a/ the extremely large number of plant variables which must be manipulated simultaneously; b/ the doubt whether there exists at all a unique optimum with regard to all variables and; c/ limitations in current sensing and control elements. Therefore instead of a true global optimum one must be satisfied with an optimum in respect of hierarchically selected goals.

iii/ Modelling of operations by computer simulation produces a mathematical representation of a physical system /an ore body, a mine, certain mining or processing equipment/ which permits experimentation when it is impossible or economically unfeasible or inconvenient to experiment with the real system. Simulation consists of imitating performance of the system step-by-step with the aim of determining outcomes at critical points of the process. In a more popular way one can put that a computer simulation permits to answer "what if" type questions. It is essential that among the variables of the system only those should be represented in the model that have substantial effect upon the performance. In response to the need for lower unit costs and high recoveries, investigations by simulation advance rapidly.

iv/ Data bases developed locally, in a single country like AMIS /=Automated Minerals Information System/ provided by the US Bureau of Mines, Washington, D.C., USA, or by international efforts like IMMAGE /=Information on Mining, Metallurgy and Geological Exploration/ provided by the Institution of Mining and Metallurgy, London, U.K., form the up-to-date source for information. Such data bases might contain in record files structured information on the technical literature, standard reference data for measurements, financial information about the international market and also any locally collected data from the fields of geological survey, planning, laboratory tests, personnel division or management that are worth storage and presumably will be needed for comparison or analysis at any later date. Data bases need extended storage media and an efficient text editing and information retrieval software that are commercially available with most microcomputers. Access to international data bases can be assured via telecommunication means /cables, microwaves, satellites/ or through information delivered batchwise on storage media like magnetic tapes or disks. In the first approach the local mini-or micro-computer may serve as an on-line terminal hooked to the information center.

v/ Routine financial calculations like payrolls and maintenance cost analysis etc. can be carried out very effectively by means of microcomputers.

Concerning market analysis and especially market predictions there arose in the last decades some doubt. The seeming lack of confidence in mathematical models of market behaviour might be a consequence of the apparent failure of such models to predict long range market developments over the past decade. Where computer modelling and forecasting is undertaken the purpose is usually to describe short term market trends and the preference shifted to "experience and judgement" type predictions. It must be admitted that reliance on statistical techniques became fairly widespread by the early 1970s because no dramatic changes were expected. In fact the dramatic changes that have befallen the mineral industry during the late 70s and early 80s could hardly be predicted by statistical methods. Therefore the computer came to be regarded as of only limited use to market analysts, no matter how excellent a tool it proved to be in the hands of accountants and financial experts in analysing sensitivity and risk factors.

Nevetheless, a feasibility study must be conducted in each case ahead of any mining investment. General principles of computer-assisted work in this field can be found e.g. in the book written by Marvin P. Barnes 2/. More specifically: COMFAR 3/ is a microcomputer based model for feasibility analysis and reporting developed by UNIDO in 1984 and available now upon license agreement to institutions or agencies interested in this software. The COMFAR system is a very flexible tool and based on a few essential input data it produces complete tables on initial and current investment, sales and production programs, production costs, cash-flow tables for financial planning, net income statements, projected balance sheets, discounted cashflow and financial ratios. The use of this complete program package facilitates the fast computation of the statements needed for economic and financial analysis of feasibility studies and consequently yields assistance in contract negotiations.

The above applications of computers in the mineral industry brought about /i/ reduction in cost partly by diminishing the demand for manual labour /measurements, data processing in quality control, accounting and finance/; /ii/ increased timeliness of results in the form of high processing speeds and access to large data bases /control, information/; /iii/ and expanded interpretation capabilities for modeling and data analysis /ore reserve calculations, mine planning, pricing/. The benefit of eliminating human error sources from data acquisition, handling, processing and storage can hardly be overemphasized especially if there is a shortage of highly skilled personnel.

The scope of the present guidelines will be restricted to the use of microcomputers in mineral processing laboratories to obtain technical parameters for determining the fair value of minerals. Although only this thin sector of the wide range of applications will be described in some detail, the reader can now find the place and weight of this theme within the broader context of "computerization in the mineral industry". It must be underlined that once an appropriate computer system is installed it can be used for more than one purpose almost simultaneously. A worldwide assesment of most profitable computer applications 4/ revealed that the benefit/cost ratio is the highest for integrated systems in which several of the possible applications are implemented.

EQUIPMENT AND PROCEDURES IN THE LABORATORY

Recently there has been tremendous change in the organization of work in many laboratories. The introduction of microelectronics and the closely related computer controlled instruments transformed the entire concept of measurement and experimentation as compared to the classical one.

Current instruments are fairly compact and easy to operate because they work under programmed microprocessor control. There are almost no manual controls but only a few keys to enter instructions when the program asks for them through questions /text/ appearing on a video display. The commercial programs usually contain also help routines for additional explanation. This means that if occasionally the operator needs detailed information regarding the exact content of a question or the consequences of a definite answer, help can be called up from the storage and displayed in the form of explanatory text. Usually the software system includes a standard text editor which can be utilized to produce any help-texts deemed necessary for the local operating staff or to translate the commercial sentences to a language better understandable for them. As an extreme one could state that any person capable of reading could operate such apparatus.

Microcomputers allow to prepare measurement programs for several users. Each program is identified as a separate job and can be accomplished sequentially if only a single instrument is available, however, if more units are linked to the computer it can control them simultaneously while executing several jobs in parallel. Such multiuser operation renders evident that assignment of separate data files to each measurement is an essential part of the program assembly.

After actuating a single START button very complex functions can be accomplished by the system without operator intervention. After the evaluation of a sub-set of measured data the control can even modify the parameters in order to obtain optimum performance. System errors are largely eliminated because the microprocessor will permit no measurements to be made until and unless all parts of the system are tested and are in perfect working condition. The same microprocessor which controls the measurement can carry out calculations and display or print the results in different formats as required by the user. The general scheme of a microprocessor control unit can be seen in Fig. 1.

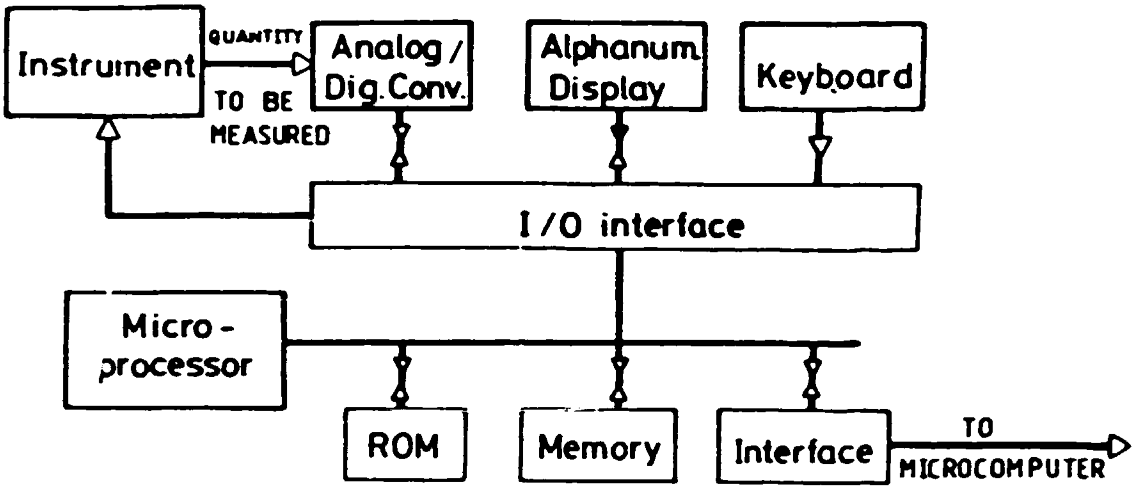


Fig. 1. General arrangement of a microprocessor controlled measurement

The digital results are also available at an output and can be directly transferred to another instrument or a computer for higher level of processing. This possibility is usually provided by linking all units of the system to a common interface bus. The compatibility of instruments and computers is assured by the application of standard interfaces. The interface is a shared boundary between instrument and computer providing for information transfer. In physical implementation it can be a serial /slow/ or parallel /fast/ interface with point-to-point or highway /multipoint or bus/connection. There exist standardized forms for each of these. In laboratory instrumentation perhaps most widely used are those in compliance with CCITT V24 5/ or its American counterpart EIA RS232-C. The interface compatibility is an important condition to include units in such a system.

Thus usually a hierarchy is built in the laboratory where a central micro-computer manages all information and the measurements, co-ordinates the individual operations which in turn are controlled by microprocessors. A typical small-scale hierarchical laboratory computer/instrument network is illustrated in Fig. 2.

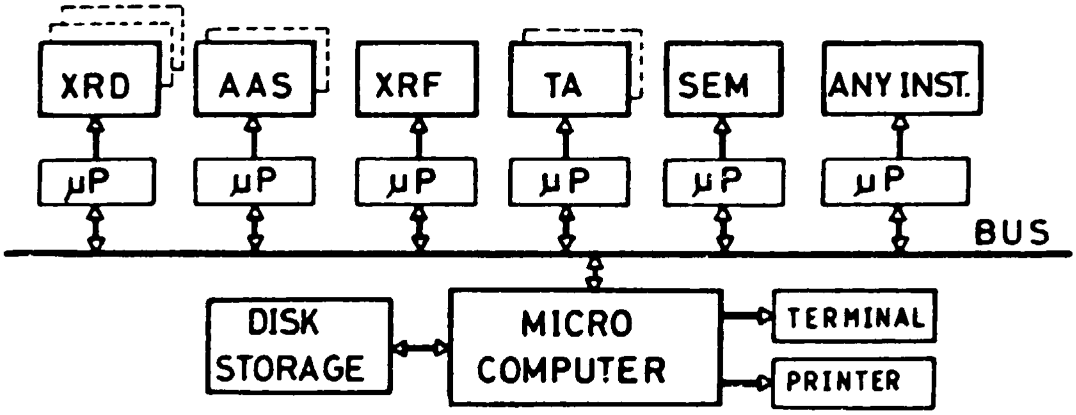


Fig. 2. Microcomputer controlled labratory network.

Microprocessor controlled instruments can be purchased from all major manufacturers "off the shelf" together with some basic software to execute certain general measurements. Unfortunately there are rarely two laboratories with exactly the same tasks therefore parts of the system must be "custom built". No matter whether this is done by the supplier of the commercial instruments or the users, an all important involvement of personnel who will finally use the system in practice must be maintained. It is also advisable to have at least one member of the user team trained in the more specialized aspects of operation and maintenance of the installed system.

With the general application of digital techniques the instruments became more sophisticated. Users should be aware that under such circumstances most important features of instrumentation are as follows:

- stability = the preservation of constant working condition despite changes in the environment /fluctuations of the supplies, temperature etc./
- reliability = high proportion between the hours when the apparatus is found in perfect order and the hours when it fails /down time/
- sensitivity = high response to slight input effects

- signal to noise ratio = the proportion between the useful response and effects irrelevant to the measurement, caused by the environment. High sensitivity is only useful if the signal-to-noise ratio is high enough
- reproducibility = a compounded consequence of the previously listed characteristics. Ability of the system to yield identical results when the mensurements are repeated after some interval.

LABORATORY INFORMATION MANAGEMENT

As a sample arrives into the laboratory for assessment it brings along definite information about its origin, eventual previous treatments and as it travels through the laboratory the measurements carried out on the sample yield additional information. Intelligence is needed to gather and use that information effectively. Intelligence for isolated tasks, like bookkeeping of the samples can be solved by dedicated microprocessors, but if an appropriate microcomputer is used it can provide for the overall control of diverse jobs in the laboratory as illustrated in Fig. 3.

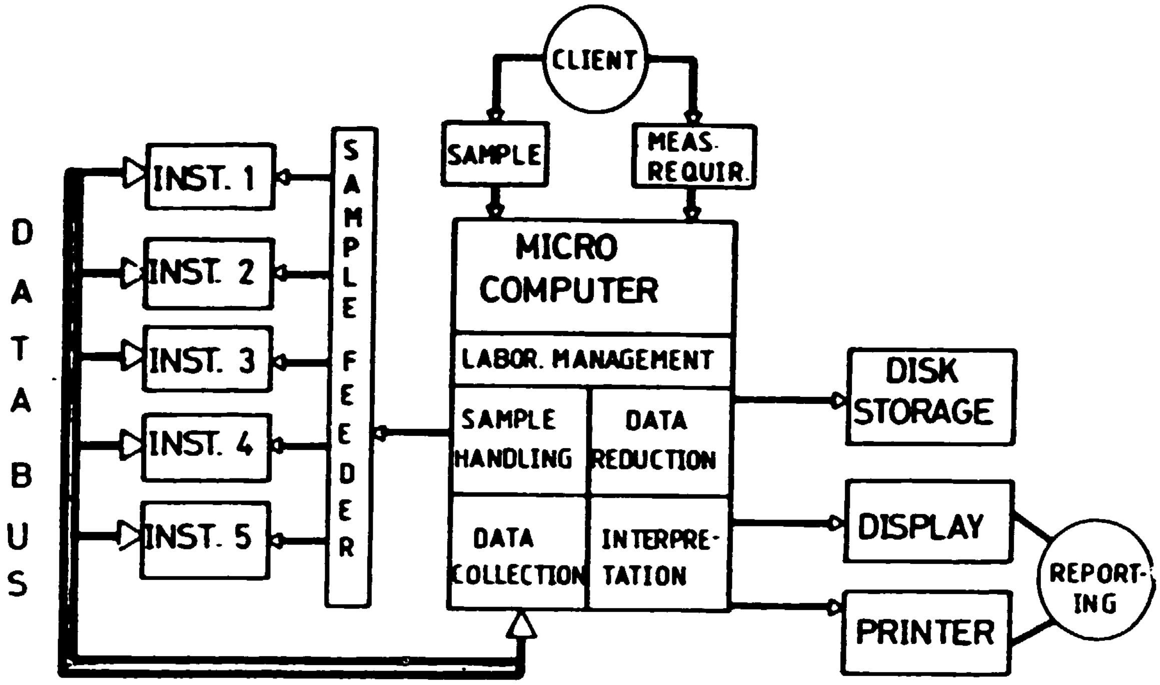


Fig. 3. Multitask laboratory automation system

The information management microcomputer will take care first of all of the identification of the samples as they arrive from different "customers" for evaluation. In the case of mineral labs Customers can be groups of field geologists producing hundreds of samples from a network of drill holes, mining engineers requiring fast quality control of the currently produced ore, and in the context of these guidelines first of all sales departments interested in the quality of averaged material to be found at a storage area or just delivered. Using several levels of identification, a clever program logs in the samples, say, by customer code /batch, lot, series, group/ and a serial number. This information must be keyed in by an operator through a keyboard or an optical decoder can read it from written information accompanying the sample. Anyhow, the person in service at this post does not need a computer science degree because commercially available programs guide all operations in the form of a dialog, the questions of which appear on a display /TV screen or window on the instrument / and only the adequate answers must be given more often than not with single keystrokes, however very carefully. Computers have very powerful intelligence to handle data, control measurements, repeat exactly the same operations, but they never can correct wrong inputs or change false semples for right ones. Microcomputer systems can offer even clear and concise error messages if the program is evidently mishandled, activate alarms when the test results are out of specification, nevertheless, there is no protection against mixing the samples, wrong characters or figures hidden in the input etc. Although the computers role is very important it must not be forgotten that it is merely a tool to be used by the analyst to accomplish their jobs. The computer permits the application of methods never before possible without its arithmetic power and provides a means by which the appraiser can seek solutions to complex problems that had been too time consuming to produce using manual techniques.

Up-to-date information management programs are as flexible as to understand words unique to any company or industry, they can be instructed in local languages, thus the terminology used in any particular laboratory or plant can be continuously used after introducing the computerized system.

Simultaneously with the logging function the computer can do many auxiliary laboratory jobs - print bottle labels, prescribe the further route of the sample throughout the lab in accordance with the type of the material and the requirements of the ordering party /worklist/, schedule the measurements with due account to priorities and special circumstances like the stability of the sample in time, give instructions about the access to the produced data if they are confidental. Advanced systems do not require for all these any programming on the users part, but offer menus whereoff individual operators can select functions they need and ignore those they do not.

The worklist finally prepared in this phase determines the operations to be carried out in the laboratory on any particular mineral sample. The instruments used for the determination of chemical composition and crystallographic phase analysis can be more or less automated. The results of those measurements which are still under human control and evaluated by manual calculations can be entered into the information management system through a terminal. In this manner subsystems of the laboratory can live together albeit their technical level can be quite different. The results will be integrated by the computer and processed uniformly.

In what follows advanced computer controlled instrumentation will be desribed for the determination of mineral characteristics.

CHEMICAL COMPOSITION

Classical wet chemistry is difficult to automate, therefore it becomes gradually replaced by instrumental methods like X-ray fluorescence analysis /XRF/, /6/ and atomic absorption spectrometry /AAS/ /7/ which readily yield for computer control.

X-ray fluorescence analysis

In the chemical analysis of ores X-ray fluorescence has several advantages therefore it has widespread application in the mineral industry. Elements of the periodic table from atomic number 5 to 92, including all metals can be quantitatively determined by this method from very low to very high concentrations.

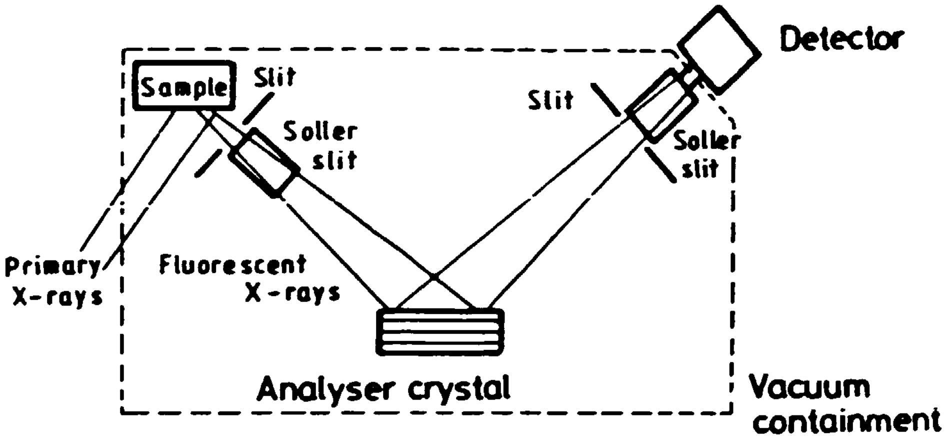


Fig. 4. Principle scheme of XRF.

The basic arrangement of a fluorescent X-ray spectrometer is illustrated on Fig. 4. The primary X-rays emitted from a spectrometric tube exite fluorescent /secondary/ radiation from the specimen. The spectrum of this fluorescent radiation is composed from peaks characteristic for the elements present in the minerals constituting the ore. The measured intensity of the peaks is influenced by experimental conditions and by the concentration of the components. After duly compensating for the instrumental effects by means of a calibration procedure, quantitative results can be computed. Homogeneity of the specimen is a crucial requirement.

In the most sophisticated equipment a few grams of the mineral sample is introduced into an automatic sample preparation unit. Here it is mixed with a flux material /$Na_2B_4O_7$ or $Li_2B_4O_7$ are frequently utilized/ after appropriate crushing and in a high frequency furnace at elevated temperature a homogeneous solution is formed. When cooled from the molten state this solidifies as a "bead". Alternatively, there exists automatic equipment to prepare pressed pellets with stable smooth surface, which can be used for measurement under certain conditions. Thereafter the specimen is placed in a holder and hundreds of coded holders can be transported by a conveyor automatically to a sample changer which brings the samples into the vacuum chamber of the spectrometer where the analysis will take place. When the microprocessor reads the code from the specimen holder all instrumental parameters are adjusted according to the needs of the analysis to be carried out on the particular material. The intensity of the exiting X-rays coming from the primary tube is controlled via the high voltage and current supplied by the generator and also by the slits, filters brought into the beam. Electronic units take care for the high stability /power fluctuations less than 0.01%/ of the supply. The type of analyzer crystal and that of the detector with the corresponding supply and the parameters of the electronic units used for radiation measurement are set automatically to obtain the required accuracy within the shortest possible time. The printed final report indicates usually the error of measurement /standard deviation/, too.

There are two main principles of detection: sequential and simultaneous. In the <u>sequential spectrometer</u> a mechanically coupled analyser crystal and counter scan the wavelength spectrum and detect the fluorescent intensity as a function of wavelength /which in fact is deduced from the angular position of the detector/. The geometric position of the analyser crystal /θ°/ and that of the detector /$2\theta^{\circ}$/ are adjusted on the high precision goniometer to an accuracy of $\Delta\theta = 0.01^{\circ}$ under program control corresponding to each chemical element. Since in this way measurements for the different elements are separated in time, stabilization of environmental conditions like vacuum and temperature are primordial. Variations of the latter are held usually within ± 0,5°C in the goniometers cabinet. Essential information on system functions is generally displayed on the instrument's front panel. Analog meters might indicate parameters while the measurement status can be followed from short text indications on another display. Vacuum, tube cooling, detector gas supply are monitored and should any of these cease to function normally, visual and audible alarms are given and the measuring will be stopped. The microprocessor will allow measurements to proceed only when all functions are normal.

In simultaneous spectrometers about 30 elements can be analysed at the same time because a separate channel is fixed for the optimum detection of each element. This assures much shorter measurement times, however, the user must pay with considerably higher investment costs for the larger throughput. The installation of simultaneous spectrometers is justified first of all in laboratories where a large number of similar samples is analysed for a pre-determined group of elements. This can be the very situation in some mineral laboratories. Sequential X-ray fluorescence instruments on the other hand are more flexible and therefore rather research oriented devices capable to analyse at a lower pace variable samples.

Energy dispersive spectrometers use stationary solid state detectors and advanced data processing for the simultaneous measurement of several elements. These spectrometers are less expensive than the wavelength dispersive simultaneous instruments but their sensitivity and accuracy is lower especially for the light elements. They find application mainly in connection with other instruments like electron beam devices and will not be taken into consideration here as general analytical instruments.

While data collection and running of the measurement programs is controlled in spectrometers by the integrated microprocessors, the more demanding data processing is transferred to a minicomputer which can be the central intelligence of the laboratory. The various measuring programs, eventually using different strategies for definite purposes, are developed and stored also here. At the start of a shift or other unit of operations the appropriate programs are selected in an interactive dialog type communication with the computer via the video terminal and then transferred for execution to the microprocessor. Although the microcomputer is free thereafter for other jobs it continues to periodically supervise the spectrometer's performance. Some extent of pre-processing, like background correction etc, can be carried out by the microprocessor but X-ray spectrometric quantitative analysis involves the use of software packages requiring processing capacities beyond the potentials of present microprocessors.

The algorithm normally used to convert measured intensities to concentrations by regression analysis can be written as

$$C_i = \left[A_i I_j + B_i\right]\left[1 + \sum_{\substack{j=1 \\ j \neq k}}^{n} \alpha_{ij} C_j + \sum_{\substack{k=1 \\ k \neq j}}^{n} \frac{\beta_{ik} C_k}{1 + C_i}\right]$$

where I = raw counts

C = concentration

A,B = straight line coefficients

α = matrix absorption coefficients

β = matrix enhancement coefficients

i = index of analyte

j,k = indices of correction elements.

The appropriate program can be implemented on 64-128 k word microcomputers and vendors must supply it together with the instrument. Fixed Winchester or floppy disk mass storage is necessary for the calibration information included in the values of proportionality coefficients /alphas/. These can be determined in a previously applied special routine from measurements on standard samples or calculated by simulation or taken from external sources. There exists some doubt about the transportability of alpha coefficients 8/. Among the reasons are failure to adequately separate instrumental and matrix dependent effects, poor quality of the calibration standards, inadequacy of the regression analysis program used in the derivation of the alpha coefficients, insufficient homogeneity of the specimens. Again it must be stressed that computers give some kind of results after each run, but these will be reliable only if the experimental conditions under which the reference data are valid and for which the program is verified, are painstakingly and intelligently obeyed. Should this be the case, the X-ray fluorescence spectrometer will analyse in a couple of minutes a specimen for 15-20 elements with an error less then 1 rel% and display, print or store the result as programmed.

X-ray spectrometers may be installed in field laboratories or even in mines, at the site of production. For special remote applications the fluorescence spectrum can be exited instead of by a primary X-ray tube by radiation emitted from a radioactive source. In this case very low power is sufficient and no water cooling is necessary for the operation of the equipment. Such instruments were introduced e.g. for quality control in copper mines. The results are usually reported by telephone to the central lab where it is entered by means of a **terminal** to the computer for processing.

There are some cases when X-ray spectrometry is used not merely for chemical analysis but also to gain supplementary information on the valence state of an ion from precise determination of peak shifts. E.g. in phosphate ores the percentage distribution of sulfur in different oxydation or chemical bond states /S^{6+} and S^{2-}, respectively/ is an important factor in value determination because it could effect subsequent thermal or chemical benefication routes. The percentages of the sulphide and sulphate components can be determined by computer aided calculations manipulating with a fair number of intensities measured around the peak. 9/

Atomic absorption spectrometry

The atomic absorption process is illustrated in Fig. 5. A light source emits the sharp atomic lines of the element to be determined. The initial intensity I_o at the selected resonance wavelength is focused on the flame cell containing ground state atoms of the material analysed. The atoms are introduced into the flame by a nebulizer device. The sample aerosol is mixed in a chamber with the fuel and oxidant gases. In the burner head combustion and atomisation occur in the flame. The initial light intensity is decreased by an amount depending on the atom concentration in the flame. The light is directed onto a detector where the reduced intensity, I, is measured. $T = I/I_0$ indicates the fraction of light which passes through the flame cell and is called transmittance. A purely mathematical quantity can be defined using the reciprocal of the transmittance.

$$A = \log 1/T = \log I_0/I$$

is termed "absorbance". Since the absorbance follows a linear relationship with concentration this quantity seems to be the most convenient term for describing light absorption atomic spectroscopy. According to Beer's law:

$$A = a.b.c$$

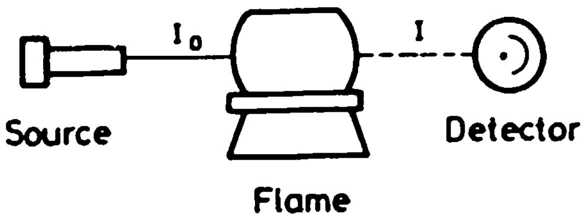


Fig. 5. The principle of atomic absorption spectrometry

where A is the absorbance defined above, a is the absorption coefficient, a constant characteristic of the absorbing species, b is the length of light path intercepted by the absorption cell and c is the concentration of the absorbing species in the cell. This equation simply states that the absorbance is directly proportional to the concentration of the absorbing atoms for a given set of instrumental conditions.

The microelectronics age brought about totally automated atomic absorption spectrometers. All parameters like the intensity of the primary source, gas flow to the burner, voltage on the photomultiplier are under microprocessor control. Setting of the wavelength in the analyser section or the adjustment of the flow rate of gas are done more accurately than any experienced operator could do it with a conventional instrument.

In the operation of an atomic absorption spectrometer safety has been for a long time a worrying concern. With the gas mixtures used there is a certain danger of explosions. Microprocessors not only monitor gas leakage and give alarm if it occurs, but prevent any backflash by igniting and extinguishing the flame in a safe order. The proper gas flow ratio is checked and gas valves operated and closed in a programmed sequence. If e.g. the incoming gas pressure is too low for safe flame operation, it can not be ignited. While the flame is lit an optical sensor watches the flame and if it goes out during an analysis the gas valves will shut in proper sequence to assure the analyst of the safest working condition. No operation will be permitted if anything is missing for total safety.

Quantitative analysis requires also some calibration efforts and corrections of the raw data. In atomic absorption spectrometry spectral interferences are virtually absent due to the strong specificity of the system composed from a modulated primary light source and a selective amplifier tuned to the same modulation frequency. However, a disturbing background might be caused by higher concentrations of molecular species, small droplets, salt particles or smoke which may absorb or scatter part of the light emitted from the primary light source. This occurs when during the atomization process a residual amount of matrix component is volatilized. When no background correction is applied this leads to incorrect analytical indications.

In most commercial designs double beam arrangement is realized with a deuterium arc lamp for background correction. The intensities of both the hollow cathode lamp used for primary source and that of the deuterium lamp are stabilized and adjusted automatically to match each other. Gains in the two beams are monitored and continuously set to assure optimal performance of the instrument at all times. Meanwhile the background correction is carried out continuously.

Matrix interferences are present when physical characteristics /e.g. surface tension, viscosity/ of the samples and the standard differ. This interferences can cause either suppression or enhancement of the instrumental indication and must be corrected to avoid erroneous results. The calibration method of standard additions make it possible to obtain accurate determinations in the presence of matrix interferences. In this mode one original sample and a number of standard additions are used. Another mode of calibration makes use of several standards to allow direct and accurate readings of concentrations even if the calibration curve shows significant deviation from linearity. The accuracy of calibration computed for non-linear relationship between concentration and absorbance depends on the number of standards and the equation used for calibration. Usually three standards are sufficient, however, for very non-linear working curves a choice of calibration with more standards is possible. In one commercially realized microcomputer controlled atomic absorption spectrometer it is feasible to use eight standards for calibration. The optimum algorithm for curve linearization is selected by the user or automatically as a function of the degree of curvature which is found, by least square fitting.

Aided by a microprocessor, manual operation consists merely of answering by keystrokes menu type dialog questions, filling in blank parameter spaces, checking displayed calibration curves and of course preparing and bringing samples to the automatic feeder mechanism.

Furthermore, most instruments can be linked to a computer via a two-way RS-232C interface. This means that the user can program complicated analytical tests or create an analytical library and store it on floppy disks for all elements of interest and the mirocomputer can in one way through the interface control all parameters of the measurement once the appropriate instructions had been retrieved from the library and loaded into the memory. Normal size sample trays accommodate about 50 samples including a blank and some standards. The lamp turrets hold 4-8 different lamps. Some manufacturers offer also twin lamps, for the analysis of two elements. Flexible programming provides then for combinations of calibration, sample analysis for the elements represented by the lamps, repetitions and so on. Sequential measurement of the individual elements in all samples is advantageous because then optimum conditions can be set for each chemical element no matter what gas-mixture is required in the burner, whether a trace element or a main component will be analysed. Typical time for analysing 5 elements in 50 samples may be about 25 min.

In the opposite way the measured and corrected data flow through the interface into the data storage will be processed and listed for the user in adequate time by the computer.

Although everything can run smoothly under the control of the microprocessor integrated into the instrument and/or under the supervision of the computer, such an assembly is very flexible and gives also room for experimentation, up-datings or any changes deemed necessary by the user. When the operators are beginners they can benefit from the tremendous general experience accumulated in the hardware and software of an advanced system, however, getting familiar with the method and instrumentation almost no barriers will be found trying to optimize the system for particular local problems. It is appropriate to emphasize here that this kind of conscious development activity becomes sooner or later a must. This might be a serious challenge nevertheless, it can not be avoided. Pushing only buttons without the knowledge of what kinds of instrumental response are avoked in this way, seems to be a very dangerous practice. Automatic instruments and computers return in most cases some results or error messages. Whether the figures read are the desired right ones or not and how to correct the errors can be decided only by operators who have fair insight into the working principles, mechanisms and algorithms utilized by the system.

This kind of awareness and caution is needed eminently in sample preparation.

The general rules of sampling are described in relevant international standards[10]. Anyhow care should be taken by adequate homogenisation and systematic diminution technique that the few grams or so of sample introduced to the measurement should be representative for the whole material graded.

Liquid and solid materials can be equally analysed by atomic absorption, however, the automatic handling of liquid specimens is more staightforward. Therefore, solid samples must be dissolved before measurement. One possible way leads through solid solution achieved by high temperature melting with the addition of a flux material similarly as for X-ray spectrometry. The mechanical propeties of the solidified "bead" are here uninteresting because it will be thereafter dissolved in an appropriate reagent. When dissolving the samples preference should be given to procedures introducing the smallest amount of foreign substances into the system. During evaluation of the raw measurement data due account should be taken of the additions that can be easily programmed in a computerized interpretation routine.

There exist several other microcomputer controlled instruments of chemical analysis. Some are of general character like emission spectrometers e.g. with inductively coupled plasma torch /ICP/ and others more restricted in applicability like neutron activation analysers /NAA/, where the success of analysis depends on the fact whether the atoms of interest can be activated or not. Nevertheless, the described analytical methods may give an idea how useful are microcomputers to the analyst in all parts of the job, far beyond "computation".

QUANTITATIVE MINERALOGICAL PHASE ANALYSIS

Exact information about the chemical composition of minerals is in many instances not sufficient to determine the commercial value. Another aspect of characterization is to determine the crystallographic phases present in the ore, and furthermore measure the quantity of each component identified. Several methods have been introduced for this purpose, however, X-ray diffraction 11/ seems to be the most generally applicable. This technique will be described in the first place and the most thoroughly. Nevertheless, in some cases other methods might be sufficient or even more adequate and more frequently than not supplementary measurements are necessary in addition to X-ray diffraction in order to obtain optimum results. From among the several reasonably applicable phase analytical methods infrared spectrophotometry 12/ and thermal analysis 13/ are included in this review.

X-ray diffractometry

Instrumentation, collection of experimental data

Powder diffractometers consist of several units. Most important of these: the goniometers should be manufactured to high mechanical precision but their working principle, as shown in Fig. 6, is fairly simple.

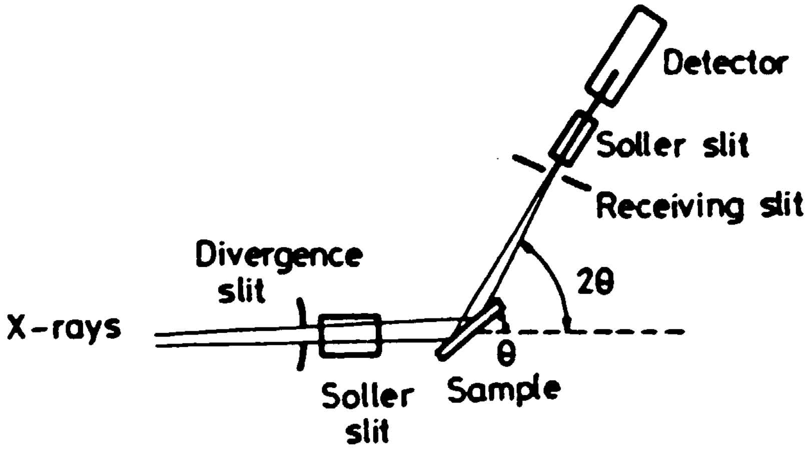


Fig. 6. Basic arrangement of an X-ray goniometer

Collimated X-rays of appropriate wavelength impinge on a flat specimen prepared from finely ground /to about 5-25 μm particle size/ mineral sample. Using a radiation sensitive detector mounted on an arm which can travel in a definitely oriented plane circularly around the sample, it is possible to measure the intensity distribution of radiation scattered by the sample. If the sample is crystalline like minerals, at certain angular positions of the detector local maxima will occur in this radiation distribution. These local maxima are referred to usually as "lines" of the diffraction "pattern". Experience proved that a unique diffraction pattern can be assigned to each mineral in the sense that the peak intensities /lines/ appear at locations and with relative magnitudes characteristic for the mineral species investigated. Chemical information enhances this uniqueness.

For good definition of the line positions a so called parafocusing arrangement is used in the goniometers. This requires that the X-ray source, the sample and the detector should be on a circle co-planar with the incident and reflected beam as well as with the normal to the surface of the flat specimen. Moreover a coupling is established between specimen and detector movements in a way that the surface of the specimen bisects the angle between the incident and reflected beams. As a result of this $\theta:2\theta$ coupling the specimen rotates with half speed /θ/sec/ as compared to the detector /2θ/sec/ and the specimen's surface is always tangent to the focusing circle of continuously varying radius.

Recently manufactured goniometers are equipped with 20 - 35 position automatic sample changers which in the same way as all other mechanically moving parts are remotely controlled by digital signals acting generally on stepper motors.

The peaks of reflected intensity are measured against a background and the inherent signal-to-noise ratio is considerably improved if a monochromator is applied to the reflected radiation in front of the detector, which is usually a scintillation or proportional counter.

Important part of the equipment is the highly stabilized / ±0.01 % power fluctuation/ generator supplying high tension and current to the X-ray tube/s/ with a maximum loadability of 3-4 kW. Water cooling of this generator and the tube/s/ is provided by a closed loop pumping/refrigerating system under electronic control.

The detector signal, consisting of pulses, is fed to electronic processors and after appropriate shaping and sorting is digitally counted by the attached microcomputer according to preprogrammed strategy.

Present day measurements are more importantly influenced by software than by the above described advanced hardware well prepared for computer control. Thus, software has a substantial share in the total prize of instrumentation.

Diffractometer manufacturers - about 10 all over the globe - offer complete systems including in modular arrangement hardware and software components capable to accomplish different commonly occurring tasks. Each make is distinguished by some unique features, however, the similarities in performance are more prominent. Consequently it is viable to outline in general the state-of-the-art materialized in present day microcomputer controlled diffractometers. Software takes care for three important areas of activity: a/ setting up the measurement, b/ execution of data collecting and c/ data reduction and interpretation.

The measurement program including all experimental parameters like angular limits, continuous scan or step-by-step counting, repetitions, presentation of data in definite formats, storage on selected medium, etc. can be set up before running the actual measurement by means of a "menu" type presentation of the various alternatives on a display /CRT/. The operator has only to accept the built in default values /suggested commands of most general applicability/ or specify his decisions answering by appropriate numeric values or by "yes"/"no" to the questions appearing in plain language and rarely requiring the use of mnemonics or codes. /Fig. 7./ Proceeding by commands given as prompted by the line-by-line

```
SAMPLE ID(16 CHAR): IRON ORE 6284121

X-RAYS KV=40:Y
       MA=50: Y
STARTING ANGLE = 5.0: Y
FINAL ANGLE = 100: 60
SCANNING SPEED (0.125;0.25;0.5;1;2  2THETA/MIN): 0.5
STEP SIZE N(0.01XN): 5
CRT DISPLAY (Y/N): Y
HARD COPY RECORD (Y/N): Y
DATA STORED (Y/N): N
```

Fig. 7. Typical "set up conversation"

guidance of the "menu" is a relatively slow process, however, when the user accumulates more experience it is possible to claim several commands in one line and speed up thereby the operation.

During the data collection phase the computer controls the automatic execution of the desired measurements and the raw data /i.e. 2θ positions of the detector together with the corresponding I intensities/ are stored in the appropriate files allowing repetitive treatments or processing of the original data sets.

Once the measurement is started it is continued autonomously, if necessary 24 hours a day, while the computer can be exploited for other tasks like preparation of further diffractometry programs or processing of already collected data.

Data reduction entails several steps of processing in order to gain from the as measured data quantitites which are more directly related to the identity of mineral components and their quantity present. These are the locations and the intensities of the peaks. Some kind of more or less arbitrary definition must be accepted for these in order to be able to determine them from a set of measured 2θ-I data /Fig. 8./. First of all the background radiation must be substracted to find the baseline relative to which the diffracted radiation due to the crystalline sample must be taken into account. The background falling under the baseline is caused by instrumental imperfections, by cosmic radiation, natural radioactivity and by eventual noncrystalline components or fluorescence of the mineral sample.

Various algorithms can be used to determine the baseline as cited by Bárdossy et.al 14/. These authors use e.g. the fllowing three step routine:

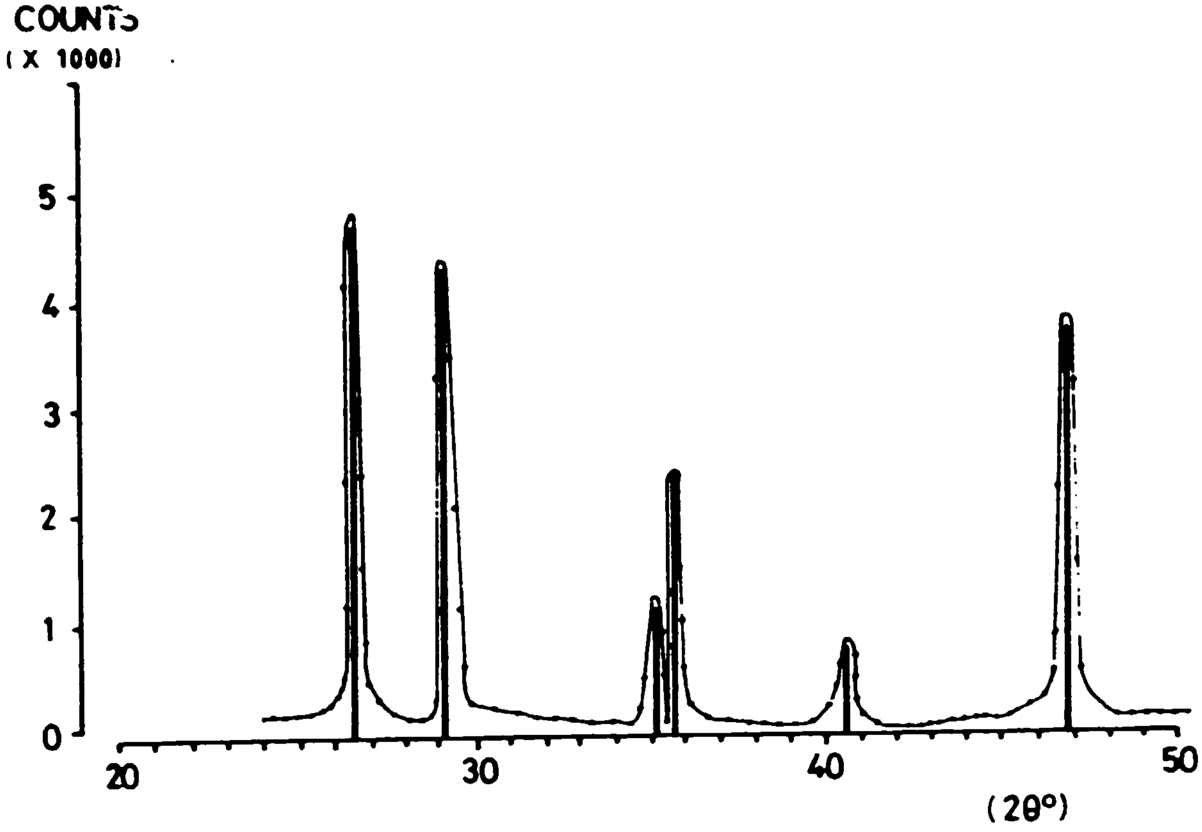
/a/ the measured counts are gathered into groups of tens, and then the average value within each subgroup is assigned to the first point;

/b/ a set of averages monotonously decreasing with the 2θ angle is selected; and

/c/ the final baseline is fitted to those points of this set which can be connected by straight lines with decreasing slopes all way.

Many microcomputer programs apply peak search by second derivative technique, because the peaks of the second derivative function indicate very sensitively the peak positions in the original pattern even in the case of serious overlappings.

The 2θ locations of the peaks are then transformed



PEAK POSITION	WIDTH (DEG)	HEIGHT (CPS)	BACKGRD (CPS)	D (NM)
26.620	0.16	4858	159	3.3441
29.350	0.22	4396	119	3.0389
35.095	0.21	1056	92	2.5535
35.605	0.15	2470	88	2.5181
40.830	0.22	918	88	2.2071
46.960	0.28	3931	102	1.9323

Fig. 8. Raw and reduced data of a diffraction pattern

to a set of d_i values by the simple /Bragg/ equation

$$d_i = \frac{\lambda}{2 \sin \theta_i}$$

where λ is the wavelength of the radiation.

The angular position corresponding to a local maximum intensity, the center of gravity of the distribution around the peak and the median of a cord taken at a definite height /1/2 of the maximum value or 1/10 of the same, are commonly used/ can equally be regarded as the position of the peak. Consideration of errors and computer time involved in the application of one or another of the above definitions can lead to the choice of a particular algorithm implemented for the determination of peak positions.

The intensity assigned to each peak can also be calculated in more than one way. The maximum value within the distribution or alternatively the sum of all counts above background in the region of the peak can be taken as well. The latter is called the integrated intensity and is less prone to errors.

Definition of peak positions and corresponding intensities as well as the choice among different computer algorithms becomes more critical when the diffraction pattern contains overlapping peaks. Thorough understanding of the underlaying physical principles and utilized computer solution might be crucial for the operator in order to obtain reliable evaluation of the data.

Application of the experimental data

When the measured quantities had been reduced by means of the microcomputer to the set of d values, peak widths and intensities, two main applications are of high value in the evaluation of ores:

a/ identification of phases and

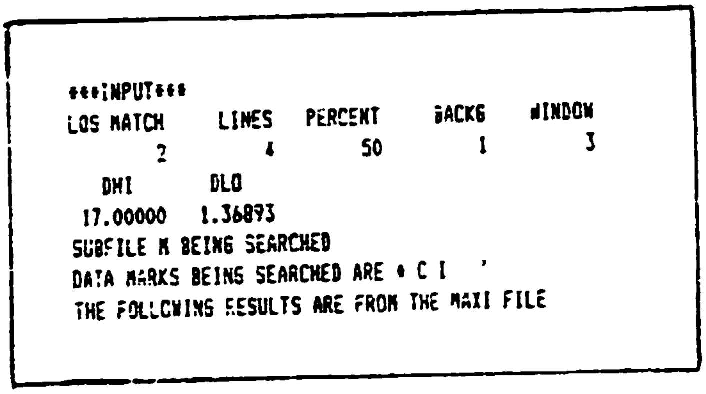
b/ determination of phase percentages.

Mineral data for identification are commercially delivered with many a computer controlled diffractometer system. The JCPDS International Centre for Diffraction Data 15/ offers data files of different coverages. The most extended one contains in its 1984 version reference data for about 46 000 substances of all sorts: inorganic, organic, metals and minerals. The storage and handling of this "maxi" file requires considerable memory and computing capacity generally beyond that of the present day microcomputers. However, the "mini" file of minerals includes only 3800 data sets, which is a manageable quantity for these devices. For identification work within a particular group of minerals the number of data sets to be compared with the unknown one can be further reduced and a "micro" bank well fitted to the individual /industrial or mining/ problem can be created.

A special mini search program is available for identifications by microcomputer facilities with video display and at least a dual floppy disk drive . This commercial software performs a search emulating conventional manual procedures on a mini file of 200 preselected patterns using 16 d values from each reference data set and up to 50 d values measured for the unknown.

JCPDS offers the service to compile mini data sets on a lease agreement according to the customer's specifications. Most proprietary programs supplied by the manufacturers of microcomputer controlled X-ray powder diffractometers allow to create a user defined data base consisting of the most frequently used 800-1000 data sets. Restrictions of the search introduced e.g. by additional chemical information render the computer aided identification with reference to user compiled subfiles extremely fast. On the other hand these restricted search operations are more than sufficient for the purposes of the mineral industry.

The JCPDS search program written by G.G.Johnson and V.Vand 16/ works also in an interactive conversational manner. A typical conversation with explanations is shown in Fig. 9. /a/-/e/. In this example an unknown mineral will be identified. 17/



```
***INPUT***
LOS MATCH     LINES   PERCENT     BACKG     WINDOW
        2         4        50         1          3
   DHI        DLO
 17.00000   1.36893
SUBFILE M BEING SEARCHED
DATA MARKS BEING SEARCHED ARE * C I   '
THE FOLLOWING RESULTS ARE FROM THE MAXI FILE
```

Fig. 9. /a/ Input conversation of the crystallographic search program

LINES indicates that that at least 4 lines above background must match for any given PDF pattern in order to be considered in the TOP ONES top-50 listing. 50 PERCENT of the lines above background in a PDF pattern must appear in the INPUT data. The background intensity is 1. A d-WINDOW of 3 is in use /this is approximately equivalent to a delta-two-theta of 0.3 degrees/. This larger window allows for shifts in the positions of lines due to solid solution that is so common in minerals. Because we know the specimen is a rock, we specify a search of only the MINERAL POWDER DIFFRACTION FILE /SUBFILE M/. In this problem no chemical information has been entered. The results will be based only on the d-I data.

```
UNKNOWN SPACINGS AND INTENSITIES WITH ERROR WINDOW

        8.5714       10       8.8106    8.3682
        8.4651        8       8.6580    8.2305
        5.3691        7       5.4496    5.2770
        4.9252        4       4.9875    4.8426
        4.8636        1       4.9363    4.7962
        4.6829        2       4.7506    4.6199
        4.5300        1       4.6404    4.5147
        4.2664        1       4.3197    4.2105
        4.0990       11       4.1580    4.0558
        3.9403        3       3.8835    3.7951
        3.7494        1       3.7951    3.7106
        3.4809       18       3.5149    3.4423
        3.4218       58       3.4542    3.3841
        3.3898       12       3.4189    3.3501
        3.3696       16       3.4072    3.3389
        3.2226        1       3.2520    3.1898
        3.1600        8       3.1898    3.1299
        3.1371       22       3.1696    3.1104
        3.0491       12       3.0817    3.0257
        3.0228       10       3.0534    2.9985
        2.8928        2       2.9197    2.8694
        2.8470        1       2.8694    2.8209
            (plus 53 additional lines to 1.375 A)
```

Fig. 9. /b/. Input data for the search program

The first output of the computer will be as shown in Fig. 9. /c/.

```
 ***TOPONES***
                                                NUM PER MIN LOG D-D D-I
  PDF     FORMULA                           REL
 NUMBER                                    FACTOR

100173 AL2 O3                              *4 66 12 100  0  25 .80 .82
310616 FE2 AL4 SI5 O18                     I4 48 25  96  6   6 .77 .64
210995 K2 MG ( S O4 )2 . 4 H2 O            I4 45  4  80 15   3 .75 .75
 70390 CA3 ( FE, TI )2 ( SI, TI )3 O12     I4 44  7  88  6   3 .71 .70
130293 MG2 AL4 SI5 O18                     *4 44 17  94  3  10 .78 .60
150800 NA2 C O3 . 10 H2 O                  *4 44  9  75 15   3 .83 .70
220018 AL2 SI O5                           *4 44 23  92  0  10 .75 .64
291036 ( NA, K ) CA ( SI, AL )6 O12 CL     *4 43  5  83 15   3 .73 .70
301351 TL2 O3                              I4 41  5  63  3   3 .73 .68
110689 SB2 O3                              *4 38  8  89  6   6 .75 .57
150776 AL6 SI2 O13                         *4 36 11  92 10   6 .69 .57
250289 CU4 ( FE, NI )5 S8                  I4 35  7  88  6   3 .57 .71
                 (plus 38 additional possibilities)
```

Fig. 9. /c/ The first proposal for identification of the search program

Here: RELiability FACTORs the closer to 100 the better the fit of d and I values of the mineral listed to the d's and I's in the submitted pattern.

NUMber is that of the lines matched.

PERcent refers to the lines of the PDF pattern that could have been observed.

MINimum difines the smallest intensity considered in the PDF.

LOG gives the goodness of fit of intensities /should be large/

D-D : delta D - overall goodness of fit in D-s

D-I : delta I - overall goodness of fit in I-s

The closer these last two are to unity the better.

Thereafter several functions are performed to present the result in form of reports.

1/ In the first report patterns with greatest RELiability FACTORs are added until a desired fraction of the intensity of the input data is accounted for.

SCALE is the fraction of the unknown's intensity accounted for by the very phase. /Fig. 9. /d//

```
***SUBSTI FINAL REPORT***

  BASED ON ORISINAL PATTERN
   PDF SCALE FORMULAE

 100173 0.553 AL2 O3                                  *4
 310616 0.162 FE2 AL4 SI5 O18                         I4
 210995 0.189 K2 MG ( S O4 )2 . 4 H2 O                I4
 220018 0.292 AL2 SI O5                               *4
  70390 0.059 CA3 ( FE, TI )2 ( SI, TI )3 O12         I4
 130293 0.083 MG2 AL4 SI5 O18                         *4
 150800 0.060 NA2 C O3 . 10 H2 O                      *4
 291036 0.031 ( NA, K ) CA ( SI, AL )6 O12 CL         *4
 301351 0.053 TL2 O3                                  I4
 110689 0.090 SB2 O3                                  *4

R FACTOR   SUM(RESIDUE)/SUM(INITIAL)=    0.259
        (SUM(RESIDUE/INITIAL))/NUMBER OF LINES=    0.197
```

Fig. 9. /d/ The first output report

2/ Report based on sequential substarction and researching of the TOP ONES for the best remaining choices. /Fig. 9. /e//.

```
***SUBSTI FINAL REPORT***

   BASED ON COMPUTER MODIFIED PATTERN
    PDF SCALE FORMULAE

 100173 0.553 AL2 O3             (corundum)         *4
 220018 0.393 AL2 SI O5          (sillimanite)      *4
 130293 0.185 MG2 AL4 SI5 O18  (cordierite)       *4
 310615 0.138 FE2 AL4 SI5 O18                       I4
 181418 0.097 W O3 . H2 O                            4
 110267 0.067 CA V4 O9 . 5 H2 O                     I4
 250285 0.168 CU3 ( ASO .64, SBO .36 ) S4           C4

R FACTOR   SUM(RESIDUE)/SUM(INITIAL)=    0.306
           (SUM(RESIDUE/INITIAL))/NUMBER OF LINES=    0.279
```

Fig. 9. /e/ The second type of report produced by successive substraction

In this last REPORT we find the 3 minerals in the specimen, corundum, sillimanite and cordierite /the names were added to the output/ plus an Fe-analog of corderite and several other minerals that the program believes would help to account for all of the intensity in the submitted pattern. It is likely that the actual cordierite specimen from which the powder data were obtained was a solid solution mineral intermediate in composition between the Mg and Fe end members.

The subtraction algorithm has eliminated patterns 21-995 and 7-390 that were listed in the first REPORT and brought the three correct answers to the top of the list in the second REPORT. Knowing that the specimen is of metamorphic origin, none of the unlikely Sb, Cu, V or M minerals makes sense in the petrological context and, of course, none would appear if chemistry had been determined and entered. The R factors in each REPORT indicate a good, but not exellent, d-I fit and are typical of work with minerals.

It must be clear that the final decision remains up to the analyst. Several runs of the search-match program with different sets of input parameters may result in better identification of the correct composition.

A more direct way of identification can be provided for by microcomputers offering a split video display. In one sector of the screen the computer plots the measured pattern and in an other sector reference data retrieved from the users data bank to be compared with the former as candidates for identification /Fig. 10/. If the patterns had been recorded under the same conditions a substraction may reveal how much or in which parts of the measurement range the patterns match. With some inventive force the user can carry out different manipulations to complete satisfactorily the identification process.

If PDF data are to be used as reference it is

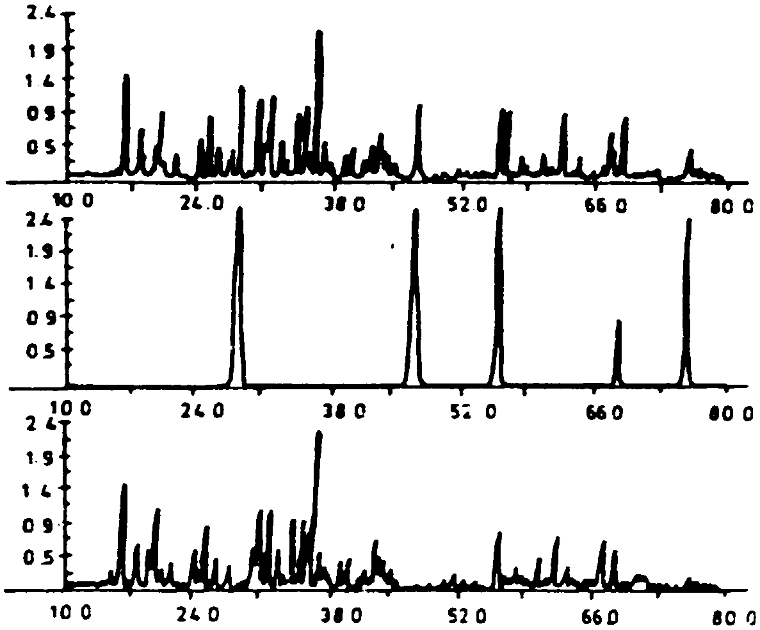


Fig. 10. Use of split screen to diplay measured and reference patterns simultaneously

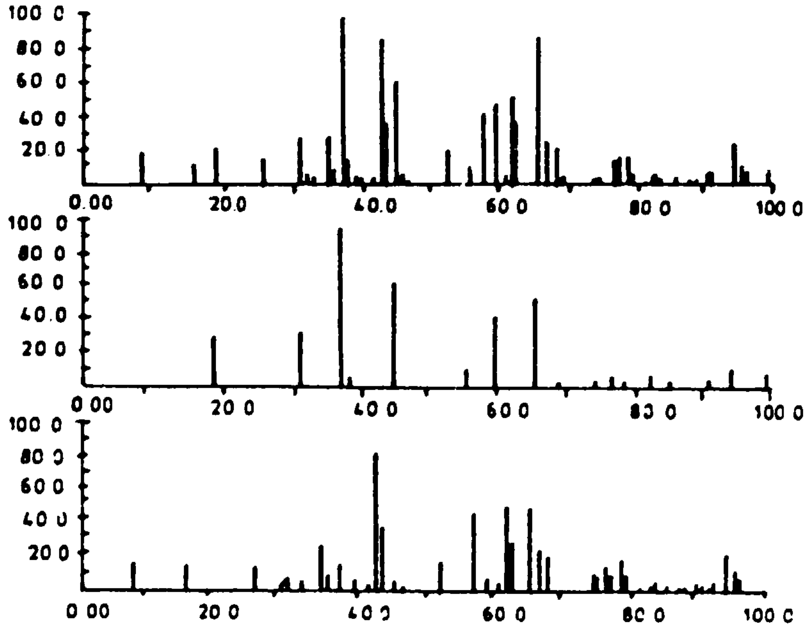


Fig. 11. Representation of data in the form of stick diagrams

comfortable to compare "stick diagrams" /Fig. 11/ since the data in the file are given ready for such presentation and the measured ones can be reduced to the same form. Subtraction and checking of match can then be accomplished on this simplified patterns.

Based on the measured or estimated intensities the JCPDS search-match program yields already a semiquantitative proposal on the concentrations of the minerals present.

However, using appropriate mathematical models the commercial softwares permit more accurate quantitative analysis of the mineral components, too. The input data required for this programs are the integrated intensities obtained after background correction and separation of the overlapping peaks done in advance as well by the microcomputer The different algorithms of concentration calculations need some constants which can be derived by calibration procedures and thereafter stored in the computer memory or backup storage and recalled each time the relevant mineral mixture has to be analysed. For multicomponent mineral systems the most appropriate quantitative analysis seems to be that of the matrix flushing introduced by F. H.Chung 18/. If it is assumed that the total concentration of the mineral components is S /usually equal to 100 %/ then the C_i concentration of the i-th component is given by the formula

$$C_i = \frac{k_i \, I_i}{\sum_j k_j I_j} S \qquad /1/$$

where I_i is the integrated intensity of a peak selected for the analysis procedure in the pattern of the i-th component,

k_i is the conversion factor for this peak,

k_j, I_j have similar definition for the j-th component and the summation in the denominator must be carried out for all components contributing to S.

P. Johnson 19/ established a dedicated mirocomputer system for the analysis of natural hydrothermal systems implementing a similar algorithm.

Bárdossy et al. 14/ used for the quantitative mineralogical analysis of bauxite in the computer input besides the measured and duly corrected diffraction data the results of chemical analysis for the main components, too. These were Al, Fe, Si, Ca, Ti and the loss on ignition /LOI/. Accurately measured shifts in the peak positions were used to determine the actual cation substitutions and in this way to refine the stoichiometry of the minerals. The chemical information is used to subdivide the complete mineralogical analysis to groups containing the same chemical element, i.e. in S of Eg. /1/ only the aluminium bearing, the iron containing, the titanium bearing and so on minerals are taken into account, subsequently. Thereby the eventual uncertainties are limited to the groups formed on the basis of common cations and the overall result are not influenced by the carried on errors. Fig. 12 is the reproduction of a typical output comprising analytical results gained by means of a microcomputer and adaquate for the estimation of the real value of bauxite to be used for alumina recovery. The

```
MINERAL        AL203%  FE203%  SI02%   TI02%   CAO%    P20%    LOI     INT.I    %
-------------------------------------------------------------------------------------
HEMATITE         0.12    7.19                                          19972    7.3
BOEHMITE        29.48                                            5.20  72588   34.7
GOETHITE         1.48   10.61                                    1.46  21045   13.6
GIBBSITE        10.21                                            5.40  22866   15.6
KAOLINITE        8.69           10.23                            3.08  10203   22.0
ANATASE                                 2.09                            9983    2.1
RUTILE                                  0.61                            2351    0.6
CRANDALL         0.72                           0.26    0.90     0.30   1025    2.2
ADS.H20                                                          0.71           0.7
-------------------------------------------------------------------------------------
CALC.CHEM.      50.70   17.80   10.23   2.70    0.26    0.90    16.15          98.8
CHEM.ANAL.      50.70   17.80   10.23   2.70    0.30    0.90    16.20          98.8
```

Fig. 12. Output table of mineralogical phase analysis of bauxite

accuracy is about 5 %/rel/ and an up-to-date microcomputer configuration can yield the results almost simultaneously with the end of data collection.

Since X-ray fluorescence measurements for chemical analysis and X-ray diffraction runs for mineralogical analysis can readily be controlled by the same microcomputer all required data can be collected automatically and manual input can be absolutely avoided.

Even if interactive control at the intermediate stages of data processing is exercized - which is often recommendable - the interpretation of measured data can be carried out in a few minutes, the exact time depending on the extent of operator corrections necessary and on his or her skill.

Infrared spectrometry

Although IR absorption spectrometry can be applied in the mineral industries similarly for the identification and quantitative determination of the components, the basic principle here is different from that in X-ray diffraction and this permits to obtain unique information by this method.

Interaction of IR radiation with material is due to the fact that the bonds existing between atoms

/ions, ionic groups/ can be changed slightly via the absorption of appropriate amount of energy. The range of wavenumbers 4000 - 200 cm^{-1} represent IR radiation with just right energy quanta to be absorbed by the cation-oxygen, cation-hydroxyl, oxygen-hydrogen etc. bonds characteristic for minerals or more generally speaking for inorganic materials.

The specimen is usually a transparent pellet pressed from a homogenized mixture of KBr with a small addition /1 - 3 %/ of the finely ground material to be analysed. Most instruments work on the double beam principle, where a reference pellet /e.g. pure KBr/ is placed in the second beam. By electronic manipulation of the signals from the two channels it can be acheived that the resulting output is the difference of the two spectra, i.e. the absorption spectrum of the sample itself. The absorption spectrum of siderite, the metal bearing mineral in many iron ores can be seen in Fig. 13. Here, as usual in infrared spectrometry, the ordinate represents the percentage of transmitted IR radiation as a function of wavenumber /abscissa/. In some cases the complementary quantity, absorbed radiation is plotted, using a

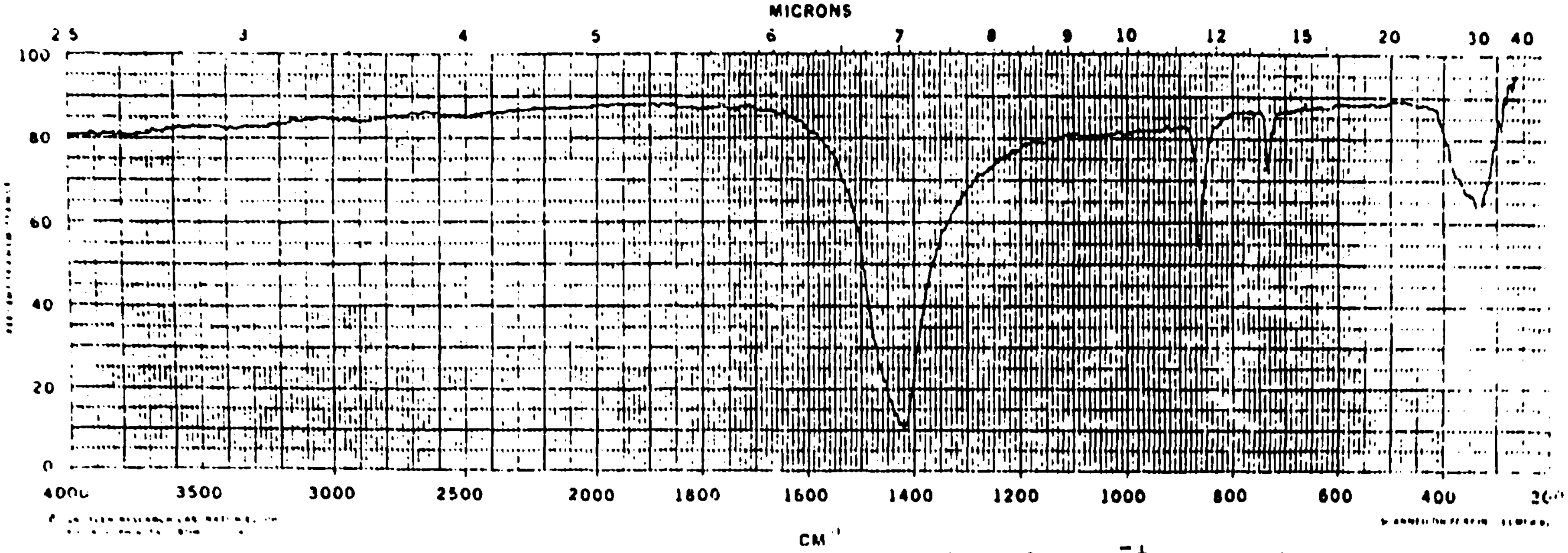


Fig. 13. Infra-red absorption spectrum in the 4000-200 cm^{-1} wavenumber region of $FeCO_3$, siderite /from Sadtler Res. Labs. Inc. pattern MN 241K, 1973./

specially defined term: absorbance. Direct transformation between these two terms is straightforward. In the latest spectrophotometers data of such spectrums are collected digitally under the supervision of a microcomputer and recorded after several steps of processing. This can be accomplished interactively by an operator, however, sets of simple commands of an IR oriented computer language can also be used to compile operating programs. Different manufacturers include for this pupose not just the same English words, nevertheless, the performance of the instruments is almost equal. Software commands of a typical IR data--control-station provide e.g. for the following:

- change to the next sample by means of an automatic sample changer
- scan defined wave-number range in given steps to measure either transmittance or absorbance, as required,
- store measured data in a specially assigned file of the storage media,
- search for stored data and copy them from the storage area into the working area,
- digitally multiply / divide / all absorbance values in a spectrum by a specified constant number,

- convert spectral data from absorbance to transmittance and vice versa,
- digitally smooth spectra to improve the signal to noise ratio using a specified window width /Savitzky-Golay smoothing procedure/,
- substracting /adding/ one spectrum from /to/ another,
- determine all peak positions and intensities in predetermined sections of the spectrum /a limit of the smallest intensity to be taken into account can be set/,
- flatten the background of the spectrum,
- accumulate data collected in repetitive scans and calculate an average from the data,
- execute a stored sequence of commands for data processing,
- store peak height and peak area determined in the spectrum of a standard sample /calibration/,
- carry out quantitative analysis using a previously calibrated system.

When the general laboratory microcomputer is linked to the IR instrument via a standard interface the relevant commands can be understood and executed by the control microprocessor of the instrument which is then overriden by the microcomputer. In a laboratory where several people work with the same instrument each can have his or her own storage media /floppy disk or cartridge, as appropriate/ for operating programs and data. In this way the individual operating habits and requirements of the various users do not interfere with each other, everybody can restore with a few keystrokes the instrumental conditions preferred.

Identification of the components can be carried out by a search program which looks for matches between the measured data and those filed in the library. In the practice of mining a given type of ore, generally it is sufficient to use a micro library consisting of some tens of data sets. Most search programs compare first the unknown with itself finding 100% overlap and thereafter measure the percentage overlap of the unknown with the library data sets. The result is a list of the labels of library data sets with higher overlap scores than say 90%. This latter figure is, of course, an optional variable of the search routine.

The detection of minor components of a complex mineral mixture /i.e. an ore/ is made fairly easy using several steps of data processing. Reference data of the major components scaled appropriately by the program can be subtracted from the spectral data of the mixture. The weak peaks in the residual can be enhanced by multiplication and thereafter digitally smoothed. Results of such a series of computations can be seen for the case of a diasporic bauxite in Fig. 14. After substraction of a standard diaspore spectrum the bands of kaolinite and other components are identified in the bauxite ore much easier.

Spectral substraction technique may be used to follow the effect of different dissolution or benefication procedures, too, which can advantageously affect the marketability and real value of ores.

Addition of spectra on the other hand can be a tool of producing a simulated spectrum matching the unknown one. The estimated proportion of the reference spectra used in adding, yield information about the composition of the ore.

Adding and averaging several scans of a weak spectrum diminishes the effect of noise and permits thereby the location of weak details. When scans are added the signal grows in proportion of the

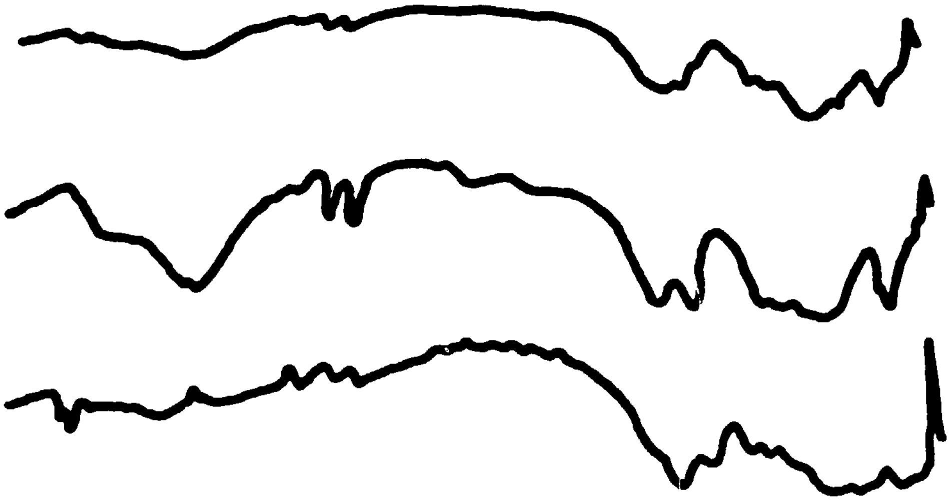


Fig. 14. Illustration of a microcomputer controlled manipulation of IR data sets. Upper curve: IR spectrum of bauxite, middle curve: IR spectrum of a pure a diaspore sample, lower curve: difference of the upper and middle curves

number of scans /N/ accumulated. Noise on the other hand, adds proportionally to $\sqrt{N}$ because it is a random phenomenon. Consequently, the signal to noise ratio increases proportionally to $\sqrt{N}$ and the resulting spectrum contains relatively less and this is very advantageous before significant expansions of the scale.

If quantitative analysis is required first some standards must run under an appropriate routine and concentration information must be supplied to the program. When thereafter a command for analysis is given the computer calculates for the peak of interest the height and/or area over a tangent baseline constructed in advance. The concentration of a component in the unknown is then determined with reference to the standard's data and a printout with detailed quantitative information is produced. Quantitative analysis by IR absorption spectrometry might become a premium as referred to X-ray diffraction when structurally disordered components are encountered /often happening e.g. with clay minerals/. IR absorption being evoked by interatomic bonds is rather independent of crystallinity, while X-ray diffraction can be very mush suppressed by the absence of long range order.

Bond strength on the other hand can be used as a direct parameter to express the industrial value of minerals in an ore. Very strong bonds can mean low reactivity i.e. resistance to solution, digestion or other hydrometallurgical processing and vice versa. Strong bonds are reflected by bandshifts towards higher wavenumbers.

Shifts of certain bands can be also interpreted in terms of cation substitutions, rather frequent among minerals. Thus, part of the metal atoms wanted to recover can be incorporated in minerals not specific for the metal requested. This is a disadvantage if occurring in high proportiones because it either leads to losses or requires extra care in processing, with possible additional costs. E.g. such consequences appear when Fe is substituted by Al in goethite and hematite in aluminium ores. Proved absence of such disturbing substitution can support the claim for a higher price.

Consequently the exact position of particular IR absorption can be of importance. A microcomputer controlled infrared spectrophotometer can measure this parameter directly. The following steps of a procedure correspond to commands of a software typical for the spectrometric programming environment:

```
      Let N1 be the number of samples to be investigated.
      F1 = 0
    * F1 = F1 + 1
      Turn all variables to zero
      Place next sample into the measuring position
      Turn off display
```

Scan the spectrum from wavenumber w1 to wavenumber w2 n times in steps of s, calculating the average in each data point

Smooth the measured curve using 13 point smoothing window

Calculate the position of the [illegible] laying between the specified wavenumbers

Calculate delta = actual peak position -
standard value of peak position

Print F1 and delta as well as the peak potition determined in the last step before the previous one

Store the peak position and delta values in file F1

Check if N1-F1 is positive

If YES repeat the procedure beginning with the command *

If No, turn on display

Display "Measurements ready"

Give every 10 seconds a warning beep signal.

This program will automatically control the measurement of the position of a given peak, calculate the shift referred to a standard position, print and store these data for further use in another program eventually determining in money terms the value of the mined product.

Thermal analysis

Since all ores contain more or less adsorbed water and most of their components also include crystalline water the measurement of moisture content is indispensable in the mineral industry for the full chemical analysis as well as for the determination of the value of mined products. Transportation of useless moisture together with the metal bearing components may cost a lot and the elimination of water requires substantial energy input. Therefore the moisture content influences in one way or another the attainable gain.

The determination of water content can be carried out using relatively simple classical tools: a balance, crucibles, a furnace and a stopper watch. Even unskilled personnel can easily measure the weight loss occurring at a certain temperature during a definite time interval. However, this kind of measurement is slow, inaccurate and needs much labour. Modern instruments operating e.g. on a coulometric or gravimetric principle permit to conduct moisture analyses and hydration level measurements in 15 to 25 minutes. The measurement conditions can be programmed for automatic execution including the printed output of data, but through a standard interface the measurements can be controlled and the data collected for integrated processing by a microcomputer hooked up eventually with other instruments as well.

Thermal analysis /TA/, however, includes several methods of more general applicability. Current TA instrumentation comprises a furnace in which the sample is heated according to a previously determined program in a controlled atmosphere. Changes in the material properties are monitored by a selective transducer which generates a voltage signal characteristic for the parameter investigated. This signal is then amplified, stored on a magnetic disk along with a direct temperature response from the sample. In TA systems designed according to a modular approach the same temperature control, data storage and analysis, display and plotter can be used with alternative measuring cells. Moreover, in a multitasking environment several measurements can be run simultaneously.

Methods of thermal analysis like differential scanning calorimetry /DSC/, differental thermal analysis /DTA/ and thermogravimetric analysis /TGA/ can readily be applied for the detection of physical or chemical changes taking place in solid materials when subjected to rising or decreasing temperatures. DSC is used to measure both the temperatures and heats associated with transitions in materials like decompositions, melting points etc. In DTA observation the sample and an inert reference /e.g. alumina/ are treated thermally in a common cell, nevertheless, at certain points there will appear a temperature difference between the sample and the reference which can be interpreted in terms of transitions or reactions. Measuring the temperatures at which heat related phenomena occur in materials, DTA provides the same qualitative information as DSC. However, in higher temperature ranges /above about 600°C upto 1600°C/ usually only DTA apparatus can be used, therefore the latter seems to be very important for applications concerning minerals. TGA involves the measurement of weight change as a function of temperature. The determination of transition temperatures is rendered more accurate by using derivative thermogravimetric analysis /DTG/. Sophisticated enough instruments provide data for the latter, too. In some instruments throughput is increased by arranging several samples in the same chamber. Over and above the information obtained from the reviewed methods of thermal analysis TGA can be used for the quantitative determination of those minerals which undergo decompositions accompanied by well determined weight changes /loss of hydrate water, CO_2 evolution from carbonates, oxydation and so on/.

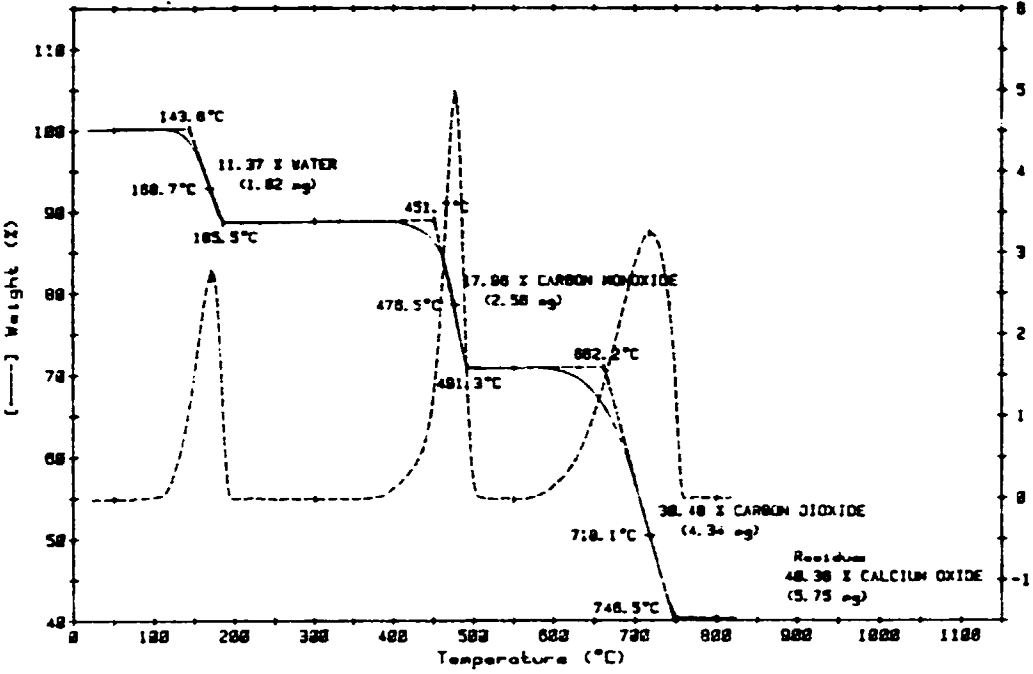
The technique of TA has been greatly enhanced and simplified with the advent of microprocessor technology which is incorporated in most instruments offered on the market recently. Furthermore, a microcomputer can here as well be used to override the local control of the thermal analysis system and set up/run the experiment, store measurement programs, collect and analyse data which is greatly facilitated if software is available specifically developed for such applications. The computer can be, of course, programmed for customized routines satisfying particular requirements of the user.

Fig. 15. shows e.g. the graphic and alphanumeric

Sample: CALCIUM OXALATE H2O
Size: 14.24 mg
Rate: 10 DEG/MIN 0.0 S/PT
Program: TGA Analysis V1.0

TGA

Date: 28-Dec-81 Time: 9:59:02
File: CAOX.07 K-0301
Operator: RLB 50 ML/MIN/N2
Plotted: 19-Jan-82 16:02:40



Transition	Onset [°C]	Inflection [°C]	Completion [°C]	Weight [mg]	Weight [%]
WATER	143.6	168.7	185.5	1.62	11.37
CARBON MONOXIDE	451.7	476.5	491.3	2.56	17.96
CARBON DIOXIDE	662.2	718.1	746.5	4.34	30.48
CALCIUM OXIDE	Residue at 825.5 °C			5.75	40.36

Modified Sample Weight: 14.24 mg

Sample: CALCIUM OXALATE
Size: 14.24 mg
Rate: 10 DEG/MIN 0.0 S/PT
Program: TGA Analysis V1.0

Date: 28-Dec-81 Time: 9:59:02
File: CAOX.07 K-0301
Operator: RLB 50 ML/MIN/N2
Plotted: 4-Feb-82 9:00:12

Transition	Onset [°C]	Inflection [°C]	Completion [°C]	Weight [mg]	Weight [%]
CARBON MONOXIDE	451.7	476.5	491.3	2.56	20.24
CARBON DIOXIDE	662.2	718.1	746.5	4.34	34.35
CALCIUM OXIDE	Residue at 825.5 °C			5.75	45.40

Modified Sample Weight: 12.64 mg

RECALCULATED FOR
ANHYDROUS CALCIUM OXALATE

Fig. 15. Output curves /upper half/ and numeric data /lower part/ of thermogravimetric analysis carried out on calcium oxalate monohydrate

output of thermal decomposition analysis of calcium oxalate monohydrate 20/. The computer controlled Du Pont 9900 Thermal Analysis System utilized TGA and DTG in combination for this purpose. The TGA Analysis program evaluated quantitatively the three steps of basic weight loss. The first represents a mole of water, the second CO and the last one CO_2. The peaks of the derivative curve permit to locate accurately the temperatures of highest rate of weight loss.

Depending on the nature of components thermal analysis can in some cases supply alone data sufficient for mineral identification if duly complemented by chemical information. Since percentages can also be derived, a target oriented reliable and sensitive thermal analysis system might be the cheapest solution for quality control. Although in other situations the performance of thermal analysis in itself is not enoughc, it is still needed as a supplementary method because some mineral species /e.g. those with high crystal water content/ can be evaluated more accurately by TGA than by X-ray diffraction or IR spectrophotometry.

Microcrystallographic characterization

Another important aspect determining the value of an ore is the spatial arrangement of the crystalline components, the morphology of the constituent minerals. The classical method for the investigation of the relevant parameters has been for a long period optical microscopy. Although still in use in special instances, this method is nowadays more and more replaced by techniques easier to automatize, like scanning electron microscopy.

Computer-aided scanning electron microscopy 21/

Images collected with a multi-detector scanning electron microscope /SEM/ contain a particular wealth of information concerning the morphological features as well as the physical and chemical constitution of the materials investigated. Adding the capability of image processing by coupling a microcomputer with adaqute software, this information can be correlated and quantitatively evaluated. SEM images, in fact, include such a high number of data that in many circumstances automatic processing will be the only realistic way to an in-depth interpretation. Just for illustration it can be cited that the digital storage of one standard 512 x 512 pixel /image point/

image requires 256 kbyte of data. A typical image processing function, like the calculation of a weighted average can be accomplished using 50 - 300 instructions per pixel. In order to obtain the results in a short time, say in a few seconds, special devices, so-called array processors are necessary which may provide for about 10 million multiple operations per second. This amount of calculation had not been feasible before the mid 80s and the mineral industry can benefit a lot from the recently introduced evaluation procedures.

The hardware configuration of an advanced scanning electron microscope based image processing system is illustrated in Fig. 16. Units of this setup assure the generation, collection, storage and processing of several data sets as well as the easy communication between instrument and user.

Central part of the configuration is the scanning electron microscope itself. In the high vacuum column of this an electron beam travels towards the sample under the accelerating force of 5-35 kV high potential. Underways the electron beam is deflected by biased plates in the X and Y directions perpendicular to each other and to the beam. As a result the electrons repeatitively scan in a regular manner a small area of the sample surface.

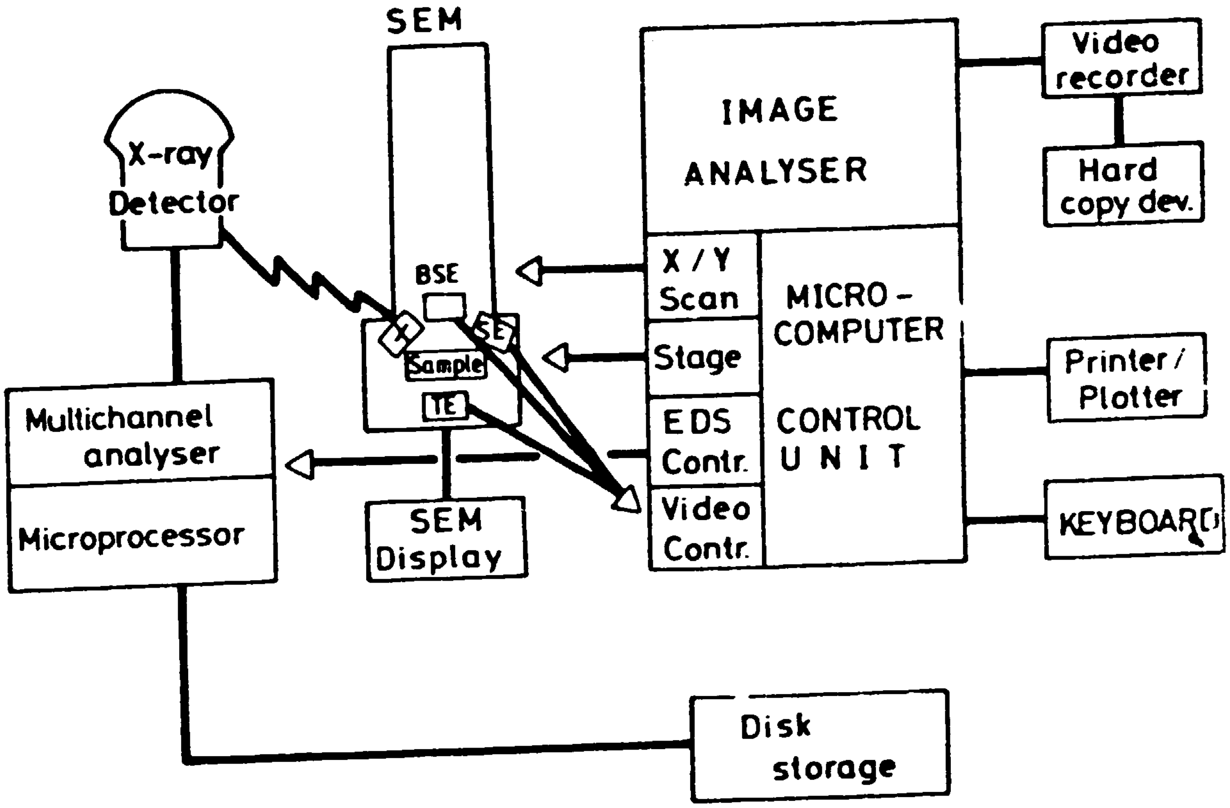


Fig. 16. SEM based system for microcrystallographic analysis

The amplitude of the deflections determines the dimension of the area scanned and if constant size analog display is used on a CRT, also the magnification of the image. In modern instruments the beam position is controlled digitally and the resolution of observation depends on the distance between subsequent measurement points.

Where the electrons hit the material there arises multiple interactions. Some electrons are absorbed by the sample, others are transmitted /TE/ depending on the average atomic number of the matter met by the beam. The proportion of backscattered electrons /BS/ is similarly a function of atomic weight. The yield of secondary electrons /SE/ in a given point is characteristic for the geometric features present, i.e. whether a smooth part of the surface or an edge, a hole or protrusion received the electrons. Thus the distribution of secondary electrons conveyes excellent 3 dimensional information. The exited X-rays can be used to identify the chemical elements constituting the material. Thus as a result of the electron-material interaction several signals can be detected the intensity of which show the strength of the interaction and these yield rich information about the properties of the material filling the very microunit of volume. The SEM equiped with several video signal detectors /e.g. for SE, BS and TE/ and an energy dispersive X-ray spectrometer /EDS/ permits the derivation of extremely valuable parameters. The electronic units of the EDS are usually controlled by a microprocessor under the

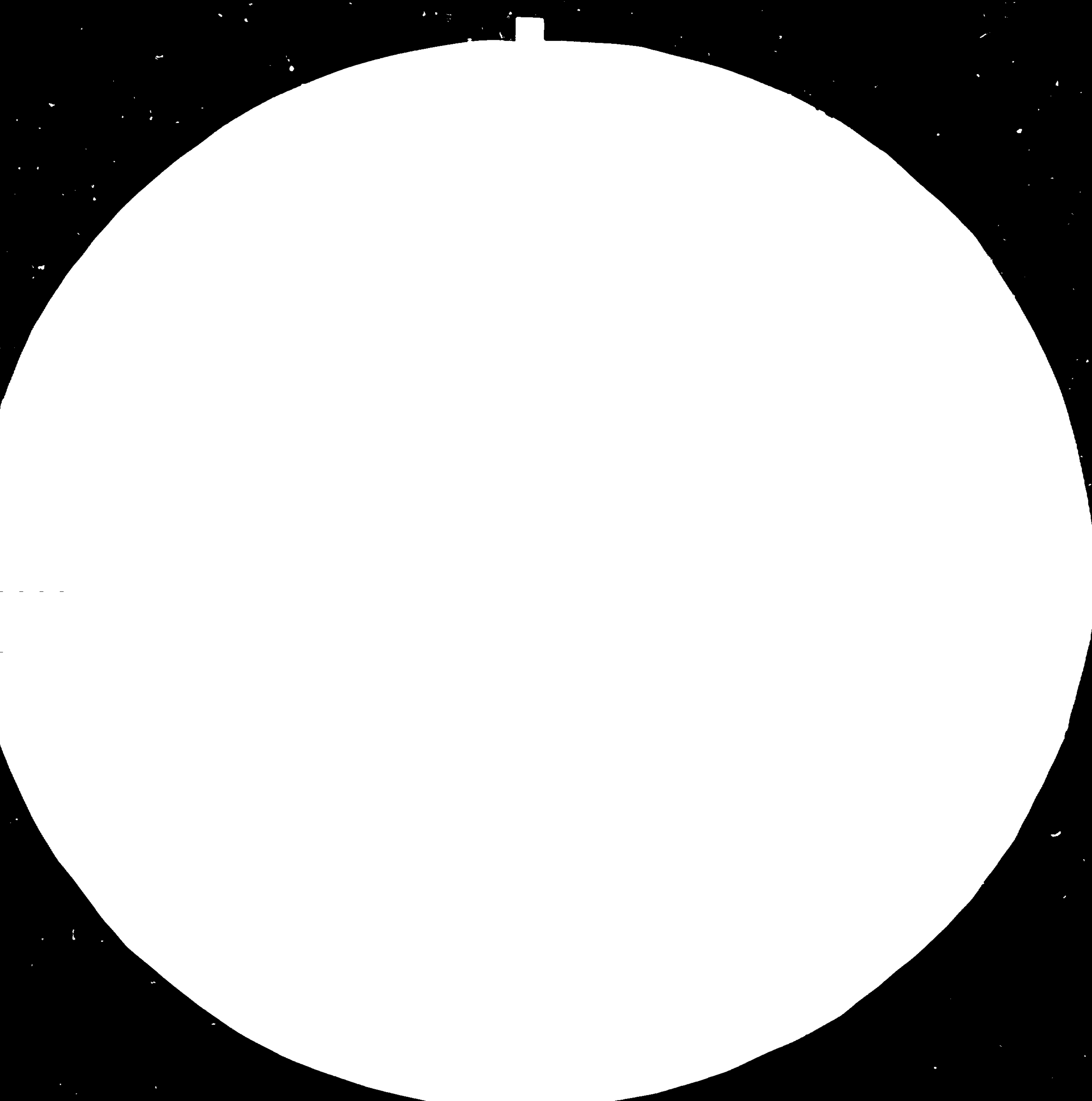
supervision of a central microcomputer providing for the global control of the system. All functions of the microscope like beam scanning in X and Y directions, positioning of the sample stage are digitally programmed and a tremendous number of observations can be carried out unattended.
The detected signals can be displayed on a CRT screen in the form of maps but in automated setups the video and X-ray data are stored for sample points as defined by the required resolution /standard 512 x 512 pixel, however generally can go up to 4096 x 4096 pixel/. Processing of these data includes the computation of several distributions, statistics and cumulative indices characterizing in different ways the material. The characterization is very much enriched by correlating spatial information with chemical analysis.

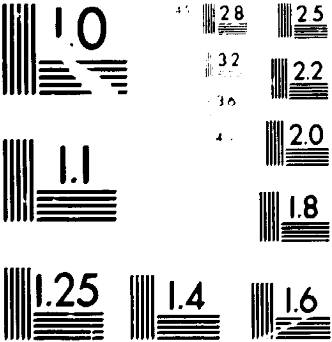
The power of the system is thus primarily based on the software functions made available. A well developed SEM-EDS image processing program provides over 100 different routines which can be combined into appropriate sequences in an unlimited variability. Among the unit function blocks are video digitization, grey level transformation, colour coding, applying filters, image quality modification /improvement/, skeletonization, generation of multiphase images, various coordinate transformations /rotating, shifting, zoom, scroll/, separating or linking different parts of the image, feature identification, measuring areas, perimeters, printing lists, preparing histograms and so on.

For the purposes of ore analysis the following parameters can be obtained from such a system by the combination of two or more of the above services:

- volume fraction of each mineral component
- weight fraction of each mineral component
- calculated bulk density
- elemental composition of particles or averages thereof /for elements $Z<9$ the measurement becomes increasingly difficult/
- surface area per unit volume for each mineral in a section
- contact surface areas between minerals
- association probabilities for mineral pairs
- grain size distribution for each mineral

and also some more sophisticated grading parameters.





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STANDARD REFERENCE MATERIAL 1010a
(ANSI and ISO TEST CHART No. 2)

CASE STUDIES

As a first example of assessing the real value of an ore the evaluation of an Iranian monohydrate bauxite will be shown as carried out and published by Solymár et al. 22/.

Assessment of a bauxite

The real commercial value of a bauxite is basically determined by the alumina content available in it and the caustic soda consumption required for the processing due to the reactive silica content. However, the contaminants have to be taken into consideration, too.

Ever since the emergence of bauxite mining efforts have been made to establish the commercial value and realistic price of bauxites. These efforts are more or less reflected in the supply contracts. Since most of the bauxite is used as the input raw material of the Bayer process for alumina production a reasonable share of profit should be aimed in these contracts between bauxite suppliers and alumina manufacturers. Correspondingly the value of a bauxite can be expressed by the formula

$$V_B = \frac{PRI_A - PRO_A - C_C - C_V}{Q_B}$$

where V_B is the commercial value of the bauxite

PRI_A is the selling price of alumina

PRO_A is the profit made on manufacturing alumina

C_C is the sum of cost element independent of bauxite quality

C_V is the sum of manufacturing cost elements dependent on bauxite quality

Q_B is the quantity of bauxite consumed, t/t alumina

From the above equation one can see that C_V and Q_B are dependent upon the bauxite quality and the lower these the higher the value of the bauxite.

Components of C_V are given by the following formula:

$$C_V = C_{Na_2O} + C_P + C_W$$

where C_{Na_2O} is the cost of replacing the Na_2O losses

C_P is the cost of bauxite preparation

C_W is the cost of evaporation of the water fed into the process with bauxite referred to 1 ton alumina produced.

Amalgamating all costs independent from bauxite quality into a single constant factor $/C = PRI_A - PRO_A - C_C/$

$$V_B = \frac{C - C_{Na_2O} - C_P - C_W}{Q_B}$$

is obtained. Q_B is determined by the total Al_2O_3

content and the "undigested" and other processing losses. C_p is related to the crystallography of the ore influencing its hardness and setting the requirement in comminution. C_W is directly due to the moisture content of the ore. Over and obove these the main task is to determine the specific caustic soda consumption due to silica, titania content and other impurities, in order to establish the real value and price of a bauxite. Clearly, this makes necessary chemical analysis, quantitative phase analysis, textural investigation and some technological tests.

An Iranian bauxite sample gave the following result in phase analysis:

Al_2O_3 in		Mass %	
	boehmite	0.8	
	diaspore	35.2	
	kaolinite	2.8	
	illite	0.4	
	chamosite	7.0	total: 46.2
SiO_2 in			
	kaolinite	3.3	
	illite	0.8	
	chamosite	4.1	total: 8.2
Fe_2O_3in			
	hematite	16.8	
	chamosite	8.9	total: 25.7
TiO_2 in			
	rutile	0.7	
	anatase	5.7	total: 6.4
L.O.I. /H_2O/		12.3	total: 12,3

Containing most of the alumina in diaspore this bauxite is expected to be hard, with relatively high C_p cost, on the other hand after digesting at 240 °C /liquor containing 410.3 gpl caustic soda, adding 4% lime referred to the dry bauxite/: the composition of red mud was:

Al_2O_3	15.0 %
SiO_2	12.2
Fe_2O_3	41.2
TiO_2	10.5
Na_2O	4.9.

Thus the given Iranian bauxite sample is characterized by the fact that its chamosite content is not reactive even under the above conditions. The chamosite is transferred unchanged into the red mud but the diaspore content can be completely digested. The so called "modified basic number" $B^{x} = A_a - 2S_r$, where A_a is the available Al_2O_3, while S_r is the reactive SiO_2 content under the given digestion conditions /both in %/ is for this case:

$$B^{x} = /46.2 - 7.0/ - 2 \times 4.1 = 31.0.$$

In this event the caustic soda loss is relatively low because only half of the SiO_2 content is reactive and consequently the processing of this bauxite may by profitable and a price near the average can be achived for it at the market /about 35 US$/MT in 1984/.

Assessment of a silver bearing lead-zinc ore

The next case study illustrates the use of quantitative evaluation of minerals by scanning electron microscopy /QEM*SEM 23//. A silver bearing lead-zinc sulfide ore will be considered.

The sulfides are economically an important group of minerals, representing the major source of most of our ores and assuring considerable income to several developing countries. In the sulfide minerals one or more metals are usually combined with sulfur, in the relevant ores several metal bearing minerals are mixed. The intimity of this mixing is an important factor in determining the real value of sulfide ores. Association of sulfide minerals is common in ore deposits. Sphalerite /ZnS/ is the major ore of zinc, however, it is often found together with galena /PbS/ in lead-zinc deposits and in association with chalcopyrite /$CuFeS_2$/ which in turn is one of the most important copper ores. Galena usually contains Ag in solid solution or as mineral impurities. In some cases galena is mined as a silver ore.

Recovery of the metal bearing minerals depends on the distribution and association of the various sulfides in such an ore. If the valuable components can easily be liberated the ore has a higher value and vice versa. Miller et al. 23/ published interesting data how this properties can be quantified using a microcomputer controlled scanning electron microscope in conjunction with image analysis and the software developed by these authors.

The carefully prepared drill core sections of the investigated ore showed the elemental concentrations:

Cu	1.5 %	
Pb	27.4	
Zn	33,4	
S	25,0	
Fe/S/	4,5	/Fe occurring in sulfides/
As	0,09	
Ag	0,92	
Sb	1,6	

The minerals could be identified by feature analysis and their volume fractions determined from the surface areas per unit volume of each mineral. Using densities taken from the mineralogical literature weight percentages could be calculated.

Mineral	Vol.%	Density	Wt. %
Galena /PbS/	20.3	7.58	31.7
Sphalerite /ZnS/	64.9	4.00	53.4
Chalcopyrite /$CuFeS_2$/	0.02	4.28	0.02
Pyrrhotite /FeS/	0.3	4.65	0.3
Pyrite /FeS_2/	3.0	5.10	3.1
Arsenopyrite /$FeAsS_2$/	0.05	6.07	0.06
Freibergite	5.5	5.10	5.8
Others	5.99		

A quantity defined as normalized association probabily /eq./4/ in /23// NAP_{ij} gives the probability of enhanced association /$NAP_{ij} > 1$/ or segregation /$NAP_{ij} < 1$/ and intermediate states for a given mineral pair i and j, respectively. For the special case of one mineral being always included within another at a given degree of comminution, NAP tends to infinity and on the other end if the phases i and j are never in contact, NAP is zero.

For the above ore the sulfide phases where found to be characterized in the drill core section by the following NAP values:

Mineral	Vol.%	Galena	Sphalerite	Pyrite	Freibergite
Galena	20,3	-	0.95/0.06/	1.99/0.33/	1.00/0.13/
Sphalerite	64,9	1.30/0.10/	-	1.15/0.19/	0.83/0.11/
Pyrite	3.0	1.63/0.19/	0.49/0.07/	-	1.51/0.25/
Freibergite	5.5	1.27/0.10/	0.73/0.09/	2.48/0.50/	-

The values in parenthesis are 2 times the estimated standard deviations and demonstrate the satisfactory accuracy of these analysis.

The normalized association probabilities show that, within 95% confidence levels, several minerals are randomly distributed with respect to one another. Freibergite, the silver rich mineral in this ore, is relatively abundant, thus enhances the value. Its association with galena is significantly above, and that with sphalerite significantly below, random expectation, and there is an appreciable association with pyrite. For an ore of this type, such results show how unliberated freibergite will be distributed with respect to amounts of galena, sphalerite and pyrite in comminuted ore, or in othwerwise processed concentrates. Such association probalities are consequntly important in establishing the real value /price/.

Recommendations

Developing countries supply a major part of the raw material input to the world economy and import in return advanced products of higher technology from industrialized countries.

The definite aim of imports should be the strengthening of their national capabilities, the updating and upgrading of means available for independent activities in the fields of production as well as in R and D. Utilizing machinery, instrumentation and other high technology goods, should create possibilities for positive development both of manpower and economy. Mere consumption should be handled as a lower preference as far as possible.

Despite the definite target of increasing the share of these countries in the world industrial output to 25% as expressed in the Lima declaration and Plan of Action of UNIDO, the dependence on imports will probably still prevail for an extended period. Consequently the exchange rate between the exported raw materials, like ores, and the purchased products of the foreign metal, chemical and machine industries has a substantial influence on the balance of the developing nations' budgets.

The selling price of ores is, of course, influenced by several non-technical and technical factors. It seems to be hard to bring the non-technical factors under control, however, enterprises mining mineral raw materials in the developing countries should be fully aware at least of the real technical value of the ores marketed by them. The latter is determined by the quality of the material as mined and the degree of subsequent beneficiation carried out by the producer prior to delivery. The real technical value can be an important ingredient in pricing policy and high ratio between value and price which renders the material competitive on the market. Buying ores of high technical value for a fair price, the owners of facilities carrying out further processing can expect due profit using reasonable technology. Low technical value may put too high a burden on the processing industry and diminish the appeal of the mined product. Thus a realistic balance should be established between real technical value and price.

This study has been prepared to give guidelines on the best possible ways of grading ores by quality and collecting technical data on which sound decisions can be based about the economically optimum degree of processing an ore before marketing.

The present state-of-art of laboratory techniques in materials research renders it imperative to use computer-aided methods in quality testing. Procedures of this kind are only sufficiently productive, applicable without high demands on the qualifications of personnel and reliable enough to yield well-founded arguments to be used in commercial trade-offs. Therefore the guidelines concentrate on the utilization of inexpensive and user friendly microcomputers in finding data to support statements on the real value of ores. The knowledge to get a microcomputer to practical application is small compared to the expertize needed to operate and maintain large machines.

Developing countries should reach a state via education, training, hiring policy, bilateral and international assistance, where they possess their own staff capable to manage at a high intellectual level all tasks in such a laboratory. The experts can be recruited from local people who have been trained in suitable environments within the country or abroad, or from consultants abroad.

Producers of mineral raw materials /ores/ in developing countries will be able to assure maximum profit to their nation from the marketing of their products if they exploit to the full extent the intelligence provided by microcomputers in the evaluation of minerals. However, it must be clearly stated that it is a wise primary governmental policy to sell ores at fair prices and the methods disclosed herein offer only tools to execute this policy on a sound basis.

Besides the field of economy, the extended use of microcomputers will have beneficial effects in many other areas, too. It will have an important contribution to increase the complexity and possible marketing prospects of the mining industry. Entering computerization stops the increasing gap in technical levels between developing and industrialized countries. Updating of know-how is fairly straightforward by software transfer once the supporting computer hardware is available.

On the other hand, after some time software can be developed and produced domestically and such software items may represent in general high value besides contributing to the independence of the mineral laboratory concerned. In the industrial sector information system products will be exported under international competitive conditions. In the academic sector expert centers contribute and expand the international state-of-the-art of information technology. This kind of activity can be organized in close co-operation among several developing countries.

Nevertheless, not everywhere and not each case will be justified to install the same microcomputer based laboratory system. Different policy actions are relevant depending on the level of development a mining industry has achieved so far. A thorough study and economic assessment of the prevailing local circumstances should be accomplished before the purchasing of a particular configuration could be recommended.

For the special case of the evaluation of bauxite the document by K. Solymár: "Profile of transferring technology in testing, investigation and evaluation of bauxite" ,/UNIDO/IO.466, 15 September, 1981/ describes different complexity levels of laboratories specified according to various local requirements. The extent of computerization could be matched to the level of instrumentation in such and similar laboratories. Besides the technology tranfer on a commercial basis assistance should be provided to developing countries by international organizations and by bilateral fundings through the following arrangements:

1/ Seminars should be held for small groups /about 15 participants/ of third world decision makers in one or two important regions /Africa, Latin America or China/ to increase their awareness about the advantages of applying microcomputer controlled laboratory equipment for the testing of the products of the mining industry;

2/ Engineers and research workers from the developing countries should be provided with the possibility to get trained in the utilization of laboratory microcomputers. Grants should be assured for 10 to 20 experts for training or research fellowships at institutions and universities experienced in this field;

3/ Visiting experts from microcomputer specialization should help in selected regions /see 1./ the installation of purchased systems and introduce the local staff to the optimum usage thereof;

4/ Regional training centers with a core group of 5 to 10 experts should be established. Select for these training centres a small list of microcomputer controlled materials research instruments. Evoluate the models and standardize a few concerning hardware and software. Here visitors from the surrounding developing countries could study the application of microcomputers in different mineral industries, get profound demonstration and training individually or in groups organized for such education;

5/ Establish a maintenance organization for the standardized hardware. It is imperative that the training and spare parts for this maintenance organization are fully secured even if small industry takes the responsibility.

6/ In countries, where this is justified by demand, national training centre/s/ should be established to introduce laboratory personnel to the reasonable use of microcomputers for advanced level evaluation of minerals;

7/ An active software policy should be worked out by developing countries and especially the regional centres of laboratory microcomputers to make available program systems well adapted to the needs of local mineral processing users. Steps necessary to develop such an independent policy are described in general in the study "Guidelines for software production in developing countries" /UNIDO/IS.440, 10 February 1984/ written by Hermann Kopetz.

8/ Regular advanced education, supply of the latest technical literature, grants for higher studies in avant-garde international centres should be provided to the core personnel of the regional training centres in order that they should not remain passive users of the procured apparatus but innovative developers of their own systems, fully understanding the scientific principles on which the automated measurements are based and able to communicate and exchange information with their colleagues working in the industrialized countries.

Realizing that societies become increasingly dependent on computerization, in summary it is recommended that abundant investment costs should be devoted to the foundation of microcomputer controlled laboratories in developing countries. This system seems to be promising among others in finding technical data to determine the best way of marketing and fix the fair price of ores. They might have rather positive effect on the viability and competitiveness of the mining companies in these countries. The conscious application of computerized systems will aid to diminish the intellectual gap between engineer's performance in industrialized and developing countries at large, as well as to overcome the shortage of well trained specialists in the field of material science.

It is hoped that these guidelines may contribute in some way to realize the stated goal.

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Annex I

MICROCOMPUTER SYSTEMS

There is no unique definition of the term "microcomputer". In general those computers regarded as belonging to this category are designed to be used for general purposes and in basic configuration do not cost more than US $ 20 000. This figure is fairly constant although the price of the incorporated large-scale-integrated /LSI/ semiconductor components is falling steadily. The balance in price is maintained by the increasing requirements, the growing share of software and attached /peripheral/ devices in the value of systems. Another possible characterization of microcomputer points out the fact that they do not require any special premises but can be directly plugged into the voltage supply and are ready for work.

In the mid 80's about 70 firms produce more than 200 types of micros of very different performances. The difference in performance can be observed even within the same type because of the generally accepted modular principle of contruction.

A common architecture of microcomputers is shown in Fig.A1. The most important features of the hardware

are as follows:

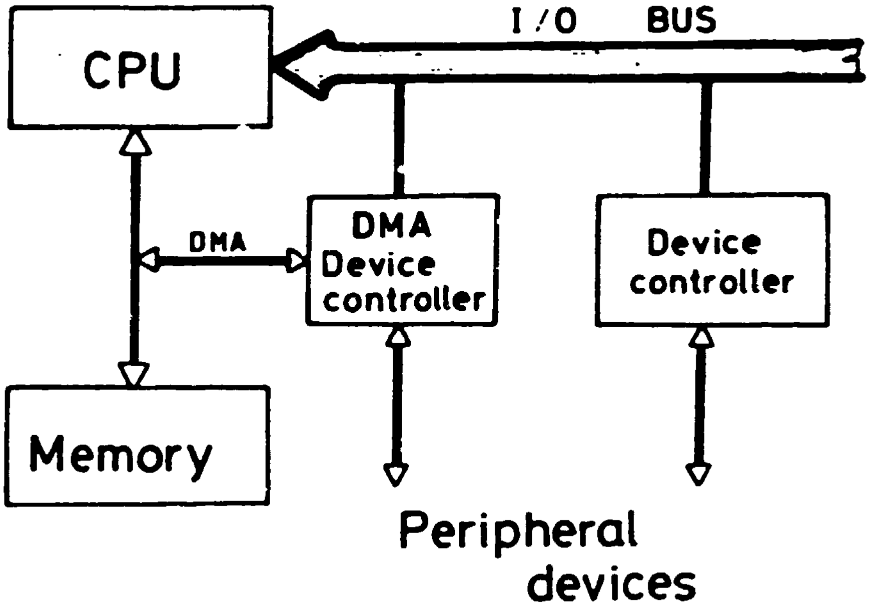

Fig.Al. Simple microcomputer architecture

The central processing unit /CPU/ is responsible for the arithmetic operations which are carried out usually in parallel on 16 bit long words. The CPU takes also care for the orderly execution of program instructions. The length of these instructions is typically one word of the memory, 16 bits. With the usual division of these 16 bits into 6 bits for the code of the operation, 2 bits for indicating the mode of addressing there remain another 8 bits for actual addressing and in this way 256 addresses can be reached directly in the main storage. Other locations must be thus addresses indirectly, i.e.

the directly addressed memory location does not contain the operand but a second address where the program continues. This involves a further cycle, therefore microcomputers are not extremely fast and the cycle time /200 - 500 ns/ is an important characteristic of the storages. Cycle time is what elapses between two consecutive memory operations. Access time /20-50 ns/ is another parameter defining the period necessary after addressing to make available the desired information. The memory size can be in most cases optionally varied between 64 and 612 Kwords using plug in modules. This concerns read/write memory accessible to the user. Additional read only memories /ROM/ can contain often used routines, programs, compilers increasing considerably the power of the system. The main storage can be implemented using magnetic cores semiconductor devices. The information stored in semiconductor memories is lost when power is disconnected from the computer therefore they are called "volatile" and while they are smaller and cheaper, this feature seems to be disadvantageous. The required size of memory is correlated with the length of the data words and instructions. This is the number of bits read from or written into the memory in a single cycle. Longer words result in higher precision and more efficient operation, however, the corresponding hardware will be more expensive. The usually 16 bit word length in microcomputers represents a reasonable compromise. The last area to be identified in a microcomputer is the input/output section which forms the contact points with the surrounding world. The computer architecture determines to a great extent the way in which it transfers information to the outside world. On Fig.Al direct memory access /DMA/ is indicated which provides for the highest data transfer rate. If such a DMA channel is available the program needs only to indicate to the peripheral control the number of items for transfer and their destination and then to avait for a signal indicating that the transfer is complete. Otherwise each word transfer between the main storage and a periphery must be programmed and this will be accomplished by the CPU registers. When DMA is used the program actions continue undisturbed during data transfer.

In order to use a computer for real time control /acting simultaneously with the events/ in a multi-measurement environment there must be possibility for program interruption. Some errors, illegal instructions, power failure as well as immediate servicing requested by an instrument or periphery may cause program interrupt until the most urgent problems are treated. Microcomputers for laboratory use should have several levels of interrupt capabilities with strictly programmed priorities for each measurement.

The laboratory computers are first of all attached to instruments as peripherals. Instruments to be included into a computerized control system must be carefully selected from the point of view of compatibility with the computer. When a laboratory is established in our era of computerization and perhaps a single expert or consulting firm prepares the specifications for the computer as well as for each piece of the equipment it is easy to satisfy this condition. It is a typical situation that one instrument is purchased with a powerful microcomputer and others with microprocessor control are linked to this computer in order to utilize its free capacity. The problem becomes more difficult but generally not hopeless when existing instruments should be controlled by a newly acquired computer. Hundreds of instruments in all fields of chemical, physico-chemical and physical analysis techniques are manufactured with standard V24/RS-232C interfaces which are commonly used. From the side of the system application engineer the instrument is just one periphery among many others.

However, more general input/output units are also needed and these must be selected with clear conception in mind regarding the forms in which the produced results will be used or demanded data will be entered into the computer. Questions which should be answered during the specification of an installation are mostly concerned with the media on which information is and should be recorded, the relative importance of facilities and their technical characteristics, the supplementary services to be gained from a system by adding a certain periphery.

Most popular devices for mass storage in conjunction with micros are the floppy disk units with a master drive and one or several slaves under the control of the previous. The changeable diskettes have usually a storing capacity of 200-500 kbyte with an average access time of 0.1 - 1 s. Much faster are the Winchester drives with hard disks and an average access time of 0.01-0.1 s. The usual capacity of such a unit is 10-30 Mbyte.

There is a considerable technical improvement in the performance of tape cartridge drives. No doubt, they offer the cheapest solution for storing about 100 kbyte information per cartridge with an average access time of 10-300 s. However, it seems to be questionable whether they can compete in the long run with the more attractive disks.

Human communication with the computer takes place in small laboratory systems usually through a video terminal. This consists of a keyboard for input of commands and data as well as a TV screen for visual display of messages, dialog questions and results. To produce hard copies of any information, often dot matrix printers are utilized. These form each character from dots in a 7 x 5 or 9 x 7 array either by impact of fine pins through an inked ribbon or by thermal effect from heated wires in contact with sensitive paper. The latter printers are absolutely silent. Some of the matrix printers incorporate microprocessors to calculate the shortest distance for the head to move from its last position to the point at which it is to print next. Character sets are changed by inserting an appropriate ROM. The printing speed is generally between 50 and 600 characters. Some matrix printers are quasi graphic devices being able to produce graphs and line drawings made up from individual dots at the right positions across the page. More expensive terminals provide full graphical capabilities both in video and in print. For the presentation and interpretation of certain measurement results this might be very advantageous, if not indispensable.

Relatively low cost graphic output devices are the incremental plotters where precision movements of a fine pen in tiny steps in X and Y directions are controlled by computer resident software. They may provide for multicolour A4 or A3 size drawings with fairly good line definition and resolution. Of course, higher precision, larger size, more colours and similar "luxuries" enhance the price. Since the microcomputer systems are preferred for their low prices, small volumes and simplicity it seems to be odd to instal complicated interface, expensive or rather sophisticated peripherals. However in principle this might be possible and special requirements might even justify it.

This attitude becomes still more pronounced with the personal computers /PC/ or professional PC-s, which are marketed for very modest prices of about US $ 10 000 for a workable system. Once again this limit can be considered as the determination of this category. Perhaps one point can be added: they usually have a fixed language which is stored in ROM and becomes immediately operative when the machine is switched on. In microcomputers the selected language usually must be loaded into the main memory from a backup storage media. Otherwise there is not much difference between the two groups of intelligent devices, especially not from the point of view of laboratory management systems.

With increasing integration degree of components distinctions between a microcomputer and a microprocessor also became blurred. Microprocessors frequently do the same or similar jobs as microcomputers. Microcomputers can be based on microprocessors, which are essentially CPU-s built on a single piece of semiconductor, a "chip", however, contains in addition a considerable amount of memory and the ability to communicate with all kinds of peripherals.

Laboratory microcomputers were defined as general purpose machines and it is important that they should be compatible with a wide variety of instruments and accept programs for various experimental tasks without having to worry which particular computer is used. This can be realized by high level languages one of the major aims of which is machine independence: the capability to transport programs from one system to the other without serious modifications. In this way general users may benefit from the program libraries' resources and do not need to duplicate existing routines but use easily ready made software.

At the lowest level each computer may be different in "understanding" instructions given in its own machine code closely related to the architecture.

All computers can be programmed more efficiently the more familiar the programmer is with technical aspects of command execution and more cleverly if he/she takes these into account in giving the instructions. However in general mineral laboratories the users probably will not be programming specialists and therefore instructions similar to those used in everyday communication would be preferred. This will add a definite amount to the hardware cost but since this component of the investment is decreasing there is a pronounced tendercy towards languages providing the highest comfort in application /even the possibility of using local languages appeared recently/. This means that the programmer makes notations in a form manageable for him or her and a translation program produces therefrom a code executable for the machine. Besides the appropriate hardware capacity this requires some time, too.

It seems to be difficult to list and characterize all the languages implemented in laboratory computer systems. Even if stated that in the past decade BASIC has been most popular in developing interactive, time sharing software to control measurements, one must admit immediately that BASIC has many modifications some of which are proprietary to an instrument manufacturer. The programs used to execute particular analytical measurements and material tests are in most cases proprietary and secured against reading, modification or transfer to other systems. The instructions can be executed within the framework of a standard language /e.g. FORTRAN, PASCAL, PL/1 or BASIC/, however, bacause of the existing modifications it is highly recommended to check software compatibility before a new piece of instrument with its own operating code is linked to a system. It might happen that extensions of the standard form are needed but are not available.

New programs to satisfy local needs can be written exclusively if a powerful general language can be used on the system. Therefore laboratory microcomputers should not be constrained by the specialized instrument oriented languages but supplied with at least one high level language including all accessories /editing, debugging, compiling or interpreting and utility softwares/.

Annex II

ACTIONS NECESSARY TO ESTABLISH A TESTING LABORATORY FOR MINERALS

In establishing a microcomputer controlled mineral testing laboratory for a developing country or in a region of developing countries the following steps should be taken under the direction of one person made responsible for the project:

1/ Determine the specific ores which will be evaluated in the laboratory

2/ Define the analytical, material testing, microcrystallographic measurements that must be carried out on the mineral samples for assessment purposes

3/ Select the instruments and accessories necessary to accomplish the measurements defined in 2/. Optimize the group of instruments including microcomputer control, with respect to available financial resources. Place the corresponding orders providing for appropriate quantities of spare parts and consumables

4/ Assign or plan and build the premises where the apparatus will be set up. Consider auxiliary functions, too.

5/ Based on definite job descriptions recruit and train personnel for the operation and maintenance of the selected instruments. Assure them the possibility for practice at home and/or abroad. Make available to them the technical literature relevant to their job.

6/ Develop the software to be run for the anticipated local tasks on the controlling microcomputer.

7/ Install the equipment purchased. The supplier/s/ should give comprehensive introduction to the operating staff and maintenance group about the instruments.

8/ Hire experienced consultants for the guidance of local personnel during the running in period of the mineral testing laboratory.

Annex III

SPECIFICATIONS AND TECHNICAL DATA

In the following tables information is compiled on some commercial instruments which the author knows to be appropriate for utilization in mineralogical laboratories for the evaluation of ores. These data must be regarded as a set of examples, not exhaustive by any means. The specification of the individual items is also not full because rather biased by the point of view of these guidelines. Thus it is strongly recommended to contact the suppliers for more details before actual ordering. Moreover it must be taken into account that in the field of instrumentation, automation and computer applications the pace is extremely fast, thus it can be predicted that the farther the reader will find himself/herself from the time of editorial deadline the more obsolate the included information will be. It is therefore possible that new manufacturers' brand new products are likely to appear and some of the existing ones may disappear. Therefore an actualization will be a must whenever using these guidelines, nevertheless, it is hoped that they will be a useful aid in specifying orders for a long time.

TABLE C-1

TYPICAL MICROCOMPUTERS FOR LABORATORY AUTOMATION /Professional personal computers included/

ommercial name	Micro or prof.pers	Memory size ROM	RAM	Mass storage	Number of interface ports	High level languages	Supplier	Price US$ /1984/
PDP - 11	M	Boot strap	Ex-tendable in moduls 512 kbyte	Floppy, hard disk	UNIBUS	BASIC FORTRAN COBOL PASCAL	DEC USA	20.000
HP-86B	PPC	56-104 kbyte	128-640 kbyte	Floppy, Winchester	HP-IB for 14 devices	BASIC	Hewlett-Packard 3000 Hannover Street Palo Alto CA 94304	15.000
VT 16	M	Boot	128 kbyte /+ 128 kbyte opt./	Floppy, Winchester	CCITT V.24	FORTRAN BASIC CP/M	VIDEOTON 1021 Bp. Vörös Hadsereg utja 54	18.000
	LABORATORY MANAGEMENT COMPUTERS							
ALM	M /PDP-11/		As above under PDP-11			FORTRAN 77	Philips S I Div. Building TQ 111-3 5600 MD Eindhoven, The Nederlands	30.000
BSAM/3350 oftware/	M /HP A600+/	Up to 8 Mbyte		HARD DISN, WINCHESTER	MULTIPLEXER WITH 8 RS 232-C	FORTRAN PASCAL BASIC MACRO	Hewlett-Packard as above	50.000 - 100.000

TABLE C-2

COMPUTER COMPATIBLE INSTRUMENTS USABLE FOR ORE EVALUATION   X-ray fluorescence spectromet

Designation	Control	Program Data Storage	Software	Communication port	Supplier	Price US$ /1984/
ARL Model 70000 Simultaneous X-ray fluorescence spectrometer	Microprocessor based electronics Optional DEC computer	Dual floppy disk drive	Fully quantitative regression analysis FORTRAN IV BASIC	RS-232-C	Bausch LOMB ARL Div. 9545 Wentworth Str. P.O.Box 129 Sunland, CA 91040	195.000
PW 1400 Sequential X-ray fluorescence spectrometer with PW 1500 sample changer	INTEL 8080A microprocessor 16 kbyte EPROM 2 kbyte RAM	Built in semiconductor storage	Quantitative regression analysis	Optically isolated current loop or RS-232-C	Philips S I Div. Building TQ 111-3 5600 MD Eindhoven The Netherlands	150.000
PW 9500/80 Energy Dispersive X-ray Spectrometer System with automatic sample changer	LSI 11/2 micro-computer /32 kword, 28 kword addressable/ or LSI 11/23 computer with 64-256 Kbytes	Double-sided dual floppy disk drives or 8-30 Mbytes Winchester disk drive	Choice of five quantitative models in analysis	-	Philips as above	70.000 150.000

TABLE C-2 /cont'd/

COMPUTER COMAPTIBLE INSTRUMENTS USABLE FOR ORE EVALUATION Atomic absorption spectrometers

Designation	Control	Program Data Storage	Software	Supplier	Communication Port	Price US$ /1984/
PU 9000 multi-element atomic absorption spectrophotometer with autosampler and PU 9090 data graphics display	PU 9007 data/control station Professional microcomputer	Floppy-disks	Background correction Calibration AAS Cookbook Graphics display CORAL, BASIC	PYE Unicam York Street Cambridge CB1 2PX, U.K.	2-way RS 232-C	16.000
IL 751 or IL 951 two channel video atomic absorption spectrophotometer with FASTAC autosampler	30 kbyte 8 bit proprietary micro computer	Floppy disks	Background correction Auto-calibration Display control	Instrumentation Laboratory Inc. Jonspid Rd. Wilmington MA 01887/USA	Standard Teletype or RS 232-C	14.000

TABLE C-2 /cont'd/

COMPUTER COMPATIBLE INSTRUMENTS USABLE FOR ORE EVALUATION Infrared spectrophotometers

Designation	Control	Program Data Storage	Software	Communication port	Supplier	Price US$ /1984/
SP 9510 os SP3-300A IR Spectrophotometer plus SP3-080 Data control and SP3-040 automatic sample changer	INTEL 8080A2 microprocessor 4 kbyte ROM 48 kbyte RAM	140 kbyte data cartridges	Infrared system program Applications software Quantitative package Library of spectra and library search	RS 232-C	PYE Unicam York Street Cambridge CB1 2PX U.K.	32.000
Model 680 IR Spectrophotometer plus Model 3600 IR datastation	MOTOROLA 6800 8 bit microprocessor /2 μsec cycle-time/ 12-164 kbyte ROM 48-52 kbyte RAM	Dual micro-floppy disk drive, 80 kbyte per side	PETOS operating syst. PECDS modular appl. program OBEY program language adapted to the spectrographic environment EDIT for writing automatic user routines		PERKIN-ELMER Co. Norwalk, Conneticut USA	40.000

TABLE C-2 /cont'-d/

COMPUTER COMPATIBLE INSTRUMENTS USABLE FOR ORE EVALUATION Thermal analysis

Designation	Control	Program Data Storage	Software	Communication port	Supplier	Price US$ /1984/
9090 Computer/ Thermal Analyser 910 DSC with 1600°C DTA Cell, 951 Thermogravimetric analyser, 903 Moisture evolution analyser, plus 1092 Data analyser	Texas Instr. Professional Computer 56-248 kbyte RAM	Dual 5 1/4 inch floppy disk drives with 360 kbyte capacity each /Enough for 8-320 hours data collection depending on sampling rate/ 10 Mbyte Winchester disk drive	Du Pont operating system and TA software library BASIC FORTRAN PASCAL	RS 232-C	Du Pont Nemours Company Instruments Div. Concord Plaza Mckean Bldg. Wilmington, DE 19898, USA	12.000 - 25.000

TABLE C-2 /cont'd/

COMPUTER COMPATIBLE INSTRUMENTS USABLE FOR ORE EVALUATION X-ray diffraction

Designation	Control	Program Data storage	Software	Communication port	Supplier	Price US$ /1984/
PW 1700 automated X-ray diffraction system /PW1730 generator, PW1050 goniometer, PW1780 sample changer, electronic units/	PDP-11	Optional floppy, hard disk	Assemble jobs, data collection, data reduction, phase identification, user reference file generation, search/match, utilities quantitative analysis	optically isolated current loop or RS 232-C	Philips S&I Div. Building TQ 111-3 5600 MD Eindhoven The Neuerlands	60.000 - 88.000
D 500 Diffractometer System	DACO MP FALCON SBC 11/21 micro-computer 32 kbyte PROM 28 kbyte RAM /DEC - PDP/11/	Built in for 10.000 measurement points	Possibility for multi-user operation via RSX-11M and overriding micro-/mini/ computer Basic units of diffractometric data processing	RS 232-C	Siemens A.G. E 689 B Salzufer 6-8 P.O.Box 110560 1000 Berlin 11 West Berlin	45.000- 90.000

TABLE C-2 /cont'd/

COMPUTER COMPATIBLE INSTRUMENTS USABLE FOR ORE EVALUATION

Scanning electron microscopes and image analysis systems

Designation	Control	Program Data storage	Software	Communication Port	Supplier	Price US$ /1984/
SEM 505 with 6791/00 interface	Optional Computer or EDAX Energy Dispersive anal. System DEC LSI-11	Dual floppy disk drives	EDAUTO, EDL SCAN MICROGRADIENT IMAGE ANALYSIS	RS-232-C	Philips S I Div. Building TQ 111-3 5600 MD Eindhoven The Netherlands	190.000 - 300.000
IBAS -SEM-IPS /coupled to any SEM/	Microcomputer based on Z80A 64 kbyte RAM Microprogrammable array processor for image analysis 16 kbyte graphics memory	5 1/4 inch floppy disk 540 kbyte 2 Mbyte RAM for image analysis	Quantitative image analysis Feature identification /video and EDS correlation/	2x RS 232-C 1x Centronix	Kontron Bildanalyse GmbH D-8057 Eching bei München	180.000
JSM-840 SEM with LINK systems 860 series 2 analyser	Link 860 microcomputer	Floppy disk	DIGIPOINT - quantitative anal.in predetermined points MULTIPOINT - specimen stage control DIGISCAN - feature detection DIGIMAP II - acquisition,processing, replay	Optional	JEOL European Headquarters Jeol House Lowther Rd. Stanmore,Middlesex HA7 1EP, U.K. LINK System Ltd. Halifax Rd. High Wycombe Bucks, HP12 2SE,U.K.	350.000