Table 1. *Relevant data from Tables* 1 *and* 2 *of Hart et al.* (1990)

		2θ(true)	$a_{\rm Si}/a_W$	error (parts in 10^6)
$1\frac{1}{4}$ Å	Si 531	83·58107 (30)		
	W 222	84·05750 (50)	1·715 754 5 (97)	±5·6
$1\frac{1}{4}$ Å	*W* 220	66·27478 (20)		
	Si 422	66·98578 (20)	1·715 776 6 (64)	±3·7
1 Å	*W* 220	53·22322 (10)		
	Si 422	53·76909 (10)	1·715 757 1 (42)	±2·4

Table 2. *Relevant data from Tables* 1 *and* 2 *of Hart et al.* (1990) *containing large systematic errors*

		2θ (obs.)	$a_{\rm Si}/a_W$
$1\frac{1}{4}$ Å	Si 531	83·5765 (3)	
	W 222	84·0527 (5)	1·715 751 3
$1\frac{1}{4}$ Å	*W* 220	66·2780 (2)	
	Si 422	66·9887 (2)	1·715 784 4
1 Å	*W* 220	53·2150 (1)	
	Si 422	53·7608 (1)	1·715 756 3

agrees precisely with the above values. Note, however, that the present values have slightly smaller error bars. The unweighted mean value in Table 1 is 1·715 763 (10) where the error is indicated as the standard deviation of the mean of the three results. This is slightly larger than the *a priori* error estimate.

The influence of systematic errors

In Table 1 the Bragg angles 2θ(true) are corrected for systematic goniometric errors of up to 0·07017° for the 1 Å data and 0·0412° for the $1\frac{1}{4}$ Å data. The determination of the systematic corrections involves non-linear least squares and determines, incidentally, the required result $a_{\rm Si}/a_W$. The present analysis algorithm is thus redundant in principle unless the method can be applied to the observed (uncorrected) data. Table 2 shows the result.

The errors are of course the same as given in Table 1. The mean of the three results is 1·715 764 (14) (standard deviation).

In conclusion, the suggested algorithm leads to lattice-parameter determination with errors of 8 in 10^6 using uncorrected data, known to include systematic errors of up to 500 in 10^6 (> 0·04° on 70° 2θ). The difference between the lattice parameters determined previously and those determined by the present simplified analysis is only 1 in 10^6.

References

Baker, J. F. C. & Hart, M. (1975). *Acta Cryst.* **A31**, 364–367.

Deslattes, R. D. (1979). In *Neutron Interferometry*, edited by U. Bonse & H. Rauch. Oxford: Clarendon Press.

Hart, M. (1981). *J. Cryst. Growth*, **55**, 409–427.

Hart, M., Cernik, R. J., Parrish, W. & Toraya, H. (1990). *J. Appl. Cryst.* **23**, 286–291.

J. Appl. Cryst. (1991). **24**, 190–193

Diffractometer devices controlled by a personal computer.

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Dedicated to Professor Dr K. Fischer on the occasion of his 65th birthday

Abstract

The application of single-board microcomputers as programmable interfaces simplifies the construction of complex diffractometer control units. The amount of hardware components of the control units is reduced and the structure of the circuits is easy to survey. These intelligent multipurpose single-board microcomputers unburden the personal computer and simplify the development of the diffractometer measuring program. The presented solution is based on an Atari 1040 STF. The concept, however, can be applied to any type of personal computer.

Introduction

Since the introduction of four-circle diffractometers for the measurement of integrated intensities approximately 25 years ago, the usual way to drive these devices under computer control was in the following manner:

A process computer was connected to the units of the diffractometer devices by a more or less complex interface (*cf.* Fig. 1*a*). Since the different properties of the device modules demand a fast reaction from the computer, two conditions had to be fulfilled before the system would operate correctly:

(i) the process computer had to have a fast interrupt ability;

(ii) the interface had to be equipped with a rather large amount of basic logic components, constructed by the user (or the factory).

In many cases, old devices are still reliable with respect to their mechanical accuracy, but their electronic systems have often broken down. It is the aim of this paper to propose a solution for the reconstruction of such instruments that makes use of the recent technological developments, namely the very powerful personal computers (PC) and single-board microcomputers (μC), both commerically available at low cost.

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Basic considerations

The main advantages of a PC are:

(i) it is a low cost device;

(ii) the computation power is comparable with computers like the PDP 11/34 up to the PDP 11/70 or even larger;

(iii) compilers for Fortran, Pascal or similar languages have become available;

(iv) most are equipped with graphic devices or can be fitted with them.

The most important handicap is the absence of a complete microprocessorbus plug connection, *i.e.* the hardware properties of a PC are not directly at the user's disposal, *e.g.* in the form of a bus foundation module. This disadvantage, however, may be compensated for by the use of low-cost single-board microcomputers. Many devices of this type are now available commerically.

Single-board microcomputers can be used as an intelligent interface. The complete control program (*e.g.* the control of the movements for positioning of an axis, the activation of shutter or attenuator magnets *etc.*) can be displaced from the main computer to single-board microcomputers. This program can be stored in erasable programmable read-only memories (EPROMs) or read-only memories (ROMs) of the μC which means that only a small amount of information is necessary to start the movement process or other processes by the PC. The PC governs the process by a number of slaves, the μCs replacing a complex interface. The software for driving a μC can normally be developed by using the μC itself (as a developing system) in connection with the PC (as an input–output device). In accordance with these ideas a diffractometer control unit arrangement is given in Fig. 1(*b*).

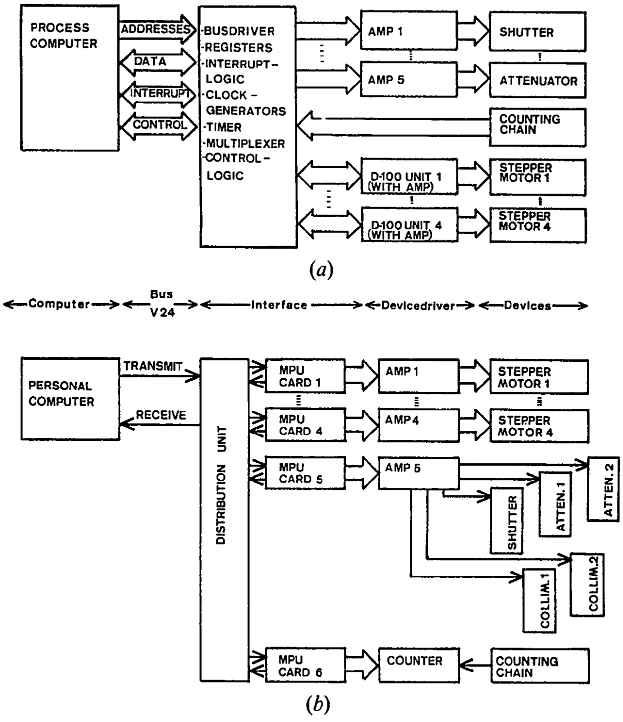

Fig. 1. (*a*) Construction scheme of a conventionally organized diffractometer control unit. (*b*) Construction scheme of a diffractometer controlled by a personal computer.

The PC is connected to the different μCs *via* the distribution unit. Each μC receives two pieces of information if it is selected, namely its selection parameter and its information parameters for correct operation. In order to avoid communication conflicts between the different slaves, the feedback information will only be given if it is requested from the PC.

A comparison between Figs. 1(*a*) and (*b*) shows that the interface module can be replaced completely by the combination of the distribution unit and the μCs.

The connection to the main computer is reduced to a serial interface.

This concept allows the extension of a system very easily. The number of μCs may be increased with very small changes of the distribution unit. This concept is independent of the choice of the PC and the μC devices. Several technical realizations were presented at the XI ECM in Vienna, 1988 (Burzlaff, Lange & Neugebauer, 1988) and at the XII ECM in Moscow, 1989 (Burzlaff & Lange, 1989).

A technical realization

This concept has been realized for different diffraction devices using an Atari 1040 STF with 1 Mbyte memory as a PC. The μC used is the so-called EMUF 08, which was described in detail by Himmeröder & Mayer-Gürr (1987). The Atari 1040 STF is equipped with a serial interface RS232. The used lines are the transmit, the receive and the ground line. The other lines are not connected, since the diffractometer-control interface can also be used in connection with simple PCs without any possibility of handshake. The handshake is realized by echoing the data in both directions, 'transmit' and 'receive'. A high communication speed of 19·2 kbaud allows this procedure.

1. Essential components of the distribution unit are two chips in the minimal configuration. The first is the open collector driver IC1 which connects the TTL (transistor–transistor–logic: 0 V and 5 V levels) transmission lines of the μCs *via* a level converter (TTL level to V24 level: − 12 V/+ 12 V levels) IC2 to the PC. Each of the open collector-driver chips contains four units and can connect up to four μCs. For more than four μCs more open collector-driver chips are necessary. The receiving lines of the μCs are directly connected with the transmission line of the PC. This is a very simple and cheap solution for connecting one master computer (the PC) to several slave computers, the μCs.

2. The MPU card (μC) is a single-board computer, which occupies 3/4 of an Europa-Karte (size: 100 × 160 mm). The main components are the microprocessor MC 68008, an 8 MHz clock generator, an EPROM (8 to 64 kbyte), a random-access memory (RAM) (8 to 32 kbyte), a versatile interface adapter (VIA) 6522 with 20 input–output lines, an asynchronous interface adapter (ACIA) 6850 and two eight-bit drivers with memory function (latches) with 16 output lines.

The EPROM contains the control program for the diffractometer devices and is about 1 to 3 kbyte (depending on its function). The RAM size is 8 kbyte. The main part of the memory is used for storing the acceleration- and deceleration-function graphs for the motors. These functions depend on the parameters of the motor circles, like moment of inertia and frictional force, and can easily be changed by the Atari *via* the serial interface. It is possible to choose the acceleration (deceleration) time, the start and the stop velocity of each motor. This procedure must be carried out only once after switching on the complete interface. The parameters can be changed at any time.

The motor-control program on the μC contains different practical routines: a fast reference position searching routine, a step error-detecting routine, an offset routine to change the diffractometer constants at any time and an acceleration and a deceleration routine, as described above. These routines are activated by one command of the PC.

The VIA is connected to several control switches of the motor circles (*e.g.* zero switch) or is used to read the result of the counter. The ACIA is set to 19·2 kbaud communication speed. The latches are connected with current amplifiers of the motors or the shutter magnets.

The program for driving the shutter, attenuator and collimator magnets controls the mechanical function of the magnets by installed switches. The EPROM of each μC contains several diagnosis routines. With the aid of these routines, the user has the possibility of detecting errors in the complete diffractometer-control system. A diagnosis card is necessary to support the error-detecting process. This diagnosis card is of low complexity (less than one Europa card).

It contains some LED (light emmiting diode) display units and some switches. The μC is able to drive the LEDs and to read the switch positions. This diagnosis card and the diagnosis routines allow the user to test the V24 transmit–receive lines, the memory, the motors by single step and normal operation, the microprocessor on the μC card itself, the switches like zero switch *etc.* and other functions.

For the μC EMUF 08 an operating system, called KAT-Ce is available with a 68000 assembler/disassembler, Pascal language and monitor. A paper on this operating system was published by Scherer (1987). The assembler programs for driving the diffractometer devices were developed with KAT-Ce and the μC EMUF 08, with the support of the Atari 1040 STF as a terminal for this single-board computer EMUF 08.

3. The main component of the counter is a single counter chip with 16 bit counting capacity. 16 bits corresponds to 65535 events. The μC divides the counting time into *n* units of 1 ms. So the counter is started from the μC *n* times 1 ms.

In theory, this procedure facilitates counting up to more than 65 million counts s^{-1}. In practice, the counting rate is restricted by the frequency of the reference clock oscillator. The maximum count rate is two million events s^{-1}. The maximum counting time is 99999 ms. Deadtime correction can easily be performed by a suitable function. The function constants are transferred to the counter MPU card in the same way as the acceleration parameters are transferred to the motor MPU card.

4. The current amplifier for the motors is a simple five-phase amplifier for five-phase motors. This amplifier is selected from the sensitive metal oxide semiconductor logic (MOS) of the μCs by optocouplers. The connection to the μCs consists of five lines, the phases. At the output of the amplifier five power transistors drive the coils of the stepper motor. The same amplifier is used for activating the shutter, attenuator and collimator magnets. Every output transistor drives one magnet coil. So one amplifier can drive up to five units like this. The only difference between motor- and magnet-unit drivers is the assembler program in the EPROM of the μC.

Example: the reconstruction of a Hilger & Watts diffractometer

A 22 year old Hilger & Watts diffractometer Y290 was equipped with a control unit, as described above. Each DC motor was replaced by a five-phase stepper motor from the Berger company, the axis was equipped with a spring press and the complete fringe gratings and reading heads equipment was replaced by one zero switch for each motor and

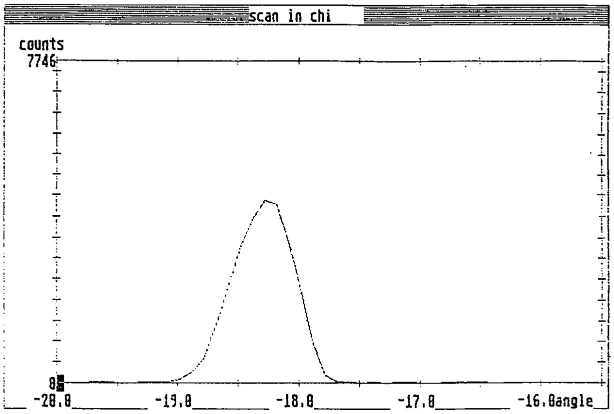

Fig. 2. On-line reflection plot (hard copy from the screen).

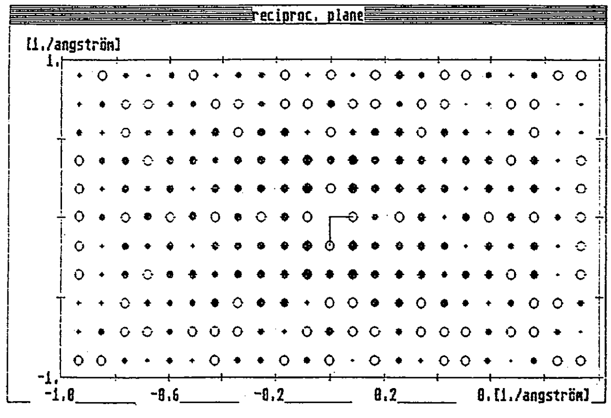

Fig. 3. Screen simulation of a precession photograph. Crystal: L-asparagine. Wavelength: Mo $K\alpha$. Selected reciprocal plane (spanned by): (100) and (001). Space group: $P2_12_12_1$. Black dots: area of one dot is proportional to the logarithm of the intensity. White circles: very weak or extinct reflections. Time of exposure: about 15 min.

two limit switches for the ω, χ and 2θ motors. The exact zero position (one step accuracy, *i.e.* 1/250 and 1/500°, respectively) of each circle is realized by an AND function of the zero switch signal and a light barrier signal, directly connected on the axis of the motor. These functions are carried out by the μCs automatically.

The detector circle is equipped with three selectable collimators, one fixed 5 mm and two variable collimators (3 and 1 mm). So it is possible to select three sizes by two magnets. These two magnets, the beam stop and the two attenuator magnets, are driven by one μC and one amplifier. The detector assembly Y318 (scintillation counter and preamplifier), the high-tension power supply and the discriminator (with main amplifier) is used without changes and directly connected to the μC-driven counter unit.

The possibilities of X-ray tube alignment are increased. The complete PDP-8 digital computer and the teletype model 33 automatic send and receive set is replaced by an Atari 1040 STF with high-resolution monitor and coprocessor, a Megafile 30 mass storage, a printer Star LC10 and the control interface.

The software is completely redeveloped with graphic fitting [*e.g.* graphic presentation of reflection plots (Fig. 2) or high-speed precession simulation on screen instead of film (Fig. 3) *etc.*]. Alignment routines, orientation-matrix refinement, peak hunter, data collection, base finder and several other useful programs and routines have been rewritten. Further information is available from the authors.

References

BURZLAFF, H. & LANGE, J. (1989). XII Eur. Crystallogr. Meet., Moscow, USSR. Abstracts, Vol. 3, p. 125.

BURZLAFF, H., LANGE, J. & NEUGEBAUER, H. (1988). *Z. Kristallogr.* **185**, 674.

HIMMERÖDER, H. & MAYER-GÜRR, W. (1987). c't 7/1987, *Magazin für Computertechnik*, pp. 90–93. Hanover: Verlag Heinz Heise.

SCHERER, E. (1987). mc2/1987, *Die Mikrocomputer-Zeitschrift*, pp. 101–108. Munich: Franzis-Verlag.

Computer Programs

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C3DCON: a stereo 3D electron-density cage contouring and atomic structure plotting program. By

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Abstract

A Fortran computer program is described which performs 3D electron-density cage contouring together with atomic structure model display on a Tektronix-4100 command graphics terminal hosted to a VAX/VMS computer. The program also supports ball-and-stick visualization of the model, on-line manipulation of the display and convenient hard-copy output. Such a program is useful in a research environment where an expensive graphics workstation is not readily available and hard copies of publication quality are often desired.

Introduction

C3DCON is a user-friendly interactive 3D electron-density-cage contouring and atomic-structure-model drawing program. It is written in Fortran77 and is designed to run on a VAX/VMS computer and display principally on a Tektronix-4100 graphics command-language serial terminal (Tek4100). A menu- and form-driven dialogue scheme is used to set up plots on any DEC VT100 compatible text terminal.

The primary motivation for writing *C3DCON* was to be able to do real-time 3D electron-density contouring using equipment common to most diffraction laboratories rather than a program like *FRODO* (Jones, 1985) that runs only on a more specialized and costly graphics workstation such as an Evans & Sutherland PS390. The implementation of *C3DCON*'s model-drawing capability was motivated partially by the frustration the authors have experienced and witnessed over years with *ORTEP* (Johnson, 1965) in visualizing atomic models when the thermal ellipsoids were never the interest. Figs. 1, 2, 3 show examples of stereographs produced from *C3DCON* on a DEC LN03 PostScript laser printer. Each of these plots takes about 1 min run time to draw on a Tektronix 4207 hosted to a DEC MicroVAX II.

Procedure and function

(1) *Contouring*

C3DCON resembles *FRODO* in its functionality in contouring. The 3D density cage contours are accomplished by 2D contouring layer after layer along the crystallographic *a*, *b*, *c* axes of the unit cell, using a single contour line tracing algorithm (Sutcliffe, 1980). The 3D cage contours are then parallel projected to the 2D viewing plane after optional 3D clipping. To speed up contouring, *C3DCON* requires the input 3D electron-density file to be pre-treated by a subsidiary routine *MAPACK*, which reads the floating-point density values sampled on the 3D grid, converts them to the 8-bit byte integers dynamically, and

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