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21st October, 1963.NI/63/21NATIONAL INSTITUTE FOR RESEARCH IN NUCLEAR SCIENCEGOVERNING BOARDA High Flux Beam Reactor for Solid State ResearchNote by J. M. Valentine

The Research Reactor Committee at its meeting on 27th June, 1963 appointed a Panel, with Professor E. W. J. Mitchell of Reading University as Chairman, to look into the scientific case for a high flux beam reactor for solid state research. The report prepared by the Panel was considered by the Committee at its meeting on 10th October, 1963.

The Research Reactor Committee felt that there was a very strong scientific case for building a high flux beam reactor, preferably as a national project although a European project would be a satisfactory alternative subject to certain conditions. The Committee recognised that there was no hope of new money being made available for a high flux beam reactor in the near future but they felt that every effort should be made to keep the project alive so that the scientific aspects could be considered carefully and its priority as a major project assessed.

The Research Reactor Committee approved the report and asked that it be submitted to the Board for their consideration.



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Membership of the Panel

Professor E.W.J. Mitchell - Chairman

Dr. W. Cochran

Dr. P.A. Egelstaff

Dr. W.M. Lomer

Dr. J.M. Valentine

Mr. G.L. Cooper

} Joint Secretaries



### Summary

In this proposal we outline briefly the history of the development of solid state physics, and emphasise the extremely important part that neutron techniques are playing in increasing fundamental knowledge of the solid and liquid states of matter. Experiments on crystals using beams of neutrons include the determination of atomic positions, studies of magnetisation distribution and studies of structural defects, while techniques which have been developed more recently enable the dynamical properties of solids such as spin waves and lattice vibrations to be investigated. We forecast that the use of neutron techniques will be as important for furthering a knowledge of the structure and dynamics of liquids as the use of X-rays was for solids.

Further advances in these fields depend on the availability of intense beams of thermal neutrons. The A.E.R.E. research reactors PLUTO and DIDO and the A.W.R.E. reactor HERALD, each of which produces a flux in the range  $1$  to  $3 \times 10^{13}$  n/cm<sup>2</sup> sec, are used by about 20 A.E.R.E. scientific staff and about 10 university staff and research students who at present work in this field. The realisation of the importance of this field, and recent improvements in the ease of operation of the equipment, is now making it practicable for many more solid state physicists to make active, part-time use of the equipment. By about 1970 there will be a strong demand for facilities to accommodate about 100 users. We state the case, on scientific grounds, for the construction of a British high flux beam reactor for solid state physics research having a flux of about  $10^{15}$  n/cm<sup>2</sup> sec. Its construction by 1968 would enable this country to maintain a leading position in the field. The cost of constructing and equipping the reactor would be about £10M, and operating costs would be about £2.5M p.a. This is rather less than the cost of a national particle accelerator project.

If this proposal is unacceptable on financial grounds, we conclude that subject to certain conditions of siting and organisation, a reactor operated jointly by European countries would be a satisfactory alternative. The British contribution, in money and personnel and the number of British scientists served would then amount to about one quarter of the figures mentioned above.



## A HIGH FLUX BEAM REACTOR FOR SOLID STATE PHYSICS

### 1. Introduction

About one half of the world's physicists are engaged in the study of the solid and liquid states and both the U.K. and Europe have traditionally been in the forefront of the developments in this field. The basic components of solids and liquids - the atomic nuclei and their associated electrons - interact according to known laws. Even so new features emerge when large numbers of particles interact simultaneously. It is salutary to remember that no detailed study of the interaction of water molecules can yet explain the simple collective motion of waves on the sea. The identification of collective motions and their interpretation in terms of individual particles and their interactions is an integral part of advance in the physics of the solid and liquid states (the state of 'condensed matter').

We are emphasizing the fundamental science of the study of condensed matter as a part of the general scientific progress, of the increase of man's knowledge of the world around him. At the same time, however, we are aware that there is a complex interplay in this part of physics between fundamental science and technology. For example, many technological applications of physical ideas have required the development of very pure materials, which, having been prepared, have enabled further and more penetrating studies to be carried out. In fact, the technological developments in the field of solids in the last 20 years have been phenomenal: transistors, photosensitive detectors, nuclear radiation detectors, masers, lasers ..... with superconductors around the corner. We strongly take the view that the earlier fundamental studies formed an essential basis for the growth and that the continuing fundamental study is an essential condition for the ever increasing application of solid state technology.

Since the war the study of some collective motions and other fundamental problems of the solid and liquid states has been stimulated by the availability of beams of neutrons. Primarily because of its mass in relation to the masses of atomic nuclei, and of its absence of charge, the neutron has become an essential tool in the study of condensed matter. The present proposal is for the establishment, either nationally or in Western Europe, of a High Flux Beam Reactor (H.F.B.R.), designed specifically to provide beams of neutrons for this work. It is felt that the provision of a H.F.B.R. is essential to progress in this part of physics.

The provision of a High Flux Beam Reactor will ensure that from 1969 - assuming an early start - we shall continue to be on equal terms with the rest of the world in this major part of physics. For a relatively modest outlay it will be possible to provide physicists both in Government Establishments and Universities with the principal incentive which can be given, that is, facilities which will give them the opportunity of doing the best work that can be done. An essential part of the pursuit of science is enthusiasm and it is difficult to maintain enthusiasm if one knows that the important and crucial experiments are all being carried out elsewhere with superior equipment.

The important characteristic of the H.F.B.R. is that it will produce intense beams of low energy neutrons (thermal neutrons). Whilst we think that the proposal has to be discussed in relation to the study of condensed matter, nevertheless there are important experiments in other fields which the existence of intense fluxes of low energy neutrons will make practicable. Notable examples occur in the fields of nuclear physics and radiochemistry.



## 2. A Brief History of the Development of Solid State Physics

### Developments up to 1925

Since the days of Faraday and Maxwell, Europe has been in the forefront of the fundamental advances of what is now known as solid state physics. These advances have come from a series of interlocking and interweaving studies, each advance a result of more and more detailed techniques of examination being brought to bear on better and better defined problems. The study of solids is essentially the study of crystals and crystalline aggregates. The properties of crystals were first studied by mineralogists, natural crystals being the only pure materials available. As chemistry developed, more pure substances showed themselves to be crystalline and impure substances were shown often to be crystalline on a microscopic scale.

The study of the thermal properties of solids has resulted in many important advances over the years. Towards the end of the 19th century, it became possible to reach temperatures low enough to reveal some puzzling anomalies in the specific heats and these were satisfactorily explained only when the concept of the quantum was introduced by Planck and Einstein in Germany and Debye in Holland. Since then each major advance in low temperature technique has brought to light new physical phenomena which have led to a more detailed understanding of the crystalline state. High pressures and high magnetic fields are further new environments which enable our theories to be tested and our knowledge extended.

The most important advances in our detailed knowledge, however, have come from the study of the interaction of radiation with matter at ordinary temperatures, pressures and magnetic fields, each new type of radiation providing a further major advance. The basic laws of the interaction of electromagnetic radiation with matter were formulated by Maxwell, the emphasis at that time being on the interaction with light. Later X-rays were discovered by Roentgen and shown to be part of the electromagnetic spectrum. The interaction of the new radiation with matter was studied by von Laue and the Braggs and they showed how from the diffraction effects the relative positions of atoms in crystals could be accurately determined. From that time the U.K. has held a leading position in atomic structure determination, even to the present day work in molecular biology.

The discovery of the electron by J.J. Thomson in 1897 and the brilliant analysis of  $\alpha$ -particle scattering carried out by Rutherford in 1911 had made the basic structure of the atom clear. This knowledge together with that derived from the study of the series of spectral lines which were observed when light interacted with the isolated atoms of gases led to the Bohr quantum theory. But still no way of generalisation was found, nor of application to condensed matter and another crucial discovery was awaited. This discovery came about by the study of the interaction of a further type of radiation with matter, although in this case the immediate conclusion concerned the radiation rather than the matter. Electrons were found by G.P. Thomson and the Americans, Davisson and Germer, to exhibit diffraction, as had X-rays, in their passage through matter. From this the ideas of the wave nature of electrons were developed by de Broglie, leading finally to the Schrodinger equation. Since electrons were a major constituent of atoms the methods for understanding the properties of atoms could then be fully developed, as in fact they were, by Schrodinger, Heisenberg, Born and Dirac.



## The Modern Theory of Matter

At this stage all the necessary developments had occurred which could be expected to lead to major advances in the study of condensed matter. These developments had taken place as a result of the study of the interactions of different types of radiation with matter - light,  $\alpha$ -particles, electrons and X-rays. The theory of the atom which had been constructed from the study of the first three could then be used to examine the properties of assemblies of atoms in the positions determined from the study of the diffraction of X-rays. In this way began the study of the ideal crystal.

Europe made major contributions in the period 1925 - 1940 through the work of Sommerfeld, Wilson and Mott, with corresponding contributions from Wigner, Slater and Seitz in the U.S.A., to the development of the framework of modern solid state physics. More recently, and in particular after 1945, it became apparent as a result of a complex interplay of experimental and theoretical work, that many important physical properties were determined not only by the given rigid ideal structure, but by departures from rigidity - atomic vibrations - and departures from the ideal structure - imperfections. The interactions of ultraviolet, visible and infrared radiations with matter continued to be of major significance in the experimental work. The use of microwave radiation, which was developed for radar, gave rise to new detailed knowledge of the behaviour of electrons in metals, semiconductors and especially in magnetic materials, and has added considerably to our knowledge of the role of specific impurities and of the simpler imperfections in crystal structures. Oxford has been one of the originating centres in this field.

A quite distinct area of solid state physics has grown up since the War on the borderline of metallurgy and engineering. This is based on the concepts of dislocations - lines of discontinuity in the regular pattern of crystal structures - and their interactions, and in the years 1945 to 1950 the U.K., virtually alone, developed the whole subject and still holds a commanding lead. The electron microscope has played an important part in this development but all the general methods for the study of defects in crystals are, to some extent, also applicable.

During the period between the World Wars considerable progress was made in the experimental study of liquids. The most striking development was the use of X-rays to measure the positions of atoms in liquids. This followed the development of the techniques used for the study of crystals and was initiated by Debye and Zernike on the Continent. These results showed that the atoms in local regions in the liquid were arranged in a manner not far different from similar atoms in a solid, while at large distances the atoms were randomly arranged. Following these experiments there were many theoretical attempts to represent liquids as disordered solids. Prominent amongst these was the cell theory of Lennard-Jones and Devonshire. Although it is now possible to calculate the X-ray scattering from liquids almost from first principles, this has not given the understanding of liquids which it was hoped to achieve. The main reason for this is that the motion of individual atoms or groups of atoms cannot be studied with X-rays. Such a study has had to wait until the advent of copious sources of neutrons.

Neutrons, which had been discovered at Cambridge in 1932, became available with the rapid development after the war of nuclear reactors. Physicists were quick to realize that the interaction of this new type of radiation with matter would again lead to major advances in our understanding of solids. The first type of work to be done was neutron diffraction, precisely equivalent to X-ray diffraction, but taking advantage of some favourable nuclear parameters to determine atomic positions not capable of being studied with any accuracy by X-rays. The



neutron also interacts through its magnetic moment with the magnetic moments arising from electron spins in atoms giving rise to magnetic scattering. This enables magnetic structures to be investigated for the first time. These developments have taken place in the atomic energy laboratories of the World where reactors are situated, and not the least at Harwell.

Perhaps of greater interest now and in the future, however, is the use of neutrons for studying the dynamic and static imperfections in crystals. In the former case it turns out that thermal neutrons have just the appropriate energy/momentum relationship for studying the atomic vibrations in molecules and solids. In the study of static imperfections one utilizes the fact that the neutrons are scattered by the nuclei and are relatively unaffected by the distorted electronic structure near the imperfections. The favourable properties of neutrons also make it possible to study the atomic motions as well as positions in liquids. This is the step which is likely to be as significant to the study of liquids as was the Braggs' work to the study of solids. As with neutron diffraction these activities have occurred at atomic energy laboratories and Harwell has been in the forefront of the field as well as the North American and European centres. In the U.K., through the co-operation of the Atomic Energy Authority and latterly of the N.I.R.N.S., the Universities have contributed to a small but increasing extent, particularly Cambridge, Reading, Sheffield and Birmingham.

### 3. Current Neutron Beam Experiments and their Limitations

The preceding Section has already mentioned briefly some of the main uses of neutrons in the study of condensed matter. In this section we outline the current limits of application of neutron techniques; detail has been relegated to Appendix A. Because the neutron has no electric fields associated with it, but does possess a magnetic moment, it is unique amongst available radiations in being able to react to the magnetic state of materials. Because its mass is comparable with that of atoms, it is possible to measure energy and momentum changes in the range significant for the dynamics of atom movement. To restate the energy condition, thermal neutron energies are  $1/40$  eV so that changes of energy corresponding to the quanta of processes with a resonant frequency in the region of  $10^{13}$  per second are easily measured. Electromagnetic radiation of this frequency has a wavelength of one three-hundredth of a centimetre, and so cannot be used for investigation of spatial detail on an atomic scale. Conversely electromagnetic radiation with wavelengths of atomic dimensions - X-rays - has such high energy ( $\sim 10^4$  eV) that the energy levels of thermal interest cannot be studied. The ability of the neutron to respond to atomic positions and magnetisation on the atomic scale, and to exchange energy of thermal magnitude with a scattering sample, enables us to make unambiguous deductions about many basic properties of those crystals which we can investigate. It is in terms of these basic properties that results of experiments using other techniques must be interpreted, but it is exceptional for any other techniques to isolate the individual effects so convincingly as can the appropriate neutron experiment. Perhaps it is worth noting that it is this certainty of interpretation that characterizes neutron beam experiments rather than any major extension into new fields of physics, (in sharp distinction to the situation in high energy physics).

The importance of attaining the highest possible neutron flux is illustrated by the following simple calculation. Neutron beams from the highest flux reactors at present available are produced by collimation from a total thermal flux of about  $10^{13}$  n/cm<sup>2</sup>/sec, or a few times higher. A well collimated beam, say  $\frac{1}{2}^\circ \times 1^\circ$  divergence,



selects only  $1.6 \times 10^{-5}$  of the original flux, so that a  $10 \text{ cm}^2$  source in a flux of  $10^{13} \text{ n/cm}^2 \text{ sec}$  yields a collimated beam of this area with a total flux of  $1.6 \times 10^9 \text{ n/sec}$ . This includes neutrons of all thermal energies; if a wavelength spread of a few per cent about the mean is called for, the best flux will be about  $5 \times 10^7 \text{ n/sec}$ , or  $5 \times 10^6 \text{ n/cm}^2 \text{ sec}$ . After partial scattering by the sample another such selection of directions and energies may be required, so that even with samples of many square centimetre cross-section, counting rates in some experiments are reduced to a few counts per second. Some weak scattering processes have been studied at significant counting rates of only 5-10 events per hour. At such levels random spurious counts can easily defeat an experiment.

At present fluxes the solids which may be studied are necessarily selected far more by consideration of whether a sufficiently large crystal of adequate perfection can be grown, than by their intrinsic scientific interest. It is not only a matter of crystal growing technique (though that is of course highly important), because the need for big samples rules out the possibility of experiments on compounds containing strong neutron absorbers, and on samples made from costly separated isotopes. Each increase in flux by a factor ten enables experiments of present quality to be carried out on a wider selection of substances; probably it is no exaggeration to say that a hundred times as wide a choice is available for each factor ten in size of crystal demanded.

In addition to this freedom to investigate more types of substances, the availability of higher fluxes would enable more significant experiments to be carried out on those few large crystals that are available.

Some experimental work has been conducted using particle accelerators as pulsed neutron sources, but at the present time they produce lower thermal neutron fluxes than the best reactors even if multiplying targets are used. Although it may be possible, eventually, to develop accelerators to the point where they are competitive for time-of-flight experiments, we shall not consider this possibility here for several reasons. First the accelerator schemes require development in contrast to a high flux reactor which could be built now. Secondly the cost, time scale and performance offer no improvement on the reactor schemes listed in Section 5. Thirdly much of the crystallographic and defect programmes listed below, which are normally carried out using continuous neutron beams, would be prejudiced by a restriction to pulsed beams.

We have highlighted some of the activities and difficulties of the current neutron programmes.

(a) Magnetisation distribution studies in crystals

Despite the fact that the close connection between strong magnetic properties and the anti-symmetry condition for electron wave functions was recognised by Heisenberg in 1926, we are still unable to predict magnetic structure. Even in technologically important materials such as ferrites and garnets we have only a skeleton empirical knowledge of the facts and this has been provided mostly by neutron techniques. The magnetic electrons are the outer valence electrons of interest for chemical as well as physical reasons. There are only four full-time scientists using as many diffractometers engaged on this work in the United Kingdom compared with about 400 scientists engaged in X-ray work - a highly unsatisfactory situation in our view. At present, single crystals for this work must be comparatively large (approaching 1 cc.) This is a very serious limitation since large crystals are generally difficult to make and has for example stopped studies of  $\text{CrBr}_3$ , a ferromagnetic



salt of great theoretical interest. Because of this limitation work has concentrated mainly on alloy systems where large single crystals are readily available and has partially neglected oxides. An increase of neutron flux would enable smaller crystals to be used and make possible a much wider range of investigations.

(b) Phonons and spin waves

Inelastic scattering of neutrons from crystals in which the neutrons experience a change in energy gives us a direct method of studying the vibrations of atoms in crystal lattices and even similar vibrations in the magnetisations (see Appendix A2). The very first vibrational studies to be completed in detail (at Chalk River in Canada) showed that whilst some of the forces between atoms in a metal were best thought of as comparatively local, some are of very long range, and probably represent forces derived from the electron gas in some way. In ionic and covalent crystals the phonon frequencies showed some unpredicted effects, now regarded as evidence for polarisation by deformation. A study of lead shows anomalies due to the interaction between the electron Fermi surface and the phonons - the interaction which is the basis of the current explanation of superconductivity. Many substances await study on the two time-of-flight spectrometers (instruments for measuring velocity changes of neutrons) available at Harwell and must take their turn with other programmes mentioned below. The same apparatus is used for spin wave studies in ferromagnets, antiferromagnets and ferrimagnets, and once again this is the only available method for work on bulk substances (there is a resonance technique available for thin films of ferromagnets). The explanation of the results is still uncertain, especially in metallic systems where inadequacies in the approximate formulation of the problem used earlier are now clearly exhibited for the first time. Most of these studies demand samples, some 20 cm<sup>3</sup> in volume, and are therefore limited to compounds of elements with low neutron absorption of which very large single crystals may be grown. On a high flux reactor with large crystals such as these, some experiments on the life time of phonons would be possible, and a detailed picture of the basic processes determining thermal conductivity should result. These experiments are quite beyond our reach with currently available fluxes.

(c) The dynamics of atoms in liquids

Inelastic scattering from liquids allows us to study the dynamics of atoms in liquids. For many years, the correlations of atomic positions in liquids have been known from X-ray studies. With inelastic scattering techniques, it is possible to study correlations of the velocities of the atoms, and already it has been found that their translational motion, which distinguishes a liquid from a solid takes place in groups of ten to a hundred atoms, in a sort of local swirl. So far, there are only two or three completed experiments on liquids, because of pressure of work, and proper interpretation has not begun. The present apparatus is presenting tantalising results, which will be far more useful when a small factor of improvement on energy and momentum resolution is available. A flux increase of factor ten would meet this requirement.

(d) Defect scattering

Long wavelength neutrons may be scattered from crystals only by deviations from the crystal perfection, so that the scattering of neutrons originating in a cold moderator, or otherwise selected to have low energy, gives a powerful method of studying defects on a



size scale of 2-10<sup>0</sup>Å. This is just below the electron microscope resolution, and there is considerable promise in this method of study of radiation damage. Foreign atoms in magnetic substances may disturb the magnetic structure, so that we can study local modifications of the magnetic lattice. This had already thrown new light on the alloy behaviour of nickel and iron based alloys and provides a searching test of the validity of band theory for alloys. Two rather different types of apparatus exist with long programmes of exciting work ahead of them. Very large samples of highly controlled perfection are demanded by these programmes, and samples, two, two or three inches square and a quarter to half-inch thick are required. Where such samples can be obtained, a higher flux would yield essential information on the wavelength dependence of the scattering. Where smaller samples only are available results of the present useful quality would be obtained for many more samples.

(e) Neutron crystallography

Light atom positions, and differentiation of atoms of similar atomic number in structures may be explored with neutrons, thus removing an irritating set of restrictions on X-ray work which has held up studies of hydrogen bonding, ammonium ion dynamics, hydride structures, heavy element oxides, carbides and nitrides, and studies of ordering in many interesting metallic systems. Single crystal work on comparatively simple, non-hydrogenic substances with, with about thirty atoms per unit cell requires, at present fluxes, samples of volume 0.1 to 1 mm<sup>3</sup>. Complex hydrogenic substances, such as the simplest crystals of biological interest, may require volumes greater than 1 cm<sup>3</sup>. All polycrystal work requires bigger samples, which are nevertheless easier to produce, and is far less rewarding in detail. An increase in flux would widen the field of application enormously, would allow use of separated isotopes, and would bring us to the borderline at least of a study of the role of hydrogen in simple substances of biological interest.

(f) General summary

To investigate the structure, vibrational and thermal properties, magnetic properties, defect structure, or electronic levels of solids or liquids, some important features can be defined only by the use of neutron techniques. United Kingdom work in this field, carried out almost entirely on the A.E.A. research reactors has resulted in the development of a wide range of experimental equipment and techniques. The specific apparatus which is currently in use, or nearing completion on A.E.A. reactors is as follows:-

- (i) about six diffractometers, of varying degrees of sophistication, suitable for structural studies of all kinds, some accommodated two per reactor hole.
- (ii) two large spectrometers suitable for work on polycrystals.
- (iii) two polarised beam diffractometers
- (iv) three fully-equipped time-of-flight spectrometers, one fitted with a cold source. A second cold source is being constructed. A fourth spectrometer and hot source are being designed.



- (v) two high intensity pulsed long wavelength equipments of different design for defect scattering.
- (vi) one small angle scattering apparatus
- (vii) a triple axis spectrometer for inelastic scattering experiments is under design.

This equipment represents a balanced basis for a national programme of research, and there is no item which could be abandoned without detriment to some branch of the study of condensed matter. Substantial improvements in every category are looked for as a result of higher fluxes, so that we must argue that any high flux reactor scheme should allow our scientists access to all categories of instrument, and that use of a number of instruments in some categories is desirable.

#### 4. Present Reactors and Future Needs

At the present time three reactors are in use in the United Kingdom for neutron beam experiments; these are DIDO and PLUTO situated at A.E.R.E. Harwell and the HERALD reactor at A.W.R.E. Aldermaston\*. The former reactors operate at a power of approximately 15 MW while the latter operates between 3 and 5 MW. These should be compared with the power of the University teaching reactors of about 0.01 to 0.1 MW and with the 70 MW of the proposed high flux beam reactor. In the case of DIDO, PLUTO and HERALD neutron fluxes available at the end of the beam tubes vary between 1 and  $4 \times 10^{13}$  n/cm<sup>2</sup>/sec. which may be compared with figures ranging up to  $10^{15}$  n/cm<sup>2</sup>/sec. for the high flux beam reactor.

The Harwell reactors were designed as a compromise to meet the needs of both irradiation and beam experiments and consequently are not fully satisfactory for either purpose. For example, the experimental conditions at the reactor face are less than ideal for beam experiments because of high radiation backgrounds and limited working space. The flux at the end of the beam tube for a given reactor power is limited by the design of the core, and the operational programme of the reactor is compromised by the need to allow for the demands of irradiation work. While these disadvantages are accepted at the beginning of a programme they become less acceptable as experiments move towards a higher level of sophistication. Thermal neutrons have been used in solid state research at Harwell for over ten years, and over this period both the equipment and the techniques of interpretation have been developed to a high level. They have now reached a point where they can contribute in a major way to the development of solid state physics and some examples of this were given in the previous Section. To achieve this full potential however, a high flux reactor designed specifically for beam experiments is required.

During the past ten or fifteen years while the neutron techniques have been under development, the number of workers in the United Kingdom - both U.K.A.E.A. and University staff - employed in this field has been relatively small. At the present time approximately twenty A.E.A. scientists are involved in this field of fundamental research while the number of University users engaged is about ten; in addition there are several more engaged on nuclear physics experiments using reactors. In many cases the Authority and University staff work in close collaboration putting a given

\*The NRU reactor at Chalk River has also been used with the permission of the Canadian authorities, but only on a very limited scale.



piece of equipment to more than one use. Over the next few years it is expected that the Authority's work in this field will increase slowly compared with a rapid increase in the Universities. The University interest has always been strong, and because the techniques have reached the point where they can be exploited effectively, there are now many experiments in which they wish to collaborate. The holding item at the present time is the number of experimental facilities fully commissioned, but this situation will be eased when the items listed in Section 3 become available. As a broad estimate, the number of Authority and University workers in this field will be about equal at twenty-five each in three or four years time, and thereafter the University numbers are likely to exceed the Authority's. By the end of the 1960's it is possible that the University numbers would be double those employed in the Authority. As an example of the potential effort in this field we cite the case of neutron diffraction. In this area a small fractional interest among the 400 or so X-ray crystallographers in the United Kingdom would produce a very heavy strain upon existing facilities and even on the proposed facilities.

By taking together the list of apparatus given in Section 3 for a well equipped laboratory and the number of scientists and students who it is anticipated will join this field, one can deduce the number of high flux beam holes which are required by the United Kingdom. On the assumption that each user will require on average two months of running-time per year, it will be necessary to have approximately twelve high flux neutron beams and a number of lower flux supporting holes, for the use of the United Kingdom. This argument suggests that the demand in the United Kingdom alone is sufficient to completely fill a high flux beam reactor of the type proposed for Europe. It may prove possible to accommodate two pieces of equipment on a proportion of the high flux holes, so that the reactor as a whole may serve perhaps 150 part time users.

#### 5. Possible Reactor Proposals

It has been shown (Appendix C) that the cost of a beam reactor to meet the needs just described and to give parity with or slight superiority over any known proposal in the world, is about £7M, which with all proper supporting facilities, would total about £10M. This overall cost depends on the site, and what existing services may be used. In any event the net outgoing capital must be between these figures. The running cost would be about £2.5M per year\*. Thus over a period of ten years, say, the total cost of the reactor project would be £0.35M per scientist - about one-third of the corresponding cost of a national accelerator project.

There are three methods of organising a reactor project of this type. They are, in order of decreasing cost:

- (i) the reactor is built in the United Kingdom for national use;
- (ii) the reactor is built in the United Kingdom in collaboration with ENEA for joint use by European countries;
- (iii) the reactor is built in continental Europe in collaboration with ENEA for joint use by European countries.

The major difference to the user is that the proportion of time allocated to the United Kingdom and the ease of access to the reactor site decreases as we pass from (i) to (iii).

\*When in full operation it would provide beam facilities for about 100 scientists.



The construction of a high flux beam reactor by the United Kingdom for national use would more than meet the immediate demand, though it would not be excessive relative to the demand which will exist at the earliest possible completion date (1968). Solution (i) is therefore by far the most attractive.

The figure of £10M may seem large for a field that has previously spent only small capital sums. Accordingly, it is worth examining the cost and utility of an international collaboration (either of solutions (ii) and (iii) above), which would make available a properly equipped central reactor to deal with those critical experiments which cannot be accommodated at the national centres. The direct capital cost to the United Kingdom of joining a European project of total net cost £10M is not easy to estimate. It seems to be commonly accepted that the host nation, on whose territory the project is sited, would pay a disproportionately high cash contribution, say 30-35% as against 20-25% for an overseas project. This difference is largely recouped on a national basis - though not on a Treasury basis - in terms of building and civil engineering contracts which draw their labour from local sources and the continued local spending associated with the centre. A net capital cost of £2.5M should be foreseen for our participation in such a project. Of the total running cost of about £2.5M p.a. the United Kingdom might bear £0.6M p.a. In return, we would expect about one quarter of the available facilities. French and German interest is as keen as ours and there can be no doubt at all that soon after its first operation time on the reactor facilities will be severely scheduled.

If solution (iii) is adopted the role of the existing reactors in the United Kingdom assumes a greater importance, since they would then certainly be used for an indefinite period for most of the United Kingdom programme. The experiments transferred to the ENEA reactor would only be those most demanding in flux or with other special requirements. Students would in general be trained on the home reactors before sending them abroad. Through the national experimental programme a reservoir of experts would be maintained ensuring that the United Kingdom contribution to the ENEA reactor is a worthwhile investment. Thus the importance of a strong home base cannot be over-estimated, and significant sums of money, probably of the order of £2M will need to be spent on developments and improvements to existing reactors (or similar neutron sources) in order to maintain the home base at a high level of productivity. For this reason the apparent savings in options (ii) and (iii) above can to some extent be illusory.

Summarising, there is a large expanding programme of work in the solid and liquid state fields requiring high flux neutron beams, which physicists in the United Kingdom wish to conduct; the basic reactor facilities will cost at least £5M whichever option is adopted. In the case of solution (i) a long term investment in a single project is being made, while with solutions (ii) and (iii) the cost is being divided into two parts, a contribution to a joint project and support for smaller national projects. The remainder of this paper will discuss the high flux beam reactor project only, the question of smaller national projects being deferred until a decision on the possibilities (i) to (iii) has been taken.



## 6. History of the H.F.B.R. Proposal

During the period 1956-60 reactor physicists at the Brookhaven National Laboratory in the U.S.A. evolved specialist designs for beam reactors to meet the anticipated experimental programme at B.N.L. The best of these designs was finally approved and work on a new reactor was started at the beginning of 1962. It will be in full operation by the end of 1964, roughly eight years from the earliest discussions.

By 1960 the need for more and better reactor space for solid and liquid state research in the United Kingdom had become apparent and design work on a new reactor was begun at Harwell in 1961. Basing their design upon the Brookhaven work they produced a design study report (A.E.R.E. - M.1123) in which several new features were proposed.

At this stage it was decided to link the Harwell work with the proposals which ENEA were making for joint European reactor projects. In July 1962 a meeting organised by ENEA on the "Scientific User Requirements for Very High Neutron Fluxes" was held at A.E.R.E. Harwell. This Conference concluded that there was a definite need in ENEA countries for higher fluxes than those at present available in Europe and that the need was mainly in the field of solid and liquid state physics. An under-moderated heavy water cooled and reflected reactor, based on the Brookhaven design, had been considered in the A.E.R.E. feasibility study; it appeared to be particularly suited to the requirements. It was finally concluded that an international study group should be set up to consider various aspects of such a reactor project. In November 1962 the Steering Committee of the ENEA favourably considered the conclusions of the Harwell meeting and set up a "Study Group on the Very High Flux Reactor" whose terms of reference included the possible experimental programme and design of the reactor, including cost, timescale and the siting requirements. To perform its work the Study Group set up three working parties which were entrusted with detailed studies on the reactor, the research programme and the organisation of a joint project respectively. The two working parties on the reactor and the research programme have presented a joint report, which has been approved by the Study Group for submission to the Steering Committee.

The working parties confirmed their agreement with the views reached at the 1962 Harwell Conference. The proposed reactor is a 70 MW under-moderated heavy water cooled and reflected reactor designed almost solely for the production of neutron beams. The design envisages 22 beam holes of which 10 horizontal ones will be situated in the most favourable positions and will accommodate the most sophisticated equipment. The maximum undisturbed flux at the inner end of some of the beam holes will be about  $10^{15}$  n/cm<sup>2</sup> sec. A feature of the reactor and one of the principle scientific requirements is the control of the neutron beam spectrum by the use of "hot" and "cold" neutron moderators.

The capital costs, which include the reactor, "hot" and "cold" moderators, experimental equipment and supplementary building accommodation and equipment, but excluding fuel, total £10M. The annual recurrent costs including the reactor operating cost, salaries, re-equipment of beam holes and rental of computing facilities total £2M. Regarding the siting of the reactor the working parties suggested that it should be near a centre engaged in fundamental research and which itself has reactors and associated facilities. This would ensure the proximity of experienced scientists and also result in economies from the joint use of supporting facilities. The ENEA cost estimates are based on such a site. A fuller account of the technical features of the ENEA reactor is given in Appendix B, and costs in Appendix C.



## 7. Boundary Conditions for Central Reactor Project

We do not feel that it is appropriate in this report to put forward detailed proposals for the organisation of the H.F.B.R. Centre. If the proposal to go ahead with the reactor is approved in any of the three forms described in Section 5, it will be necessary at a later stage to have a detailed report on the organisation of the Centre and on the procedure for using the reactor. Nevertheless, there are some comments which we feel should be made now. They are made in terms of an international project but most of them would apply, with some modification, also to a national H.F.B.R. Centre. One of an international project but most of them would apply, with some modification, also to a national H.F.B.R. Centre.

Whether the United Kingdom contribution is the whole - as in the case of a national reactor - or part - as in the case of an international scheme - it should be clearly seen to be a national contribution. Thus we envisage a centre for neutron beam research and any potential user who satisfies a "Users Panel" will have access to the H.F.B.R. Undoubtedly the first United Kingdom users would be from groups already active on existing reactors, primarily the A.E.R.E. and the Universities of Birmingham, Cambridge, Reading and Sheffield. However, the criteria for access should be the scientific importance and feasibility of the problem, rather than the organisation from which the problem comes.

The versatility of neutron beam research is naturally reflected in the kinds of apparatus required. It is necessary to have apparatus specialised to each type of experiment and we may easily find that at least eight or nine distinct types of apparatus are necessary (see Section 3). British scientists will expect the U.K. financial contribution to buy time on a complete set of neutron instruments. It would be disastrous if each nation were allocated two or three beam holes and uncoordinated equipments were installed on them, or if access to instruments of a particular type rested too much on the good will of the "owners" of individual holes. Within this general framework it is possible to list several specific user requirements:-

- (a) the centre should be responsible for the working order of in-pile and out-of-pile equipment.
- (b) the mounting of an experiment by a user, or the change of equipment on a hole, should be as rapid as possible to achieve a high utilization of the reactor.
- (c) the centre should be responsible for developing new equipment, with possibly the collaboration of a user who may have done some preliminary work on a national reactor.
- (d) the user during a visit should be able to decide the measurements he wants to do day by day, and determine his programme during his visit, and be able to change it if necessary in the light of results.
- (e) the centre must be reasonably accessible to all users, at least to the extent of being within easy reach of a major airport. This is of particular interest to the University users since supervisors of research students would need to visit the centre for short periods while their students were at the centre.
- (f) Adequate funds from a national source must be provided to cover the personal expenses (travel and subsistence) incurred by visitors using the centre.



We envisage three types of User visit:

- I. Short visits of one or two months. The majority of visits would probably be of this type. A User - who may be a research student or a member of the University staff, or a member of the scientific staff from a research establishment - having preferably had experience of his problem or a similar one on a national reactor, would visit the centre for the short period in order to carry out his measurements. In most cases the analysis would be done at the home laboratory but it would be essential to keep a record of accumulated experience at the Centre. It would be necessary to submit a report to the Users Panel before a further visit could be made. The report would be made available at the centre.
- II. Extended visits of six months or more. This would be necessary, for instance, when some major new experiment was being mounted. As much as possible of the detail of the method should have been developed on national reactors, but it would be unrealistic to suppose that the new versions on the H.F.B.R. could be made to work immediately. The visiting scientist would work with the appropriate resident scientist and his staff.
- III. Visits for 'Service' experiments. The type of User envisaged in I and II would have had some experience of using neutron beams. There is a class of User, however, for which this is not essential. Thus for example, a crystallographer may require the diffraction pattern and some data processing of a given sample in order to answer some specific structural problem. It should be possible to arrange a service of this type which the resident staff would provide after discussion with the User who would normally want to visit for a few days. Service experiments would also require approval by the Users Panel.

The Centre must contain a nucleus of scientific staff of high calibre who are employed on a permanent basis or on long term appointments. They would be neutron specialists who were easily available to visitors for the discussion of scientific problems. In addition to the dissemination of knowledge concerning the applications of available techniques the permanent staff would also be responsible for the maintenance of existing apparatus and the development of new and more sophisticated techniques.

In order to attract and keep scientists of the right quality the Centre must be able to offer them the opportunity to run their own programmes of research in addition to their other duties.



## 8. Conclusions

(i) The use of neutron beams is an extremely powerful technique for studying the properties of solids and liquids, and there is an increasing demand for high flux reactor facilities for this purpose.

(ii) Although the present high flux reactors in this country are being intensively used they are not able to produce the highest fluxes now required to carry out the most critical experiments.

(iii) We consider there is a strong scientific case for building a high flux beam reactor. Moreover, our estimates of the probable demand for experimental time from users in this country suggest that such a reactor could be fully occupied by British experiments and therefore we would like to see the reactor built as an entirely British project.

(iv) Failing this, a share of a European reactor would be acceptable providing certain minimum requirements in the matter of siting and organisation are accepted. Probably the most important of these is that British users should have the right of access to all the available experimental facilities provided at the reactor face.

(v) Such a reactor built either as a national or European project would provide a facility comparable to the best in the world, enabling scientists in this country to maintain their place in this vital branch of physics.



## APPENDIX A

### Details of current status of neutron programmes, and specific advantages of higher fluxes

#### A.1 Crystallographic Studies

##### A.1a Crystallography of magnetic materials

The neutron magnetic moment interacts with the magnetic moments of atoms, whether due to electron spin or orbital motion. Since both of these represent distributed sources of magnetic field, the neutron scattering cross-section exhibits a form-factor dependence on the change of neutron momentum. These form-factors are not yet particularly well known, for they involve the outer electron shells which are only moderately well calculated for free atoms, and which are subject to large modifications when the atoms are incorporated into a solid. Apart from these form-factors, the magnetic scattering length depends on the expression  $\mathbf{e} \cdot \boldsymbol{\mu} - (\mathbf{e} \cdot \mathbf{K}) (\boldsymbol{\mu} \cdot \mathbf{K})$  where the  $\mathbf{e}$  is a unit vector in the direction of polarisation of the incident neutron,  $\boldsymbol{\mu}$  - the magnetisation vector, and  $\mathbf{K}$  a unit vector parallel to the scattering vector. The magnetically scattered waves therefore are of opposite phase if  $\boldsymbol{\mu}$  is oppositely directed, as in an antiferromagnetic material. This can give rise to additional diffraction lines corresponding to the magnetic superlattice. Their intensity for different scattering vectors gives the absolute direction of  $\boldsymbol{\mu}$ . This information is not accessible in general by any other technique. The alternation of the sign of the scattering amplitude is not dependent on neutron polarisation and so the antiferromagnetic lines may be studied by the same techniques as normal nuclear neutron diffraction.

Until neutron diffraction was available, it was supposed that antiferromagnetic materials consisted simply of two sublattices of magnetic atoms with their directions of spin oppositely aligned. In the last few years however, many types of pattern have been discovered involving non-parallel spins, and spins of systematically varying magnitude on crystallographically equivalent atoms. It is now clear that a tremendous quantity of information must be collected in order to understand this class of material, whose applications are multifarious and which include nearly all transition metal and rare earth metal oxides, carbides, sulphides, complex ions and in many cases, the metallic elements and alloys as well.

In ferromagnetic materials the sign of  $\boldsymbol{\mu}$  is the same on all equivalent atoms, and so the relative phase of nuclear and magnetic scattering can be changed by changing the sign of the neutron polarisation  $\mathbf{e}$ . This gives us a great facility for studying in detail the form factor for magnetic scattering, since the nuclear scattering cross-section is well known and isotropic. Pioneer work on iron and cobalt has already been reported, but a wide range of work remains to be carried out.

At present fluxes, the single crystals used for quantitative work on these subjects must be of the order of 10 - 100 mm<sup>3</sup>, and preferably far bigger. For example, a study of Cr Br<sub>3</sub> - a simple ferromagnetic salt of great interest - had to be abandoned both at Harwell and Brookhaven because the largest crystal that could be grown for either group was "only" some 300 mg. in weight. A higher flux would open up the study to many more materials.

##### A.1b Crystallography of non-magnetic materials

The scattering of neutrons without change of energy is related to the average positions of the atoms in the scattering sample. The same is true of X-rays, and, apart from differences in the magnitude of the scattering



cross-section, neutron and X-ray crystallography of non-magnetic materials are very closely similar. There are however a few points of difference, which gives neutron crystallography a notable role to play in documenting the basic structures of materials. First, the neutron scattering cross-section is small and isotropic; there is no complicated form factor correction to be applied to compare scattering at different angles as for X-rays. Second, the majority of neutron scattering cross-sections lie within a factor ten of all others, whilst for X-rays they are proportional to the square of atomic number and so have a range of nearly  $10^4$  between uranium and hydrogen. Third, elements which consist of mixtures of isotopes, or which have nuclear spin, may show a set of unequal values of nuclear cross-sections, the average of which contributes to the structural terms, and the deviations from average contribute an isotropic structureless diffuse scattering. Fourth, by using separated isotopes, the cross-section of an atomic type can sometimes be changed.

The main application to non-magnetic studies has so far been to hydrogen atom location, and to studies of uranium and thorium oxides. Bacon has for example shown that in some half-dozen crystals containing water of crystallisation, the hydrogen atoms are often to be found lying nearly on the line between two oxygen atoms forming a long hydrogen bond, but that nonetheless the configuration of the water molecule is too rigid to allow all the hydrogen atoms to become truly colinear with the oxygen atoms. This kind of positive information could not be won by other means.

To carry out such studies, of hydrogen especially, demands single crystal techniques. Polycrystal powder techniques worsen the elastic Bragg scattering relative to the incoherent diffuse scattering, and for hydrogen the diffuse scattering cross-section is some twenty times greater than the coherent cross-section. At present day fluxes studies of crystals with say thirty atoms per unit cell, including several hydrogen atoms, demand single crystals of a cubic mm. or more in volume. To increase the flux by a factor of thirty would allow crystals of this size with perhaps a thousand atoms per unit cell to be studied so that we could truly begin to study simple biological materials, or alternatively would allow us to use crystals thirty times smaller only a few micrograms in weight. Such changes would tremendously widen the types of crystals in which we could positively place the hydrogen atoms. To be able to use small single crystals would also permit of wider use of isotopic substitution. So far the only study using a special isotope in this way has been an investigation of ordinary reactions in Fe - Ni alloys, using  $\text{Ni}^{60}$  which has a cross-section very much smaller than the value for natural iron, and involved 8 grams of  $\text{Ni}^{60}$ , which would cost about £60,000 to produce.

There is some interest too in obtaining precise measures of crystal structure factors, for though the nucleus is small its average position is not well defined because of thermal vibrations. Exact measurements of diffracted intensities can therefore give information on the time-average nuclear distribution. With neutrons there can be no confusion between such effects and the broadening of atomic electron clouds consequent on bonding which affects X-ray results. It is hoped that with higher fluxes comparison of X-ray and neutron data on similar sized crystals will give new information on electronic bonding and thermal vibrations in all kinds of solids.

#### A.1c Crystallographic apparatus required

To carry on a sensible programme of crystallography two basic types of instruments will always be necessary, viz. good accurate diffractometers suitable for use with comparatively small single crystals, and large diffractometers suitable to handle large polycrystalline samples. At some



times, high angular resolution will be desired - at others, the highest possible intensity to allow work with small samples. Work with polarised neutrons require specialised apparatus, so that we arrive at a basic minimum kit of -

- 1 high resolution single crystal diffractometer
- 1 high intensity single crystal diffractometer
- 1 general purpose polarised neutron diffractometer
- 1 large sample powder diffractometer

Whilst the work load might not be even on these instruments they all seem essential, and the overflow work would have to be carried on at reactors of lower flux. At present at Harwell there are effectively two at least of each of these types of instrument and three or four general purpose diffractometers in addition. All have programmes of work which extend beyond the foreseeable future, and which are revised from time to time as still more exciting possibilities arise.

## A.2 Dynamical studies

### A.2a Vibrational spectra of crystals

Ever since the acceptance of heat as a mode of motion, it has been realised that the atoms in a crystal are in a state of continual vibration. The theory of the dynamics of the atoms in a crystal dates from some of the early publications of Einstein, Debye and Born, some fifty years ago. The motion is described in terms of travelling waves, and the relations between the frequency and wave number of the waves, and their polarisation properties, depend on the forces between the atoms in the solid. A knowledge of this spectrum of lattice vibrations, (often called phonons to emphasise that their energy is quantised), is essential for complete understanding of the mechanical, thermal and electrical properties of a crystal. Until recently there has been no satisfactory experimental method of obtaining basic information such as the relation between frequency and wave number of these thermally-excited modes of vibration. Within the last six years it has been shown that, by measuring the change of energy and momentum of a beam of slow neutrons which has interacted with a crystal, basic information about the lattice vibrations can be obtained. As yet the method has been applied only to metallic elements such as copper and lead, ionic compounds such as potassium bromide and a few semi-conducting materials, such as silicon and gallium arsenide.

It has been shown that the formulation of the dynamics of the crystal in terms of forces between nuclei, though formally acceptable, is inadequate from the point of view of physical understanding. We must take explicit note of the function of electrons of the solid as intermediaries in the interaction. This represents a major shift of emphasis, as yet far from realised, which will one day bring together the treatment of atomic vibrations and electron states in crystals. Already certain anomalies in the vibration spectra of lead are interpreted as an image of the electron Fermi surface. In this field, above all, the importance of the neutron work lies in its definitive nature. The positive identification of a few critical vibrational energies in silicon has enabled the techniques of infra-red absorption to extend our knowledge, though the interpretation of infra-red data alone had been originally too tentative to be fully accepted.

At present, such phonon studies are limited to crystals of very large size, say twenty to one hundred grams. The value of an increase in flux for these studies would be tremendous.



#### A.2b Phonon life-times

The vibrational spectrum of a solid reflects the interatomic forces produced when atoms undergo very small displacements. It is of interest to study larger displacements and we note here that the shape and energy width of phonon states could be measured in favourable cases if a somewhat higher flux were available. No such studies have yet been carried out, for they are just beyond our present grasp.

#### A.2c Spin waves in magnetic crystals

The dynamics of magnetisation fluctuations in crystals may be studied in essentially the same manner as the vibrational motion of atoms. Just as it is easier to explain the vibrations of a particular lattice than it is to determine why it is the most stable lattice, so it is in some ways easier to analyse the spin waves than the magnetic structures. Information on the magnitude and range of the coupling between spins is now beginning to accumulate, and results are available for one or two ferromagnets, one or two ferrimagnets and a single antiferromagnet. The variation of the spectrum, and the width of the lines, should be studied at temperatures near the Curie point, to elucidate the nature of the very weakly magnetised state. Thus a recent study of nickel at the Curie point has shown that though long wavelength fluctuations are of vanishingly low frequency, those of shorter wavelengths are not, showing something of the nature of the short range order problem in magnetic systems. This work, however could not be carried out with proper wavelength resolution because of the low values of the flux available.

#### A.2d Atomic dynamics and the structure of liquids

The cross section for scattering of neutrons by liquids depends upon the momentum and energy transferred in the scattering process. By Fourier transforming the scattering function one determines the space time correlation function of Van Hove. This relates the position of an atom at one time with the position of the same or another atom at a later time and consequently contains all the information about both the dynamics and the structure of liquids insofar as it can be expressed in terms of the interaction of atoms two by two. In thinking about the dynamics it is convenient to consider separately the motion of single particles which leads to diffusion and the collective motion of particles analogous to phonons in solids.

In the study of diffusion it is possible to examine the details of a single diffusion step. The diffusive step occurs on a time scale of about  $10^{-12}$  sec, and to study that period requires momentum transfers of  $\sim 0.5 \text{ \AA}^{-1}$  and energy transfers of  $\sim 0.5$  meV. Transfers of this order have to be measured precisely and the scattered intensity at each point determined, and the shape of the curves compared to the predictions of diffusion theories. In this way one can decide, for example, whether the diffusion process consists of atoms jumping from site to site as in a solid, or combined movements of groups of atoms analogous to Brownian motion, or, as actually occurs, the process is a combination of several mechanisms. Advance in understanding of liquid diffusion is directly related to the precision of the neutron measurements, and very high resolution measurements on liquids will be one of the first experimental programmes with a higher available flux.

The discussion of the collective motion in liquids is a complicated matter since these modes are heavily damped due to their strong interactions with one another. Since it is just at this point that the theory of liquids is in difficulty the neutron measurements of this effect are eagerly awaited, but again they require accurate and time-consuming measurements. For example, at present the measurement to an accuracy of



0.5Å of the wavelength change occurring in the scattering of 8Å neutrons may take one week, whereas with the proposed reactor the same measurement to an accuracy of 0.1Å would take about one day. These figures are for reasonably favourable processes. However, some of the most interesting processes give low scattered neutron intensity and longer counting times; those occurring at the minima of the diffraction pattern for example. Most important amongst these are the study of collective modes having a wavelength of several atomic spacings, because modes of this kind determine the degree of long range order (or disorder) in the liquid.

#### A.2e. Crystal field splitting

It is also possible to explore the excited levels of atoms in crystals, if these are excited by only thermal energies. An investigation of FeCl<sub>2</sub> on these lines had to be abandoned at Harwell because of low flux, whilst it succeeded at Saclay where a liquid hydrogen moderator increased their effective flux some five times. (The cold source at Harwell was already saturated with other work and not available for this experiment.) FeCl<sub>2</sub> was naturally chosen by both groups as the freak "easy" substance.

#### A.2f. Apparatus for dynamical studies

There are two basic techniques for selecting neutron energy; direct velocity measurement by using pulses of neutrons and measuring time-of-flight, or crystal diffraction monochromators. The first method involves the production of a pulsed monochromatic beam by a pair of phased choppers, and energy analysis by the time-of-flight after scattering by the sample. The design of rotor for the choppers is determined by the resolution required and by the energy range of the neutrons. Thus it is difficult to combine in one apparatus the facilities for high intensity and high resolution work, and for large and small incident energy. At low incident energy there is great benefit to be derived from the operation of a liquid hydrogen source block, and the final resolution does not so much depend on fixed parameters of rotor design. A reasonably complete set of apparatus would then include:

1	general purpose time-of-flight instrument on cold source
1	high resolution " " " " " normal or hot source
1	high intensity " " " " " " " "

We should note that it would be possible to accommodate some very sophisticated time-of-flight equipment of these kinds on a specially built pulsed reactor-accelerator if inadequate space were available at the high flux reactor.

Time-of-flight techniques involve certain disadvantages however. They demand precision high-speed apparatus and the incident energy is preset rather than variable. A triple axis spectrometer uses crystal monochromators for incident beam and scattered beam analysis; this instrument is easy to operate but suffers from certain complications, e.g. second order reflections of half the desired wavelength. Nevertheless it is capable of very high precision, but loses intensity badly for low incident or emerging energy. All the best work has so far been done on instruments of this type and one should plan for at least:

1 triple-axis spectrometer at normal source

At present at Harwell and Aldermaston there are:

- 1 general purpose time-of-flight instrument at normal source.
- 1 (+1 under construction) general purpose time-of-flight instrument at cold source.
- 1 planned triple axis machine.



### A.3 Defect scattering

#### A.3a Structural defects

Beyond the Bragg cut-off a perfect non-absorbing crystal would be completely transparent to neutrons. In practice various types of disorder will contribute to the scattering out of an incident beam of wavelength, say, between 5 and 15Å. Point defects and simple aggregates of defects represent one such type of disorder.

The study of defects produced by irradiation using this technique is in its infancy, although various types of experiment are being studied on national reactors, particularly HERALD where a cold source is being designed for this purpose. The great advantage of using neutrons is that, contrary to any other method for examining defects, one knows the defect (nuclear) scattering cross-section (i.e. the effect per defect; compare for example the electrical resistivity of a metal). In addition, using the wavelength dependence, or preferably the angular variation of the scattered intensity and its wavelength dependence, one can obtain as direct information as possible about the formation of pairs, etc. ... under different conditions.

With the cold sources in national reactors many experiments will be possible, including the observation of the scattered radiation from defects produced by reactor irradiation and the transmission experiment using defects produced by fast electron irradiation. Using the cold source in the H.F.B.R. it should be possible to perform the most sophisticated experiment in this field: the determination of the angular variation of scattered intensity from defects produced by electron irradiation.

#### A.3b Substitutional atom defects

A further type of experiment in the field of long wavelength neutron scattering is the study of atom positions surrounding an impurity atom. At present no experimental information exists about these relaxed positions. It is hoped to obtain some information from transmission experiments in very special cases on a national reactor. But the availability of this technique for a wider variety of solid solutions, and the complete determination of the angular variation of the scattered intensity in the special cases, will both require the cold source of the H.F.B.R.

So far the only related study has been the ferromagnetic alloys, where over the last year an entirely new field has been opened up. The introduction of a foreign atom into a crystal of ferromagnet disturbs the magnetic order over a radius which is some measure of the range of interaction. This has provided a new test of theories of metallic systems which is more definitive than any previously available. Corresponding experiments in antiferromagnets demand longer wavelength neutrons to avoid Bragg scattering, and these are in very poor supply without a higher initial flux and a cold source. The significance of such experiments on ferrites and similar substances should be considered. A trial experiment had to be abandoned because of the complications due to Bragg scattering at the lowest neutron energies usable on our present equipment. This could be greatly improved by a higher flux and a cold source.

#### A.3c Order-disorder

The possibilities of detailed investigation of order-disorder reactions with neutrons are wider than with X-rays because so many interesting systems involve atoms of similar atomic number. Much of this work can be satisfactorily carried out on polycrystalline specimens, and present flux limitations are not critical.



#### A.3d Apparatus requirements

The main programmes under 3a and 3b involve the elastic scattering of low energy neutrons. The basic equipment is therefore a cold source for the neutrons, followed by a crude chopper and time-of-flight instrument to eliminate inelastically scattered neutrons. This is therefore a similar requirement to that for inelastic scattering and the necessary instrument is a time-of-flight apparatus on a cold source.

Order - disorder studies require shorter wavelengths and have so far been carried out without emergent energy resolution on conventional spectrometers. This is unsatisfactory in principle, and represents another potential call on the inelastic scattering equipment installed at a normal source position.

Small angle scattering is of particular significant for a number of reasons and a special collimation to yield a beam of angular divergence of not more than  $1/10^\circ$  would always be very valuable. Current work with three times this divergence (the best the flux will allow) tries to measure certain abrupt changes in cross-section at  $\frac{1}{2}^\circ$ , which is only marginally possible. Thus we add to the list of apparatus required one small angle scattering facility.

At present at Harwell there are:

- 1 high intensity time-of-flight instrument at normal source
- 1 small angle scattering facility

together with intensive use of cold source, and general purpose time-of-flight instrument referred to in previous section.

#### A.4 Nuclear physics experiments in a High Flux Beam Reactor

Although it is recognised that the main purpose of the high flux beam reactor is for solid and liquid state physics, nevertheless there are a variety of nuclear physics experiments which it would be worth doing once a reactor of this type had been built. Several of these experiments involve irradiation of samples inside the reactor and extracting a beam of nuclear radiation which has been produced by a thermal neutron interaction. For example, a sample which absorbs thermal neutrons strongly into a single nuclear state can be placed near the centre of the reactor and a beam of gamma-rays obtained from it. The measurement of the energy and intensity of the captured gamma-rays so produced is very important in completing our picture of the nuclear level schemes. Alternatively a fissile specimen can be placed near the centre of the reactor to give a beam of fission product nuclei, and this way one can obtain beams of unstable nuclei for special experiments which cannot be obtained by other methods. In other cases it will be necessary to extract the irradiated sample from the reactor for measurements of nuclear level schemes, and for this reason a fast rabbit would be installed. Taken together these types of experiment will represent a useful advance over the existing nuclear physics knowledge in this field.

Another and particularly important nuclear physics experiment concerns the re-measurement of the basic properties of the neutron, particularly its half life. These properties form some of the basic knowledge by means of which the theory of nuclear forces is tested, and consequently it is important that they should be measured accurately and well. The high neutron fluxes available from the proposed reactor, coupled with modern detecting techniques, should enable a substantial improvement in the accuracy of these constants to be made.



In addition to such nuclear physics experiments there is the occasional experiment in some other basic area of physics which the introduction of a new and very powerful machine makes possible. An example of this type of experiment is provided by the study of gravity with cold neutrons. In this, one measures the gravitational constant for neutrons in which the neutron spin is at first parallel and then antiparallel to the gravitational field. By a comparison of the results an upper limit to the coupling between electromagnetic and gravitational fields may be estimated for the first time. This illustrates the fact that some fraction of the time on the high flux reactor will have to be devoted to new and unusual experiments which show promise of advancing new areas of physics.

#### A.5 Radiation damage using epithermal beams

In a reactor, atoms are displaced after being struck by fast neutrons and the atomic recoil energy may be as high as  $10^5$  eV. The primary knock-on then produces further displacements in slowing down to rest and produces on a local scale considerable disturbances of the atomic vibrations. Because of the large maximum recoil energy and of the continuous spectrum of incident neutron energies the pattern of damage produced in a reactor is complex.

A considerable advance has been made in the study of radiation damage by treating separately the primary displacement process on the one hand, and on the other, the range and energy loss of the relatively massive primary knock-on. It has not been possible to obtain sufficiently intense beams of monoenergetic neutrons to work in the threshold region. Consequently threshold studies have all been made using fast electrons, which owing to their smaller mass, produce much smaller recoil energies. The electron charge, however, does introduce an unwanted complication. The motion of primary knock-ons through a crystal has been simulated by bombarding crystals with similar or identical ions to those in the crystal. This has the advantage that the energy can be accurately controlled and that fairly copious beams are available. From experiments of this type the crystallographic effects associated with the passage of a heavy particle through a crystal have been elucidated. Much work remains to be done on both of these aspects - the threshold region and the loss of energy of the massive particle.

There is no doubt however that for these two aspects to be satisfactorily joined in relation to our understanding of reactor damage it will be necessary to work with neutron beams of defined energy. First, one would work in the energy range where atoms are just displaced, and then step by step, move into the region where the damage produced by the primary knock-on becomes more and more important. We are therefore interested in beams of neutrons having selected energies in the range 100 - 10,000 eV.

Even with the high flux beam reactor it will not be possible to carry out a wide range of radiation damage studies. However, using carefully selected physical properties - e.g. internal friction, electron spin resonance and minority carrier lifetime - it is possible to detect  $10^{12}$  -  $10^{13}$  displacements per  $\text{cm}^3$ . For such experiments we require a neutron dose of about  $5 \times 10^{12}$  -  $5 \times 10^{13}$   $\text{n/cm}^2$  in the threshold region. Then, if one week were the maximum period over which the irradiation could be carried out we should require a flux of about  $10^7$  -  $10^8$   $\text{n/cm}^2$  sec. For an epithermal flux of  $10^{14}$  -  $10^{15}$   $\text{n/cm}^2$  sec. the above types of experiment become possible in principle with a not too roughly defined incident energy.



## APPENDIX B

### Technical Specification of the High Flux Beam Reactor

(prepared by Dr. V.S. Crocker)

The basic requirement is for high intensity neutron beams and it is considered that to provide the desired beam intensities the beam holes must 'view' a thermal neutron flux of about  $10^{15}$  n/cm<sup>2</sup> sec. There are few reactor types which could supply this neutron flux and the use of the reactor solely for neutron beam production again reduces the number. For neutron beam work the required neutron flux should be attained in the reflector and the beam holes should end not too close to the core (because of the possible 'background' effects from core  $\gamma$ -rays). Also to avoid rapid changes with time of the beam intensities the neutron flux should fall off relatively slowly in the reflector. It is also desirable that the power output should be kept to a minimum which leads to the choice of enriched uranium as the fuel. A heavy water reflector combined with a compact, heavy water cooled, enriched uranium core provides all the required characteristics. The thermal neutron flux actually peaks in the reflector about 6 in. from the core and then falls off relatively slowly with distance from the core. All the above reasoning and detailed neutron beam requirements have been considered in an A.E.R.E. design study (see report A.E.R.E. M.1123) which formed the basis of the discussion for the E.N.E.A. 'Very High Flux Reactor Design'. Such a reactor would fulfil all the requirements listed in this report, being designed as a specialised reactor for the production of high intensity neutron beams.

The reactor is a 70 MW heavy water cooled, moderated and reflected reactor using a compact, highly enriched core, composed of plates of magnesium aluminium alloy containing a U<sup>235</sup>/Al alloy centre. The thermal neutron flux peaks in the reflector giving a flux of about  $1.2 \times 10^{15}$  n/cm<sup>2</sup> sec. at 70 MW power. The core is located at the centre of a flask-shaped aluminium alloy pressure vessel. Heavy water enters through the neck and passes downwards through the core, then up around the outside of the core and out again through the neck. The inlet and outlet connections are made only at the top of the flask so that a fracture of the external heavy water circuit would not uncover the core. The coolant is circulated by centrifugal pumps through light water cooled heat exchangers. The 70 MW of heat transferred from the heavy water to the light water is finally dissipated in a bank of forced draught cooling towers.

To remove the heat from the core without taking the water above its saturation temperature the heavy water flows through the uranium-aluminium alloy fuel plates at a velocity of 35 ft/sec and pressure of  $\sim 250$  p.s.i.g.

Piercing the flask are twentytwo beam tubes, including one through hole. Eleven of the beam tubes (mostly tangential to the core) terminate close to the maximum thermal flux peak in the reflector and are equally spaced just above and below the core centreline. Eight beam holes (one through one) emerge at an angle to the main beam tubes and view a lower flux than the main holes. There are also three vertical beam tubes which lead into the basement beneath the reactor. Two special experimental facilities are important features of the reactor. One using a hot moderator, provides a source of 'hot neutrons', and one using a cold moderator, 'cold neutrons'. Each of these sources is viewed by a number of beam tubes. The hot source is viewed by two horizontal, one inclined and one vertical beam tube whilst the cold source has three horizontal, two inclined and one vertical beam tube. To reduce interference with the



beam experiments the hot and cold sources are loaded through angled holes above the main beam holes. These two special facilities are the main features of the reactor and should provide intensities of 'hot' and 'cold' neutrons that could not be obtained elsewhere in the world. The number of experimental facilities has been limited to provide adequate space outside the 9 ft concrete biological shield for the proposed equipment. The concrete shield has been made 'thick' to reduce the interference of background radiation and by having a 'slot' filled with removable shielding around the beam holes the shield has been made as flexible as possible besides providing the necessary shielding for experimenters. The reactor is housed in a cylindrical containment building of reinforced concrete, designed to provide the maximum working space for experiments on the main floor around the reactor.

The principal parameters of the reactor are given below:-

Purpose	-	beam research
Power	-	70 MW
Max. neutron flux		$\sim 1.2 \times 10^{15}$ n/cm <sup>2</sup> sec
Fuel	-	90% enriched U <sub>235</sub> in aluminium
Mass of fuel	-	$\sim 8$ kg U <sub>235</sub>
Length of core	-	21 inches
Diameter of core	-	19 inches
Coolant and reflector	-	D <sub>2</sub> O
Mass of D <sub>2</sub> O	-	-
Pressure at core inlet	-	250 p.s.i.g.
Max. heat flux	-	400 W/cm <sup>2</sup>
Velocity of D <sub>2</sub> O thro' core	-	35 ft /sec.
No. of beam tubes	-	22 (11 high flux)



### APPENDIX C

The following estimate of the capital and annual operating costs for a 70 MW high flux beam reactor is taken from the report of the ENEA "Study Group on the Very High Flux Reactor", April 1963.

<u>CAPITAL COSTS</u>	<u>\$ million</u>
Reactor capital cost (including heavy water and reactor development costs but excluding fuel)	20.2
Cold and hot neutron sources .....	1.5
Experimental equipment .....	4.5
Supplementary building accommodation and equipment .....	3.0
<u>TOTAL</u>	<u>\$ 29.2 million</u>

<u>ANNUAL OPERATING COSTS</u>	<u>\$ million</u>
Reactor operating cost (based upon hire of fuel and including reactor operating personnel)	2.8
Research staff	2.0
Re-equipment of beam holes and operation of cold source	0.6
Rental of computing facilities	0.3
<u>TOTAL</u>	<u>\$ 5.7 million</u>

.....

Assuming that the reactor is approved in the Autumn of 1964 and that the design team is working by the beginning of 1965 the following table is an estimate of the annual commitment of money for the following four years until the completion of the reactor. The cost of the experimental equipment is also included:

	<u>\$ million</u>
Year 1965	2.7
Year 1966	8.5
Year 1967	11.8
Year 1968	6.2
<u>TOTAL</u>	<u>\$ 29.2 million</u>