INTRODUCTION

Michael Norgett Memorial Issue (1943–2003)

This issue of *Journal of Physics: Condensed Matter* is published in memory of Dr Michael Norgett. In recognition of his contributions to the subject of computational physics. It contains articles by his former friends and colleagues and others whose own scientific work in this field—mainly materials physics—has been influenced by his. In this introductory note we will try to set his work and influence in the context of the time. He was a modest man and it is fitting that this influence should now be highlighted by this issue. Since he joined the UK Atomic Energy Authority's Harwell Laboratory in 1968 the tale is inevitably tied in part to the history of this laboratory and of its links with the nearby University of Oxford.

Norgett's first degree at Oxford (in 1965) was in chemistry. He then moved over to the Theoretical Physics Department directed by Professor (later Sir) Rudolph Peierls, but his actual research for his DPhil degree was carried out in association with Theoretical Physics Division at the UKAEA Harwell Laboratory. He thus received his early training as a theoretician in two very strong departments, both of which ranged widely in their work and interests. In TPD Harwell these derived from the nuclear and reactor programmes of the Harwell Laboratory as a whole, which at that time was concerned, among other things, with matters relating to the next generation of power reactors following the building of the series of Magnox stations. Norgett's thesis work was prompted by the need to understand the effects of neutron irradiation on oxides, especially the migration of fission gases (Kr and Xe) in nuclear fuel materials such as UO_2 [1].

From the point of view of a young theoretician entering the field of defects in solids, it was fortunate that these needs in the nuclear reactor field were already leading, not only to a great deal of technical materials data, but also to related, refined experiments on model ionic solids such as the alkali halides and the alkaline earth fluorides (which have the same crystal structure as UO_2). These experiments permitted the fundamental processes to be studied in the absence of extraneous and uncontrolled factors while their interpretation demanded accurate theoretical predictions of the properties of possible defect models for comparison with the experimental results. Such predictions demanded—as Norgett was quick to realise—a good understanding of the underlying theoretical solid state physics, an area where both Oxford and Harwell were strong, and increasingly good computational techniques. In turn the latter required not merely good programming skills but also a recognition of the advances being made in numerical analysis. So it was again fortunate that TPD Harwell had an outstanding numerical analysis team and access to what were then top of the range IBM computers. An overview of the wide-ranging, yet deep, strengths of TPD is given in [2], which celebrated the first 25 years of TPD. Norgett's recognition that these advantages could be used to produce general purpose programs—as distinct from those written in individual ways to deal with only particular models or particular crystal structures—was the key to his initial influence on computational solid state physics. Norgett also saw that since such programs ('black boxes' in the language of the day) were intended also for use by others having limited knowledge of the way they worked, they had to be user-friendly. The quality of his user guides and associated documentation was of the highest.

The first of such tools which Norgett provided was HADES, designed for the computation of defect structures and energies in model ionic solids [3–7]. It allowed numerically accurate predictions of defect structures and characteristic energies for any specific potential energy function within the class of Born models for cubic crystals without assuming any particular defect symmetry. It did so through the use of efficient minimisation routines which made limited demands upon computer memory. To verify the suitability of the assumed model associated bulk crystal properties (e.g. elastic constants, dielectric constants, etc) could be calculated by another program called PLUTO [8, 9]. These programs were avidly taken up by research students, experimentalists and other theoreticians attached to Harwell and would have been even more widely disseminated but for the commercial policies of the Laboratory at the time. Collaborations and codes sales led to HADES being used in Europe, Africa, Asia, Australasia, and North and South America. The combination of widespread dissemination, feedback, and Michael Norgett's own careful approach meant that the code earned the trust of users. This was very important in the acceptance of the idea of a widely-available, general-purpose code. A similar program for pair potential models of metals—DEVIL—which used the same efficient minimization routines and likewise provided accurate predictions followed soon after [10]. Until the time these programs were produced almost all similar calculations had contained various simplifications and approximations, so that the reliability of the results was uncertain and the meaningful comparison of different calculations was difficult [11]. The accuracy and power of these programs ensured that the subsequent use and extension of the HADES program was rapid (see, for example, the reviews by Catlow [12] and by Catlow and Mackrodt [13]). During the late 1970's and the 1980's various other developments followed; a version HADES III was developed for non-cubic crystals and for crystals with large and complex unit cells, it was re-coded as CASCADE for use with the Cray supercomputers, it also became available for use with the PC's then emerging whilst its example had encouraged the development of a number of related programs for dislocations, surface defects, grain boundaries, and thermal and lattice vibrational effects. In addition there were parallel developments from atomistic potential models to programs embodying quantum mechanical sub- routines, essential for 'open-shell' defects such as colour centres and defects in covalent semiconductors. The number of different physical applications had by this time run into hundreds.

Norgett's work and influence was by no means limited to the above examples. However, the features to be found in them—rigorous physics, good numerical analysis and efficient programming and good documentation—also formed the basis for much other work: particularly (i) his analysis of radiation effects in metals and an associated program for determining the relation between radiation dose and the resulting damage (the so-called NRT relation [14]), (ii) his HELP program for the economic analysis of strategies for electricity generating systems, which he applied to determine the economic benefits of the proposed Severn Barrage and other schemes for renewable energy sources and (iii) his work on the modelling of combustion and fluid flow behaviour.

Norgett's value to the UKAEA was well recognised by the organization and in 1988 he was appointed Head of the Computer Science and Systems Division. Ironically, the management changes imposed on the UKAEA in 1990 meant that within two years of this appointment he had to oversee the closure and dispersal of that Division. Thereafter his knowledge and insights were applied in other areas of work in the UKAEA's commercial arm—AEA Technology—as it prepared for privatisation in 1996 and after. He retired on grounds of ill health in 2000 and died of leukaemia in 2003. Meanwhile the scientific developments which he had started and fostered were carried on by others in many institutions, especially in the UK, thereby enhancing its reputation in the field of computational solid state theory.

In this note we have tried to bring out some of the factors which made Michael Norgett's work timely and important to the field of computational materials physics. The papers making up the present issue of the journal give detailed examples of work 'down stream' from his and provide a fitting tribute to his memory.

References

[1] Norgett M J 1968 *The theory of defects in crystal lattices* DPhil thesis (University of Oxford)

[2] A B Lidiard (ed) 1979 *25 Years of Theoretical Physics 1954–1979* UKAEA Report TP 843

[3] Lidiard A B and Norgett M J 1972 *Computational Solid State Physics* eds F Herman, N W Dalton and T R Koehler (New York: Plenum) pp 385–412

[4] Norgett M J 1972 *A Users' Guide to HADES* Harwell Report AERE-R7015.

[5] Norgett M J 1974 *A General Formulation of the Problem of Calculating the Energies of Lattice Defects in Ionic Crystals* Harwell Report AERE-R 7650

[6] Norgett M J 1977 *Symmetry Methods for Lattice Defect Calculations Harwell Memorandum* AERE-M2880

[7] Stoneham A M 1975 *Theory of Defects in Solids* (Oxford: Clarendon) see particularly section 8.3

[8] Catlow C R A and Norgett M J 1976 *Lattice Structure and Stability of Ionic Materials* Harwell Memorandum AERE-M2936

[9] Harding J H 1982 *A Guide to the Harwell PLUTO Program* Harwell Report AERE-R 10546

[10] The early version of DEVIL was used for several distinct applications to pair-potential models of metals. It was later developed by Thetford for use with the N-body potentials devised in the 1980's particularly for transition metals. See
Thetford R 1985 *Application of the DEVIL program to N-body Potentials* Harwell Memorandum AERE- M3507 (with an appendix on the srtucture of DEVIL by M J Norgett)

[11] See for example
Lidiard A B 1966 *Calculation of the Properties of Vacancies and Interstitials* ed A D Franklin, National Bureau of Standards Miscellaneous Publication No 287, pp 61–8

[12] Catlow C R A 1980 *J. Physique Colloque* C6 pp 53–60
Various other papers in this issue also illustrate the point being made.

[13] Catlow C R A and Mackrodt W C (ed) 1982 *Computer Simulation of Solids* (Berlin: Springer) see particularly pp 3–20

[14] Norgett M J Robinson M T and Torrens I M 1975 *Nucl. Eng. Design* **33** 50