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► **To cite this version:**

A. Bostel, Marinette Bouet, J. Sarrau. A SOFTWARE PACKAGE FOR ATOM PROBE USERS. Journal de Physique Colloques, 1986, 47 (C7), pp.C7-521-C7-524. 10.1051/jphyscol:1986787 . jpa-00225984

HAL Id: jpa-00225984

<https://hal.science/jpa-00225984>

Submitted on 4 Feb 2008

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A SOFTWARE PACKAGE FOR ATOM PROBE USERS

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Résumé - Un programme d'acquisition et de traitement de données pour sonde atomique a été développé. Il permet d'obtenir toutes les informations usuellement disponibles à l'issue de calculs ultérieurs pendant la manipulation. Il permet de montrer les spectres de masse, les différents profils ... Il supporte la multi-détection et autorise la désignation et le tri des objets métallurgiques. L'interface utilisateur est particulièrement convivial.

Abstract - An atom probe software package for on line analysis of atom probe data has been developed. It allows to get during the experiments all informations usually obtained with "off-line" treatments, such as mass spectra, multi-element concentration and composition profiles ... It supports the four sector multi-detection we developed. The designation and sorting of various phases is achieved by means of on line graphic methods. The user interface is very convenient.

I - INTRODUCTION

This software package is designed for "on-line" atom probe data collection and analysis. The objective is to create a set of programs usable by an artless computer scientist, allowing to make fast and easy data interpretation during the manipulation. The atom probes are designed for "off-line" running : they do not need any computer to operate in a free running mode. They issue messages in serial form on a EIA RS232C normed cable. The program supports data acquisition, interpretation and saving.

II - ON LINE ACQUISITION PROGRAM

The data collected are saved and interpreted. Thus, an unique structure of data suit to each individual atom. The benefit does not reside in disk space neither in speed but in treatment suppleness : all the original data are saved. There is no dependance between data structures and programs actions, allowing us to change the disposition of programs with no data loss.

The software is turned toward the end-user ; it is interactive and governed by menus. Depressing one function key performs one action : changing menu (they are connected in a tree form), making some changes or calculation works, drawing or printing some data. We take special trouble for the text describing each function ; in the

same manner we have specially chosen the functions contained in one menu, so as to preserve the logical approach of the atom probe scientist. For example, the results of calculations (drawings or texts) are always showed on the screen before they are printed, in the crazy hope to reduce paper consumption. Another example is the strategy we use to enter data. When an user begins to work, the system automatically recognize him, names the data files, and remembers the last data he used. In most cases, those data do need some modification. In the same way, the system manages a library of alloys, containing for each alloy, the mass limits for each element. This library is a collection of models. During the manipulation, the model corresponding to the alloy under study can be read, and, if necessary, modified. This model is kept in intimacy with atom probe data: all the work done during data collection is not lost.

The response time (i.e. the time delay between a request and the completion of an order) is kept as low as possible. For a screen menu change as well as for a standard request, there is no visible delay. However, heavy recalculations performed over a set of a few 10^4 atoms need a few seconds, including disk latency and read time. Every second, data tables and some immediate results are updated. I/O processor, buffers and a high priority ensures a null loss in data collection.

The functionalities are analogous to some other software products recently described in the literature (1)(2); spectra, cumulative plots, compositions, flux curves, state of manipulation... However, specific improvements are operative: the multi-detection support, the designation and sort of metallurgical phases. This can be of great help to decide whether a fluctuation can be interpreted as a phase or not.

III - MULTI-DETECTION

The software supports the four sector multi-detector (3) described elsewhere. For the whole possibilities given above, it ensures data calculation on an arbitrary chosen set of detector. The coherence of the address translation between one set of detectors to another is transparent to the user.

There is no need to remind the great interest of the multi-detection system, specially for the high data collection rates. It can be used even with a Poschenrieder atom probe. This requires however a defocalisation of the ion beam (5).

IV - DESIGNATION AND SORT OF METALLURGICAL PHASES

A mechanism of pose and release of markers on any draw involving the order of incoming ions (cumulative plots, composition plots) allows separation and naming of the various metallurgical objects (i.e. different phases, or types of planes in Long Range Order studies). These markers can be written or even rubbed out in an arbitrary order. The corresponding program structure is a binary tree, which gives always sorted data. This function supports the multi-detection. It allows to calculate the concentration of each element in the various objects, and to draw corresponding spectra. This is of great interest for Long Range Order studies, and frees the atom probe worker from a heavy load of hand-made calculations. We have also included some statistical tests (Poisson, squared-khi test...), the aim of which is to detect some deviation from a random distribution of solutes in a solid solution (6).

V - ACTUAL STATE

This product is being on test and works, but does not include all the modules : the auto-correlation is not yet implanted.

Further developments are of great help for the interpretation of various sets of data corresponding to the study of an alloy, and we develop now the collection and the choice of valid data, and their draw on synthetisis corresponding diagrams. For instance, we will draw for a α/β two phases alloy the observed composition of α -like elements versus that of β -like ones for each designated phase. Such a plot is of great interest for ensuring the data consistency. In addition, the volume fraction can be readily estimated from the well known lever rule. (4)

VI - HARDWARE AND SOFTWARE

This product is developed on HP 9000 Model 550 with HP-UX and C language. The software set furnishes a powerful help for the conception and the maintaining of complex software products. The programming aids of HP-UX are of great interest by automatizing some complex, careful and frequent works (as the make function). The bug hunting aids are also of great interest.

The calculation power of the hardware seems to be larger as needed. But the machine is able to support three atom probes ; each of them with a multi-detector. That is equivalent to a dozen of standard atom probes in terms of speed and amount of data. We also think to the future developments on a five years scale.

Acknowledgments

The authors wish to thank La Région de Haute Normandie, Le Centre National de la Recherche Scientifique, Le Ministère de la Recherche et de la Technologie for their financial support.

REFERENCES

- (1) M.K. Miller, Proc of the 32th IFES, Journal de Physique, C2-47 (499).
- (2) A. Cerezo, T.J. Godfrey, A.J.W. Moore, J.D.W Smith, Proc of the 31st IFES, Journal de Physique, C9-45(315)
- (3) D. Blavette, A. Bostel, J.M. Sarrau, Proc of the 32th IFES, Journal de Physique, C2-47(473)
- (4) D. Blavette, S. Chambreland, Proc of 32th IFES (1985)227
- (5) O. Nishikawa, K. Oida, M. Tomiori, this Symposium
- (6) D. Blavette, P. Caron, T. Kahn, submitted to Scripta Met (1986)

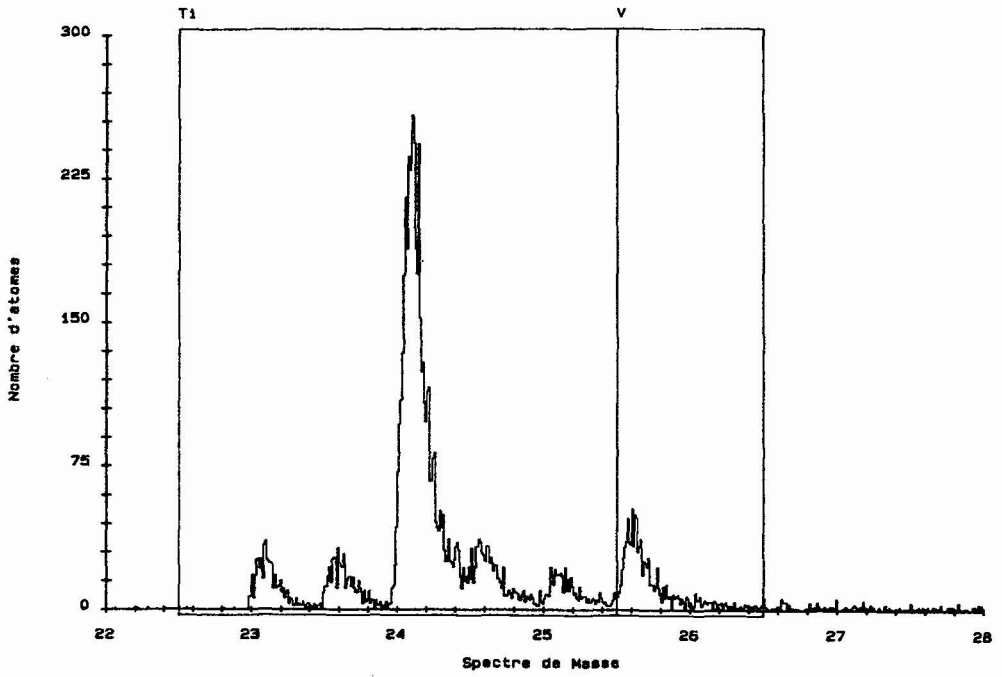


Fig 1 : Example of mass spectrum with specie designation

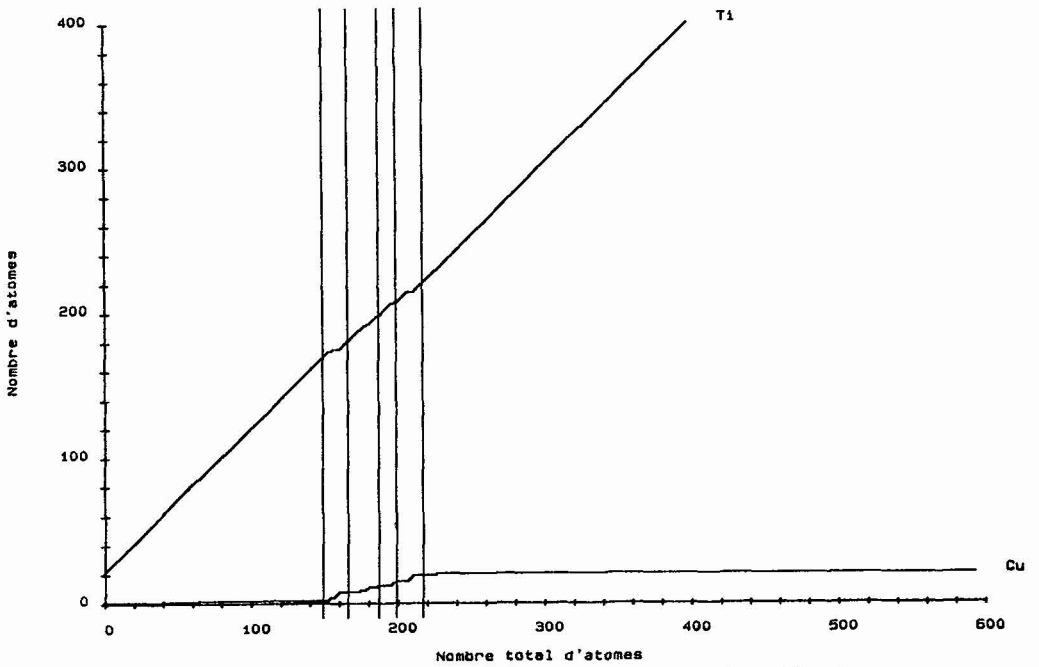


Fig 2 : Example of cumulative plot combining the layer marking as deduced from the flux curve