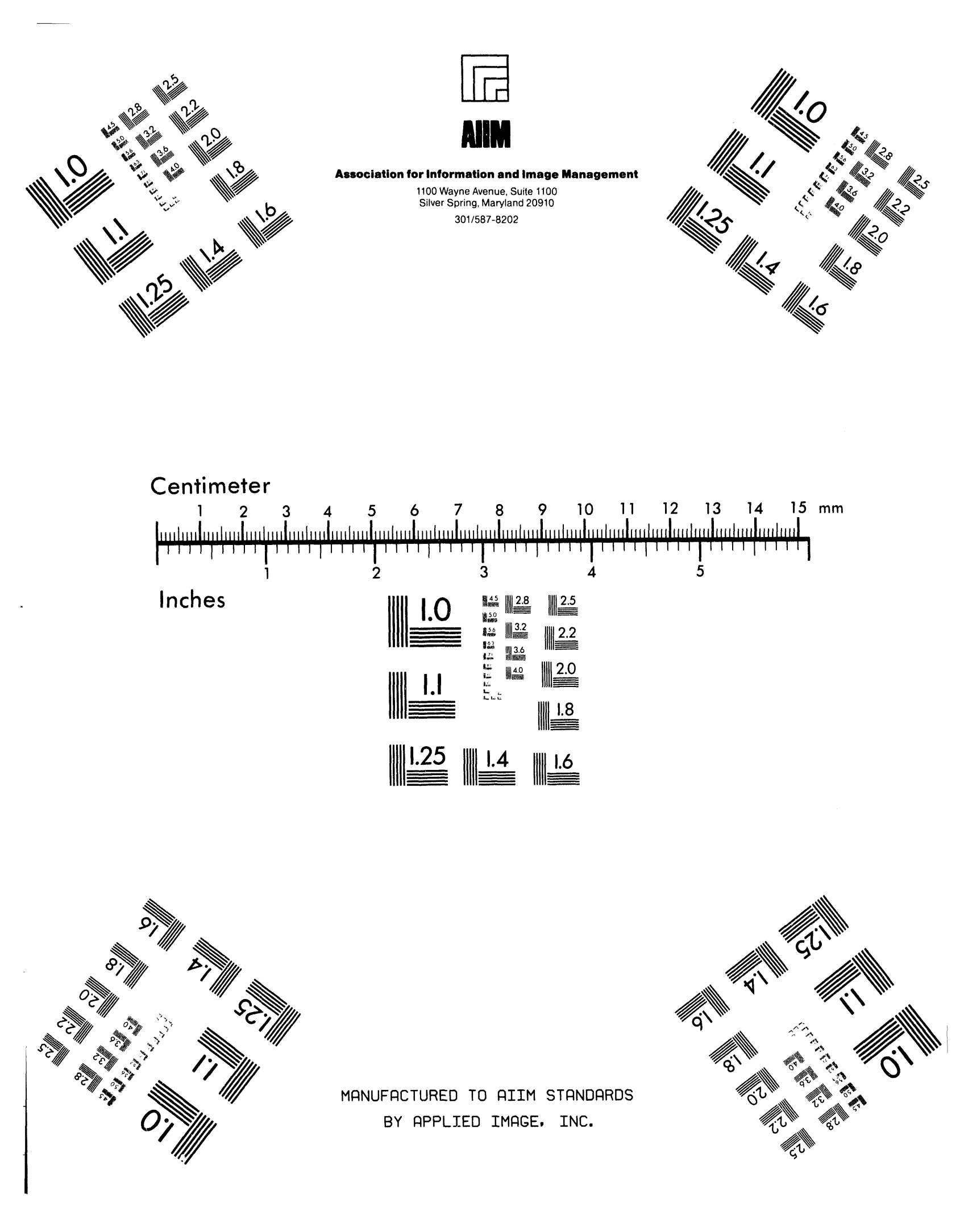
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XAMath: An XAFS Analysis Package Based on Mathematica®

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XAMath is a graphics-based interactive package written with the Mathematica® system for the analysis of XAFS data. Mathematica® offers the advantage of use on several computer platforms, including Unix, IBM Windows, and Macintosh, without any modification of the program. The portability and flexibility of this software has some cost in speed of execution.

Keywords: XAFS, data analysis, software, Mathematica®

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Numerous programs exist for the analysis of X-ray absorption spectra. Although some progress has been made in having these programs function on several computer platforms, including the adaptation of the University of Washington programs for use on Macintosh, IBM PC, Unix, and VMS systems, true portability has been an elusive commodity. The major problem has been that XAFS analysis requires interactive graphics, the development of which is often highly system dependent.

During the past two years we have created a new program based on Mathematica® [1-2], XAMath, for the reduction and fitting of XAFS data. XAMath provides the same basic functionality as other XAFS programs, including background subtraction, Fourier transforms, and fitting to reference compounds or theoretical models. In addition, the use of Mathematica® offers a route to portability which minimizes the programming effort. This approach does not eliminate the inherent problems in creating portable software. But these problems are subsumed within Mathematica®, rather than becoming the responsibility of the individual programmer. And since Mathematica's primary function is

that of a mathematical and graphics library, many basic functions, such as fourier transforms, are built in, thus simplifying the creation of new programs.

The XAMath code functions without modification on the many platforms for which Mathematica® is supported. Figure 1 shows the actual screen displays, for a single XAFS transmission spectrum of copper foil, from three different computer systems: a Macintosh, an IBM clone running Windows, and a Unix system with an XWindows environment. The XAMath codes running on each system are identical, although the original data file was translated to the proper format for each system. Functionality across platforms is the same, despite the minor differences in the display from each computer system.

Flexibility and portability in programs result in some cost in efficiency [3]. On a Macintosh, XAMath requires a minimum of 12 MB of memory. Execution is also not extremely rapid. The slowest calculation, the determination of the background spline in EXAFS, takes 65 seconds on a Macintosh Quadra 700. However, Mathematica® also supports communication via the MathLink® [4] protocol

with external programs. Sending the same calculation to an external C program and receiving the result requires less than 2 seconds. Mathematica® provides a fairly convenient process for the creation of such programs, although they must be compiled on each specific machine.

XAMath maintains a trace file in which each of the parameters used to analyze the current data set is listed. It currently supports data formats from several beamlines at NSLS and both the MIDAS and XASCollect formats of SSRL. The addition of other formats is straightforward. We have also provided an interface to FEFF3 [5] for the calculation of theoretical scattering amplitudes and phases.

Mathematica® is effectively an interpreted language. This fact facilitates alternative manipulations of XAFS data that are not specifically programmed in XAMath. This feature also simplifies the creation of new modules in the program.

XAMath provides flexibility and cross-platform compatibility for XAFS analyses at some cost in speed. In applications for which the former capabilities are important, it is a viable alternative to other XAFS programs.

Acknowledgments

We would like to thank Farrel Lytle for helpful suggestions during the development of this software. This work was supported by the Office of Chemical Sciences, Basic Energy Sciences, U. S. Department of Energy under contract W-31-109-ENG-38.

References

[1] S. Wolfram, Mathematica®: A System for Doing Mathematics by Computer, 2nd Edition (Addison-Wesley, Redwood City, CA, 1991).

[2] Mathematica is a registered trademark, and MathLink is a trademark of Wolfram Research, Inc.

[3] J. A. McCall, "Quality Factors" in Encyclopedia of Software Engineering, Vol. 2, J. J. Marciniak, ed. (John Wiley and Sons, New York, 1994), p. 958.

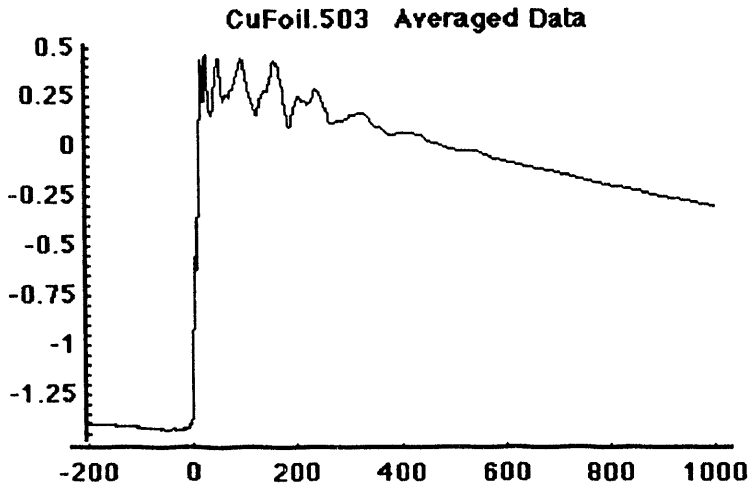
[4] MathLink® Reference Guide, (Wolfram Research, Champaign, IL, 1993)

[5] J. J. Rehr et al., J. Am. Chem. Soc., 113 (1991) 5135.

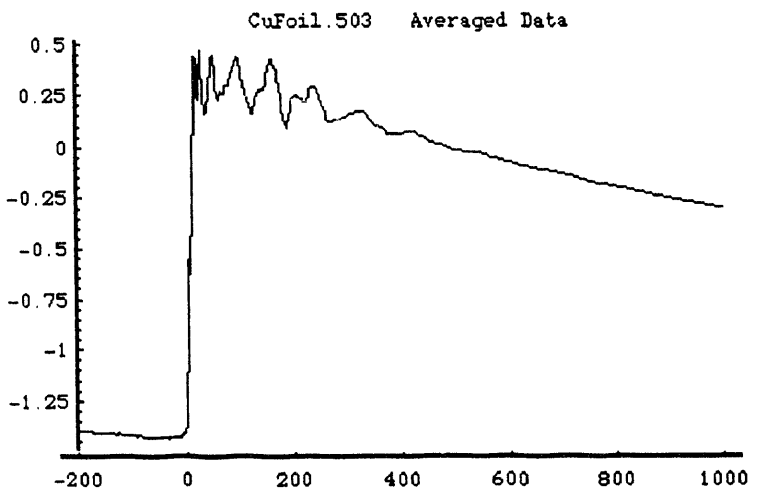
Figure Caption

Fig. 1. XAMath displays on three computer systems of the transmission XAFS spectrum of copper foil: Macintosh, IBM PC/ Windows, and Unix/XWindows. These displays are identical, except for minor differences in the screen font.

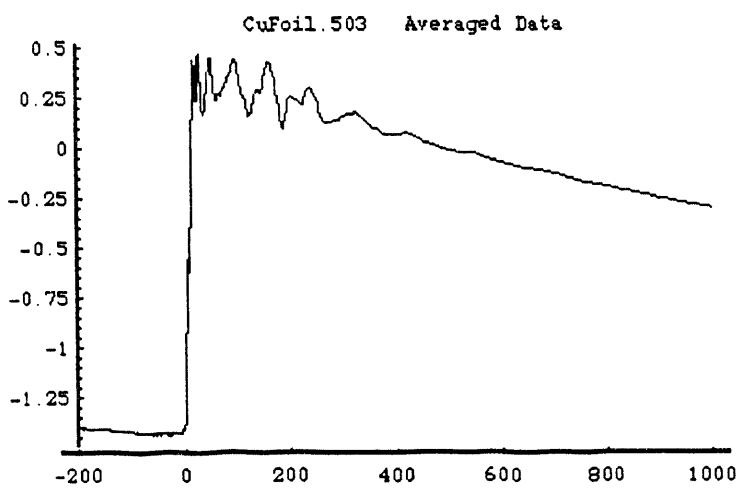
Macintosh



Unix / XWindows



IBM PC / Windows



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