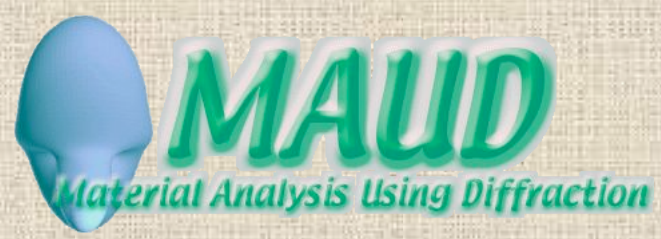

Maud: a Rietveld analysis program designed for the internet and experiment integration

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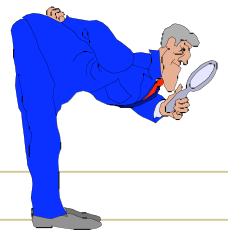
The problem



- *Carl is a PhD student in Material Science*
- *He is developing a new SiC/Si3N4 composite*
- *He want to know the SiC structure and quantity obtained*
- *He ask to Lawrence (a Crystallographer) for help*
- *Lawrence realize that is not an unknown structure and suggest Carl to do it himself just using the XRD instrument and a Rietveld program.*
- *Carl has three months to do it and he lost:*
  - *Two weeks repeating the experiment*
  - *Two months to realize how to manage the analysis*

Project Goals

- *Ultimate goal of project*
  - *Provide an analysis tool to help material researchers (non-crystallographer) in characterizing their samples*
  - *Integrating different measurements and analysis in a unique expert system*
- *Relationship to other projects*
  - *ESQUI (EU project for Diffraction-Reflectivity)*
  - *Hippo (the new Beam Line at Los Alamos)*

Description - 1

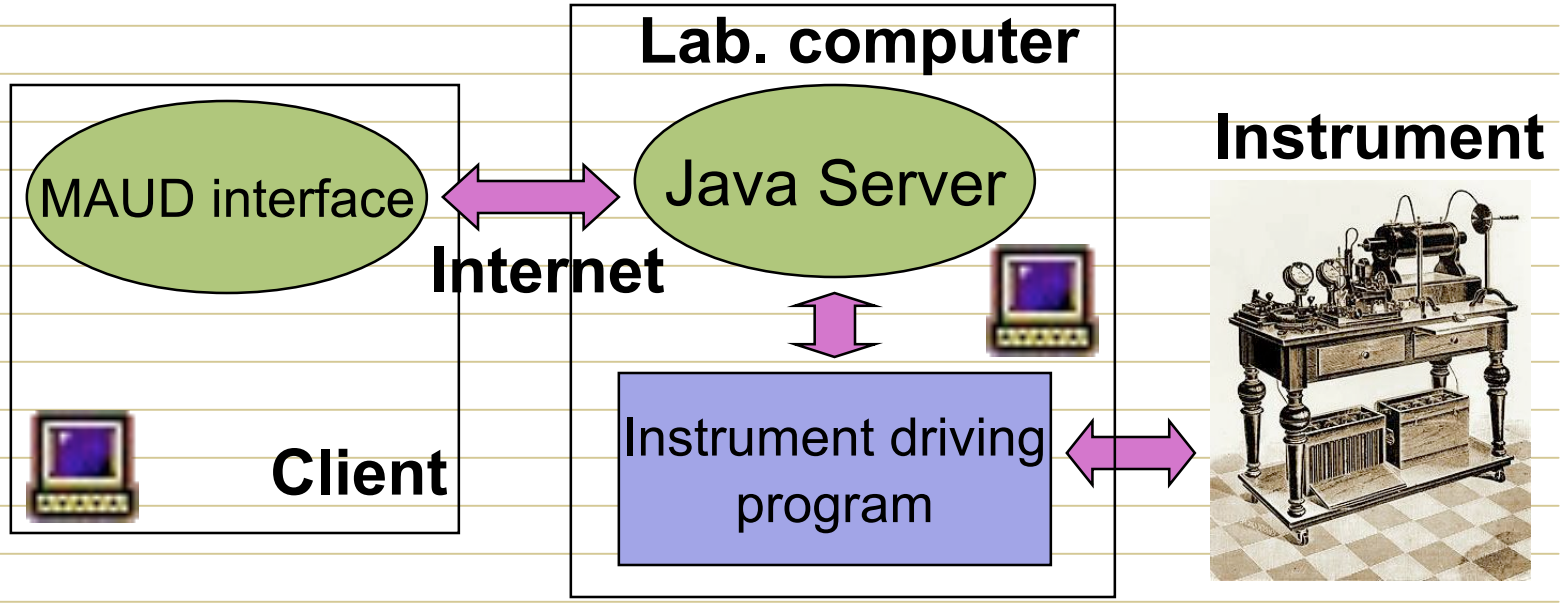
- *Multipurpose Rietveld analysis program for Material Science including:*
  - *Crystallography*
  - *Quantitative analysis*
  - *Texture, Residual Stresses*
  - *Reflectivity, Layered systems*
  - *Microstructure*
  - *……..*
- *Easy to use interface including:*
  - *Wizard for automatic analyses*

Description - 2

- *Connection to databases and use of the CIF syntax*
- *Ability to suggest measurements and to drive them locally or remotely*
- *Possibility to run:*
  - *Embedded in a browser over the internet*
  - *Locally as an application*
  - *On every platform*
- *Plug-in structure to extend easily some features*

Description - 3

- *Written in Java (OOP)*



FOR MORE INFO...

Http://www.ing.unitn.it/~luttero/maud

Methodology

- *Methodology included in Rietveld refinement*
  - *Texture: harmonic, WIMV, Entropy*
  - *Residual Stresses: Reuss-Voigt, SODF*
  - *Microstructure: anisotropic size-strain (Popa), Planar defects (Warren)*
  - *Reflectivity: Matrix method*
  - *……*
- *Standards being adopted*
  - *CIF file format (work saving, output, databases..)*

Competitive Analysis - 1

- *Advantages*
  - *Using texture for structural refinement/crystal structure determination*
  - *Global analysis in one step, automatic analyses*
  - *Correcting quantitative analysis for texture*
  - *Residual stress analysis on textured samples*
  - *Amorphous analysis (quantitative, structural)*
  - *Possibility to run on a web browser*
  - *Same program for all platforms*
  - *Plug-in structure (OOP)*

Competitive Analysis - 2

- *Weaknesses*
  - *Need a special instruments for texture-stress (Eulerian cradle + PSD detector or TOF)*
  - *Instrumental broadening should be determined*
  - *……..*

Peculiarities

- *Based on Java, full OOP Rietveld program*
- *Use directly physical quantities for fitting:*
  - *Crystallite size, microstrain, planar defect densities for peak shape*
  - *ODF for texture, Residual Stresses for peak shift*
  - *Phase quantities instead of scale factors*
- *Internet ready*

FOR MORE INFO...

Microstructure: Lutterotti, Scardi, J. Appl. Cryst. 1990.
Lutterotti, Gialanella, Acta Mat. 1998.

Texture-Stress: Ferrari, Lutterotti, J. Appl. Phys. 1994.

Maud Applet/Application

- *It run unchanged as:*
  - *An application locally*
  - *Embedded in a html page over the internet (java applet)*
- *Applet advantages:*
  - *Facilities maintain only one installation (on the web)*
  - *Users have already the last version*
  - *Run in the client (no server overloading)*
  - *Can be used out of the office/lab/facility*

Applet downside

- *Security is good (browser dependent) but if the user need to open/save files on his client:*
  - *The applet must be "signed" by a certificate*
  - *Mac OS system may release a less secure certificate but usable (at the user risk and only by other Macs)*
  - *For other systems the certificate should be obtained by a certification entity ($$$); only one in reality by the developer (?!?)*
- *Solution: buy a Mac*

Distributed/parallel programming

- *Java threading model (parallel tasks in computation)*
- *Each thread may run on:*
  - *Same machine, same processor*
  - *Same machine, different processors*
  - *Different machines, different processors (require internet connection and JPVM)*
- *JPVM (Java PVM)*
  - *Provide the infrastructure for distribute programming/processing*
  - *The computer network could be heterogeneous*

JPVM distribute system

- *Based on messaging*
- *Advantages*
  - *Speed up computation*
  - *No special computer requirements*
  - *No limits on the participating computers*
- *Weaknesses*
  - *Critical to balance computation/messaging time*
    - *Requires few long running separated threads to minimize messaging*

Current Status - 1

- *Algorithms*
  - *Completed: Rietveld, quantitative analysis, texture, microstructure, amorphous*
  - *On track (testing): reflectivity, residual stress (SODF), layered system, wizard analyses*
  - *Behind schedule: texture-structure solution, user manual*
- *Platform/Network/Internet*
  - *Completed: Multi-platform*

Current Status - 2

- *Network/Internet*
  - *On track: JPVM distributed processing, Maud-Applet (completed for Mac)*
  - *To do: Server side computation*
- *Expert system (instrument connection)*
  - *On track: Client-Server structure, experiment definitions, instrument interface exchange protocol*
  - *To do: multi-user security, instrument side interface implementation*

To finish….

- *future plan*
  - *Release first non-beta version (with manual and on-line Applet for all platforms)*
  - *Test the expert system with the under-construction ESQUI instrument (Hippo at Los Alamos delayed)*
- *People contributing*
  - *H.-R. Wenk, S. Matthies, L. Cont, A. Gibaud…..*
- *submit questions and addresses*
  - *Maud: maud@ing.unitn.it*
  - *Http://www.ing.unitn.it/~luttero/maud*