Integrated Approach to Software Environment for Nanotechnology.

Bykov V.A., Saunin S.A., Volkov A.D., Efimov A.E., Komkov V.N.

Introduction

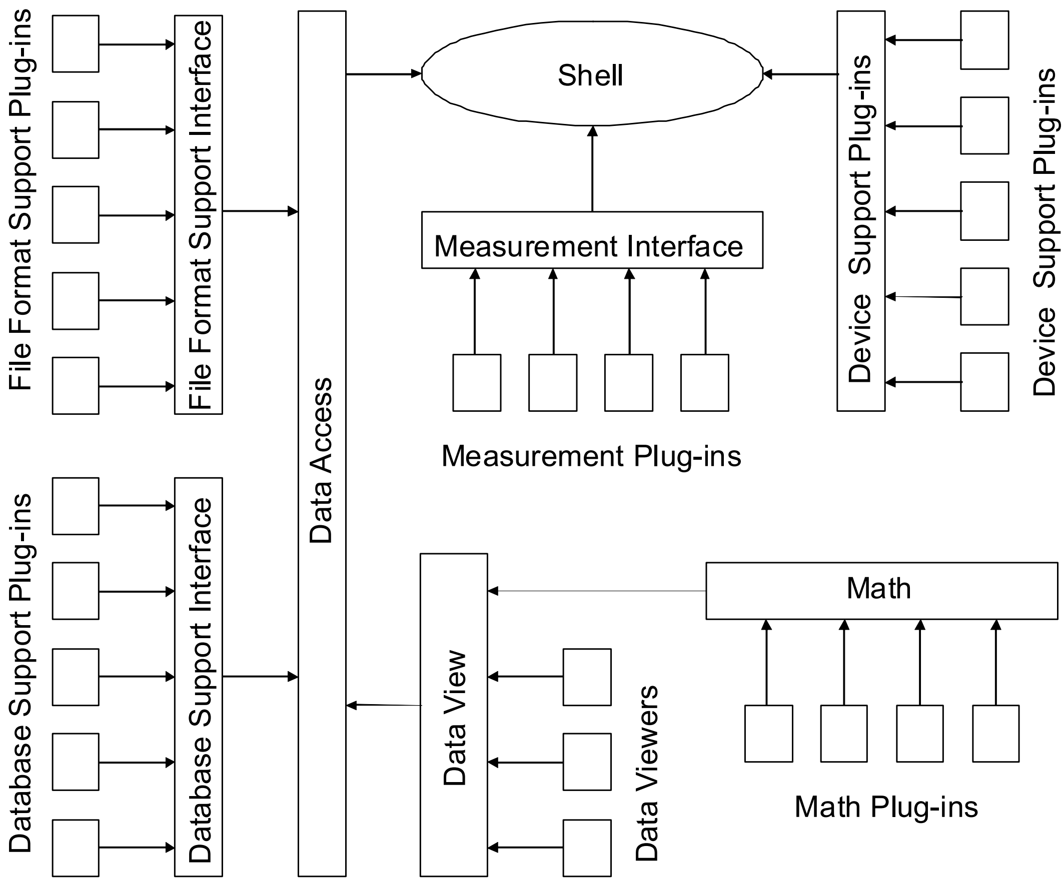
In the nearest future nanotechnology software will consist of the following parts:

1. Measurement/synthesis control workstation software.
2. Data, knowledge and computation Internet resources.

We consider transparent seamless integration of these components to be the most effective solution, combining their advantages without any loss of efficiency.

Integrated RAD technology for workstation side applications

Every modern device needs software to control it and/or acquire measured data. Up to date software needs connection to specialized knowledgebases, databases, expert systems and specialized data analysis algorithm packages. No single foundation except scientific community itself can provide all these specialized software packages or even gain the knowledge, required to build them. All these tasks require open modular software structure and extensible platform for development of local software for workstatons, controlling



nanotechnology arrangements to enable distributed software development.

This platform should also provide standard set of GUI components to force different software producers to build standard looking, seamlessly integrated GUI.

Specialized automation packages for high throughput measurements.

For next few decades one of the most perspective trends in modern science will be the high throughput measurements. The idea is to perform synthesis and successive measurements as fast as possible, trying different combinations in order to find the best one. High throughput systems require specialized automated interfaces. They should replace the qualified specialist control by automatic or at least simplified procedures because a human being, even most qualified, can't operate systems with the speed, required by high throughput measurements.

Automatical search of markers on sample substrate, connecting coordinate systems of synthesizing, modifying and measurement arrangements requires implementation of machine vision algorithms. It is possible also to connect information on sample origin and sample itself, introducing bar codes on the substrate. Bar code recognition algorithms allow to connect measurement data and sample origin data automatically. Other algorithms allow to find the same place on the sample at every stage of technological process and automatically record influence on the sample.

In collaboration with Pensa State University (Prof. Fedotov N.G., PhD. Shulga L.A.) was developed the demo-system for DNA autorecognition. It segmentates image and finds DNA parameters with required stability. Now we plan to develop analogous systems for viruses and bacteria disease diagnostics.

Large number of experiments in high throughput measurements needs a lot of samples to be prepared. If sample material is expensive enough, micrometer scale sample synthesis, SPM measurements and bulk material properties reconstruction may become a reasonable substitution for common methods in material research.

Expert systems

Another idea we should take into consideration is to make these systems interact with user through domain of his natural notions and help him even in his own field.

This requires introduction of automatic methods and expert systems.
Expert system asks user to input only information, needed to specify the task in native terms and notions of user's field. All other information should be measured or calculated by expert system itself. At the same time user still can take control over every stage of measurement process.

One of this systems is developed at the moment for basic SPM measurement techniques. On the first stage user selects sample type and measurands he wants to define. Then system identifies optimal probe type and recommends it to user. User selects recommended probe or any other on his own choice and resets set of techniques applied if needed. Then system measures probe properties, perform landing, calculates optimal parameters of measurement and starts measurements, automatically tuning parameters to achieve better quality of the scan. After appropriate processing, removing measurement artifacts and recalculating to physical measurands required, data is presented to user in the publication ready form.

Global Internet Resources.

Today SPM has become an instrument of practically every field of applied science but the price of SPM is too high for labs that do not need daily measurements. One of the possible solutions is Internet lab with access to SPM measurements from anywhere. Studying SPM methodology by specialists from other fields is still a problem, too. Internet lab and online SPM simulators can help to learn SPM before one pays for it.

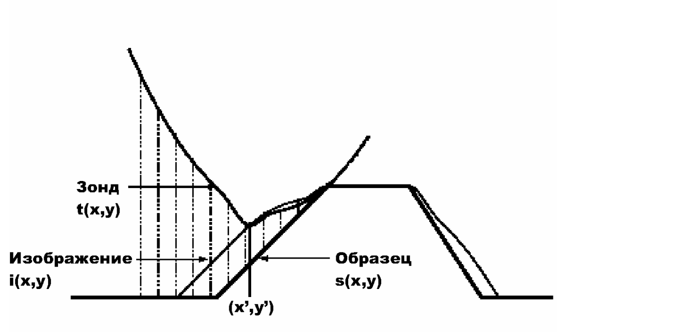
Supercomputer power and sophisticated scientific software make possible molecular dynamics and quantum mechanics calculations, modeling of processes in nanostructures and large expandable knowledgebases with real time search capability.

Workstations controlling measurement system connect to supercomputer services through Internet. Due to availability of thorough calculation instruments one can make a model of the object to measure before measurement itself. Thus he can calculate optimal measurements parameters and predict the result expected before he makes his first try. This will cause significant acceleration of methodology development.

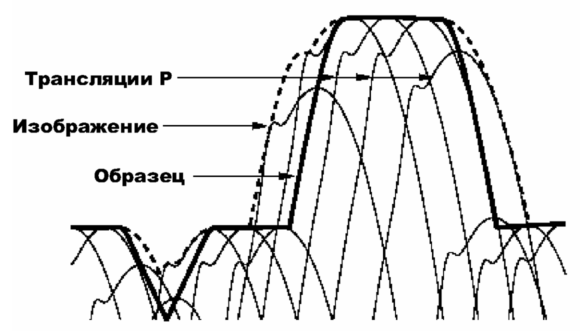
Specialized integrated database, containing results of ready SPM measurements, SEM images etc. from scientific community can serve the same goal. It should store images from different labs all over the world together with parameters of their measurement and methodology descriptions.

Local databases can be used by technologists in the lab for micro and nanomachining process development. This requires measured data to be associated with technological process description (parameters and stage of the process). Such technological high throughput system was developed for polymer synthesis labs. It imports the sample matrix synthesis information from the file of the polymer synthesis control software, automatically measures all samples in the matrix and puts measurement data into database together with synthesis parameters, automatically performs data processing algorithms set and use calculated sample properties to build parameter dependence diagrams between parameters of synthesis and sample properties.

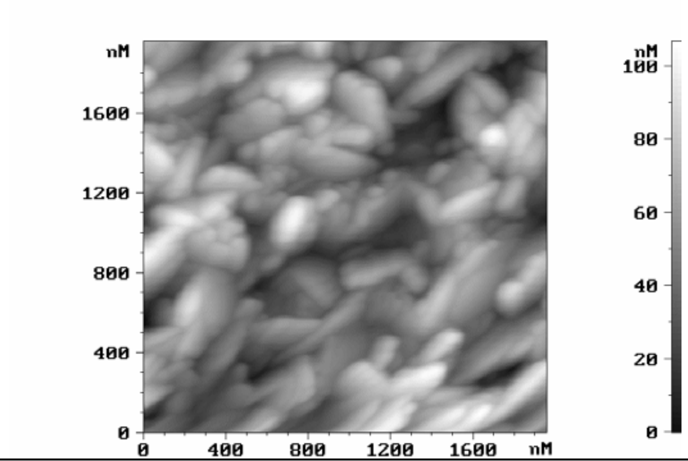
Program “DECONVO” uses morphological algorithm of blind deconvolution of probe shape to minimize systematic errors, connected with probe artifacts and calculate correct lateral sizes of measured objects.



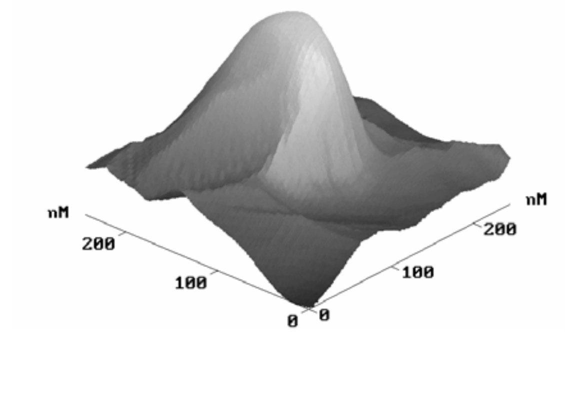
Morphological model of SPM measurement



Dilation formed image



SPM Image of Ti crystal film.



Reconstructed probe shape.

On the base of already developed and developing deconvolution algorithms for SPM, optical high aperture and apertureless probes will be created a system to solve inverse problem of sample restoration and discrimination of artifacts by probe and other parts of measurement system. These tasks are resource consuming ones and calculation on PC based workstations can take more than ten minutes for SPM images of standard size. In this situation it’s much faster to transfer the image to the supercomputer by Internet during few

seconds. Calculation and back transfer will take few seconds more. Simple deconvolution tasks paralleling makes effective the use of supercomputer. Acceleration is proportional to processor speed and total number of processors. In future number of points per scan will greatly increase and the time consumed will increase in the order of four. That's why the use of supercomputer may become the only reasonable solution.
Stable Internet connection with appropriate automatization will make this operations intrinsic and perform them for every scan not disturbing the user. This makes possible check for defective or broken probes and supply a "photo" of the probe used for every scan.

Conclusion

Effective nanotechnology development will require specialized global information environment. Searching for information is much more effective than obtaining it every time experimentally. When performing a research, it's always useful to look at results measured before. Researcher needs to think only on the problem he is working with, all other tasks should be held automatically. And of cause all this possibilities should be available directly from the workplace of a researcher – his workstation software.

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