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LECLAIR, S.  
JACKSON, A.

AUGUST 1995

FINAL REPORT FOR 10/23/94-11/09/94

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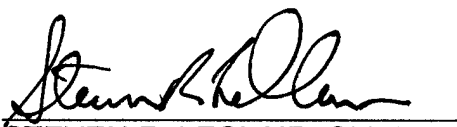
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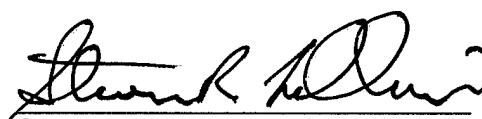
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Materials Process Design  
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## Executive Summary

The following is an in-depth report of a very successful Window-On-Europe (WOE) visit to three European countries. Before describing our visits and discussions with various materials and cybernetics scientists, we believe it is important to establish the significance of such international visits, because in times of 'military' downsizing such programs are particularly susceptible to indiscriminate budget cutting efforts.

Prior to this WOE experience, we might have been somewhat indifferent to the reduction or elimination of such programs- but no longer. It was an unexpected realization to discover that upon encountering our hosts we became diplomats of US Government interest's in the international scientific community. Also unexpected was a consciousness that if we are to sustain our stature as a 'super-power', we have a responsibility to sustain our international scientific awareness, to leverage collaborative efforts, and to stay abreast of competing research programs.

Foremost among our visits were those in the former Soviet Union. Soviet scientists have been exploring a number of uncharted areas of science and engineering, and now, for the first time in decades, we have an opportunity to 'mine' their successes and learn from their failures. Hopefully, we will not waste this opportunity. Should the openness currently exhibited by the Former Soviet Union (FSU) republics endure, it is clear that the relationships we are building can only benefit our longer term defense interests (in knowing more about the work of others - particularly potential aggressors). Direct face-to-face discussions are ultimately the best means for a genuine exchange of ideas regarding science and technology. In particular, we have learned that such opportunities are critical in overcoming the miscommunication due to language and translations.

The 'bottom-line' is that we - the Air Force Laboratories need to be heard from if we are to retain these programs. We are the customers of those who administer the 'Window-On-Europe, Asia, etc.' programs, and it is incumbent on us to communicate our support for the continuation of the program and the need for the personnel who administer it. Management needs to document their support of these programs as an essential and productive element of our in-house research program in support of Air Force missions.

# Introduction

This report will cover a three week Window-On-Europe visit to the following locations:

**23-29 Oct 94** - A.A. Baikov Institute of Metallurgy of the Russian Academy of Science, Moscow, Russia;

**30 Oct-3 Nov 94** - Institute for Applied Informatics, of the Ukrainian Academy of Science, Kiev, Ukraine;

**7 Nov 94** - Engineering Design Center, Cambridge University, Cambridge, England; and

**9 Nov 94** - Artificial Intelligence Department, University of Edinburgh, Edinburgh, Scotland.

The report will address each of the four (4) site visits and will consist of the following sections for each site:

- 1) a brief overview of the author's perception of research in material/process discovery methods,
- 2) a description of each site visited,
- 3) facilities and assistance,
- 4) research objectives and approach,
- 5) progress,
- 6) continuing activities,
- 7) potential for further collaboration.

The visits involved sites whose current research involved either empirical methods for the design of materials and resultant products, and/or the development of empirical methods of potential benefit in automating empirical research of materials and/or processing.

Subsequent to the above identified discussions regarding each site, general observations encompassing all sites are reported as follows: Travel/relocation experiences, Comments, Acknowledgments.

## A.A. Baikov Institute

### 1) Brief overview of the authors' perception of research in material/process discovery methods at the Baikov Institute for Metallurgy

Dr. Nadya Kiselyova and two researchers (Natalia Kravchenko and Vitalii Petukhov) are engaged in research on prediction, optimization and visualization of material properties as related to fundamentals of the elements and compositions of the compounds. Under the direction of Dr. Kiselyova, Vitalii, who is a mathematician, has developed a software system for prediction of material properties using a pattern recognition program, referred to as CONFOR, originated by Dr. Victor Gladun, of the Institute for Applied Informatics in Kiev, Ukraine.

The CONFOR program was demonstrated for a simple set of data. CONFOR uses the Gladun algorithm to generate a pyramidal net from a trial set of experimental data and is capable of predicting and graphically displaying the properties of compounds. Of particular interest is the property prediction of those compounds outside of the training set. Vitalii pointed out (several times) that this approach is very good for relatively small sets of data (20-50 objects), but that it also is very good for large data sets once the net has been created.

The CONFOR program is written in C, but since it originated with Gladun, any use of it should be discussed with him directly, according to Kiselyova and Vitalii. Clearly, their use of the CONFOR program is a valuable application of computers to direct the design of materials. During discussions about the Gladun algorithm and a demonstration of our implementation of it in Logistica, the issue of discretizing or binning of data surfaced repeatedly as a problem to be addressed.

A set of data on semi-conducting compounds was presented and the binning for it was questioned. This led to a discussion of how best to approach binning in order to obtain useful information from the data. Vitalii suggested training on a set of data and then removing objects one-at-a-time from the data set. Comparison of pyramidal nets is then done and the output from the net for unknowns is generated in each case. If the results do not differ then the binning choices are acceptable. If the results do change, then the binning choices were not acceptable. The above is similar to a suggestion made by Prof. W. Ziarko (University of Regina, Canada) during a recent visit to the Materials Directorate. Although intuitively appealing, this approach is 'NP complete' and our trial experiments yielded no clear direction (i.e., smaller or larger bins) much less the optimal bin size. The interpretations of the results varied considerably depending on the starting number of bins used, and there is no identifiable way to decide which beginning set of bins is appropriate. Vitalii and Dr. Kiselyova mentioned that Gladun has reported on this issue.

To complement the pattern recognition capability of CONFOR, Natalia and Vitalii have created a program called LAGRANGE for visualization and optimization of property data based on available experimental data. The approach utilizes the crystal symmetry properties, specifically a subset of the thirty two (32) point groups (23, 3m, -3, etc.) of the seven (7) crystal systems (cubic, hexagonal, trigonal, tetragonal, orthorhombic, monoclinic, and triclinic) and their associated matrix representations of the tensor quantities representing properties of materials (e.g., thermal, electric, elastic, thermo-elastic, piezo-electric, piezo-thermo, etc.) that have particular point groups in their crystal structure.

The LAGRANGE program was demonstrated with elastic constants (i.e., elements of the compliance tensor) for the cubic system with an interactive graphics capability for fitting experimental data (e.g., frequency doubling vs. crystal orientation in  $ZnGeP_2$ ). Plots of summed frequency or wavelength Vs phase angle were shown, as generated from the table of experimental data.

**Note:** The LAGRANGE program is of considerable interest because of its potential for applications involving the design of crystal orientations for all types of *thin-films and coatings*.

## 2) A Description of the A.A. Baikov Institute

A five story complex built in the early 1950s, which prior to 1994 housed over 1200 researchers, today has approximately 700, and noteworthy is the ratio of women to men, approximately 4:1. Vitalii (the only male researcher in Dr. Kiselyova's group) stated that male researchers have moved on to business-type positions, where there is more potential for higher-income. The research budget has been reduced to 1/3 of that provided under the former Soviet Union and it is obvious the Institute complex suffers as a consequence - in terms of appearance and maintenance neglect. Because of budget crisis and the abysmal researcher salary of approximately \$35/month, research direction at the A.A. Baikov Institute is guided more by outside research funding than by research management.

The material property data available to the Institute is a combination of resident Baikov Institute data together with data/knowledge provided by over 20 other laboratory groups all coordinated (distributed and serviced) by the Ministry of Science of Russia, Republican Research Scientific - Consulting Center for Expertise (RRSCCE) led by Director Vladimir L. Belousov, & Dep. Director Prof. Juri J. Degtyarev and Moscow University.

The RRSCCE is attempting to organize Russian research resources and apply them to private sector needs, somewhat analogous to the current 'dual-use' initiative within the DoD. The RRSCCE currently has government sponsorship but has been told that their survival will depend on revenues that they generate. There is an opportunity to collaborate with this organization since they are struggling to find customers, which we are potentially one, but more important is the opportunity to market their data through use.

**Note:** A science 'information highway' is slowly but surely under development in Russia, and the RRSCCE 'Materials (structure, properties and processing) Data' network is clearly illustrative of how to use the highway to bridge academic and industrial interests.

## 3) Facilities and Assistance

No specific facilities, except for the use of email, has been required or utilized. Our hosts have been very hospitable and are eager to assist us in any way they can.

## 4) Research Objectives and Approach

The Department we visited within the A.A. Baikov Institute was the Laboratory of Materials Sciences of Semiconductors (LMSS) which has several research groups addressing crystal growth of Si, SiC, BiSb, InSb, etc. to achieve both reduced impurities (space processing) and more cost-effective processing, and the thermo-electric phenomena associated with compounds such as  $\text{Bi}_x\text{Te}_y$ ,  $\text{Ge}_x\text{Te}_y$ ,  $\text{AgAlTe}_2$ , etc. for thermoelectric cooling devices (reference Bi & Sb chalcogenides brochure). It should be noted that the work on protective coatings and crystal growth of SiC (reference brochures) has been shelved for lack of funding.

Dr. Shelimova presented results of her group's research on thermoelectric phenomena in bismuth telluride's. Ternary compounds of  $\text{GeBi}_2\text{Te}_4$  with slight variations in stoichiometry of the Ge yield significant changes in crystal structure and related electrical properties. Thermal conductivity, for example, decreases by 50% with a change in Ge content of less than 5%. Bismuth and antimony chalcogenides can be produced with 30mm diameter and about 150mm in length. Thermoelectric cooling power ranges from 0.1 W to 14 W, for cooling surfaces of 2x4 to 10x12 mm. An interesting result is that by addition of Ag compounds the transition temperature is lowered by several hundred degrees C in the Bi-Te-Ge system. Work on the pseudo binary phase diagram by this group was important in assessing this Ag compound effect. These results are not yet published, and we were shown plots of the results (in Russian). Evaluation of these data remains to be accomplished, but on the surface they are very

interesting and represent the high level of research effort conducted at the Baikov by this group. Also, the Kristallit Co., Moscow, is prepared to sell devices utilizing micro coolers made from the Bi-Te based materials. A sample can be obtained by sending a request to Kristallit Co., 49 Leninsky Prospekt, Moscow, 117334, Russia. The Director is Dr. T. E. Svechnikova.

$\beta$ -SiC is also being studied and single crystals have been prepared by Si-organic compound dissociation at 1800°K and characterized, according to a brochure we received, as follows: band gap: 2.39 eV, carrier concentration  $5 \times 10^{15} \text{ cm}^{-3}$ , mobility  $1000 \text{ cm}^2/\text{V}\cdot\text{s}$ , n-type,  $4 \times 5 \times 2 \text{ mm}$ , yellow color, and  $5 \times 10^{-5}$  to  $10^{-6} \text{ wt}\%$  impurities.

**Note:** It is our belief that the above described work involving the Bi-Te-Ge system is unique and warrants further investigation to determine the potential of exploiting these materials for thermal-electric energy conversion for air and space applications as well as thermal charging systems for ground support equipment.

The only group in the LMSS which is not conducting experimental research is the group led by Dr. Kiselyova. Her research objective is to conduct theoretical design of inorganic compounds for new electro-optical, ferro-electric, superconducting and semiconducting materials, and her approach is to use empirical methods involving both computation and pattern-directed search of materials property databases. It should be noted that Dr. Kiselyova's group appears to be the best funded (nearly 100% externally funding) in the LMSS with a budget just over \$100,000. Her external funding is generally provided through a Russian enterprise to sell information over an analog to the internet. The principal buyers are Russian and German companies.

## 5) Progress

After six days of interaction, we have acquired an improved perspective of the research objectives, approaches and customer needs which are guiding both experimental and empirical research at the Baikov Institute. It is expected that future progress will be pursued via the internet and meetings at international conferences.

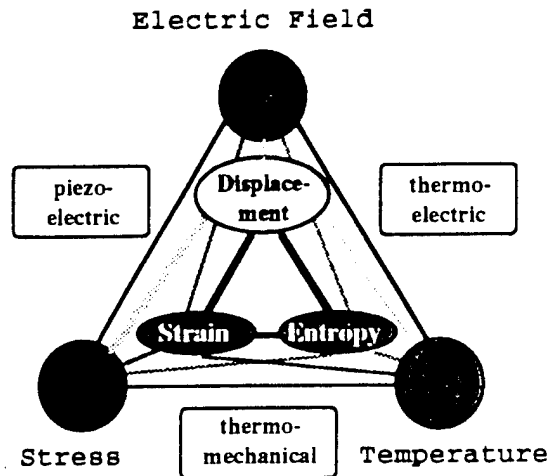
## 6) Continuing Activities

A proposal by Dr. Kiselyova has been submitted, reviewed and funded by the European Office of Air Force Office of Scientific Research (EOARD). The goal of the research is to develop a new approach to *a priori* prediction of inorganic compounds which could be usable for search of new electro-optical, ferro-electric, superconducting or semi-conducting materials with pre-defined properties.

As stated in Dr. Kiselyova's proposal, there are three ways of predicting properties of materials, 1) quantum mechanical calculations, 2) two-dimensional criteria (classification rules) by various semi-empirical approaches, and 3) methods of computer learning (cybernetic prediction). She is an advocate of the computer learning approach and uses the Gladun Algorithm (to be discussed below) to generate a nested set of patterns which characterize a selected class of materials (e.g., binary compounds with distinct birefringence properties). If a new binary is suspected to also have birefringence properties, it is compared with the nested set of patterns to determine if the new binary compound fits the class and if we can predict any of its unknown properties.

It is apparent that the Gladun Algorithm is, indeed, useful in both characterizing (for recognition purposes) and predicting material properties. But of interest is how to use this capability in a materials design environment. For example, with the Gladun Algorithm, a designer may be able to explore many unknowns relative to a new material, process, shape

design or compare various alternatives. But, it is the view of the authors that the information regarding materials must be organized as in the Nye Diagram (reference Figure 1), and then tightly coupled, via empirical (Gladun's Algorithm, Neural Nets, etc.) and/or analytic computation, to available information on shape and process.



**Figure 1. Design (Materials, Product & Process) via the Nye Diagram**

Future work involving collaborative activities will need to explore the development of a materials-process-shape *design environment* which has embedded in it fundamental (phenomena-based) knowledge of materials. Such a system will target thin-film design (such as the examples highlighted below), but of curious application is the design of bulk material applications, such as the LCB example discussed below. As we address the design of thin-film material applications from a more fundamental level (crystal structure, composition and time-temperature perspective), might we also learn how to use this more fundamental information in the design of bulk material applications. The basic construct for integrating materials knowledge in such a design environment is the Nye diagram which classifies and relates physical phenomena and associated physical properties of materials. These interrelationships serve as a foundation for the geometric (to include shape and gradient composition) and process design of various products.

- \* Electron Beam Spray Casting of Dense *Metallic and Ceramic Coatings*
- \* Accelerated and Ecologically Friendly Method for the Production of Wear Resistant *Iron Boride Coatings on Steels*
- \* *Superheated Steam Treatment* for the Enhancement of Tribological Properties of Ferrous and non-Ferrous Alloys
- \* *Multilayer Coatings* for Improved Tribological Performance
- \* *Functionally Graded Interfaces* for Improving the Performance of Hard Coatings on Austenitic Stainless Steel and Titanium Alloys
- \* *Surface Treatments* for Improving Performance of Diamond Like Coatings on Tool Steels
- \* *Diffusion Barriers/Nucleation Surfaces* for Chemical Vapor Deposition (CVD) of Diamond on Tool Steel Surfaces

-\* High Energy Electron Beam Treatment for the Enhancement of Tribological Properties of Tool Steels, Cemented Carbides, and Nitride Coated Tool Steels

- Beta Phase Processing of Low Cost Beta (LCB) Titanium alloy

\* Materials Processing at Technical Institutions in Ekaterinburg & Chelyanbinsk Russian Workshop, Oct 27, 1994, sponsored by National Center for Manufacturing Sciences.

Low cost processing of bulk LCB Titanium is dependent upon the control of crystal structure (Titanium is an allotropic metal), prior to forming, by heat treatment through beta transus as specified by the level of alloying constituents, i.e., % weight by volume of various alloying elements. The connection to the Nye diagram is as follows (reference Figure 2): The heat treatment is associated with the temperature corner (lower right). Application of heat induces entropy effects which drive diffusion processes. Thermal expansion induces strain and associated stresses which cause the material to change volume and helps drive the phase change from the two phase, alpha plus beta, to a single phase beta. By holding the Titanium alloy at this elevated temperature, a beta equilibrium phase is established. Quenching induces stresses because of the negative coefficient of expansion (contraction). These stresses provide the necessary energy to stabilize the high temperature beta phase at a temperature below which it normally occurs.

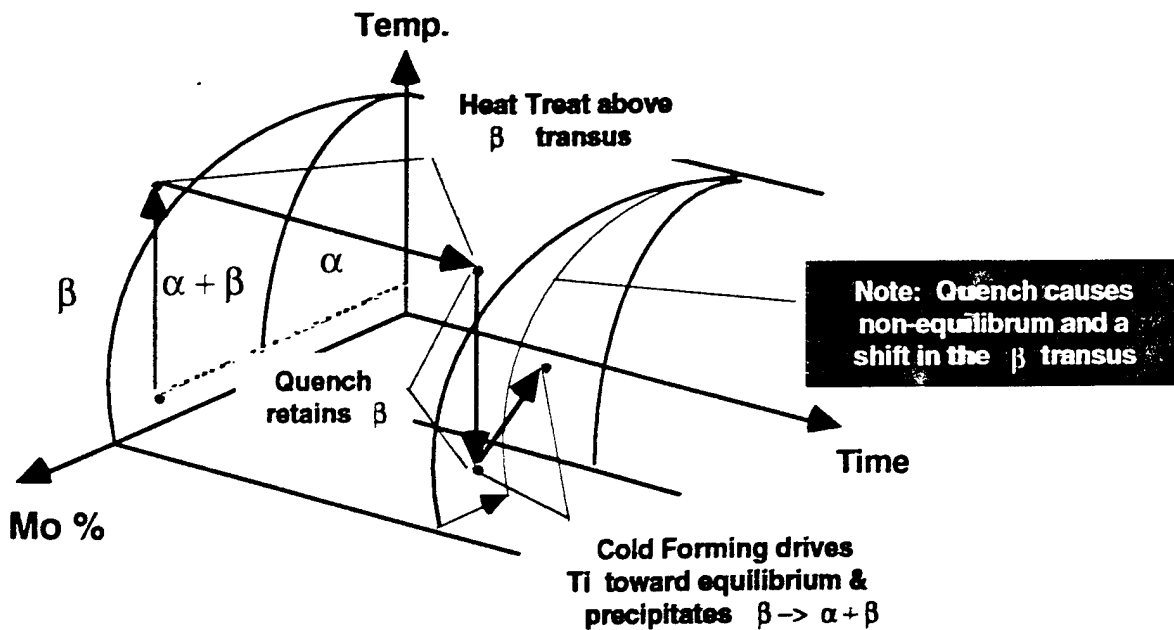


Figure 2. Time Sequenced Phase Diagram of Titanium (alloyed with Molybdenum)

This low temperature beta phase is of interest because the body-centered cubic structure of the beta phase has many more slip systems which make it much easier to deform (e.g. a stress at ambient temperature of 100 tons/in<sup>2</sup> Vs over 170 tons/in<sup>2</sup>). Hence, when cold forming is applied, the slip systems available become operative via the stress corner (lower left) of the Nye diagram. Thermal effects are induced because of the energy added via the application of stress which raises the temperature of the material. As deformation proceeds,

stored energy is released from the phase change in addition to the energy introduced because of the shape change. The net effect is to retain the new shape, but at a cost of changes in microstructure and precipitation of alpha phase via diffusion, which are aspects associated with the temperature and stress corners of the diagram.

Describing the heat-treat, quench and cold forming process from such a fundamental 'crystal-system-viewpoint' needs to be further refined to clarify the physical interactions occurring. The research question is whether an automated and/or intelligent means can be found which uses the Nye diagram to uncover the processing 'trick' explained above for minimizing the processing costs associated with cold forming a material such as bulk titanium.

#### **7) Potential for Further Collaboration**

The potential for further collaboration is tremendous. We are being exposed to a novel, radically different, approach to materials design. Further collaboration with the Baikov Institute is expected as we become better organized to exchange ideas and identify potential opportunities for cooperation regarding research objectives. Some of the future dates and opportunities to explore collaboration are as follows:

**September 1995** SAMPE Japan - Session on Innovative Materials Design

**May 1996** AFOSR Initiative Review - Presentation on Empirical Methods applied to Materials Design

**Now through 2000** Workshop and Conference Sessions focused on developing an *International* Information Highway of collaborators in pursuit of advancing knowledge and methods associated Integrated Materials-Process-Shape Design

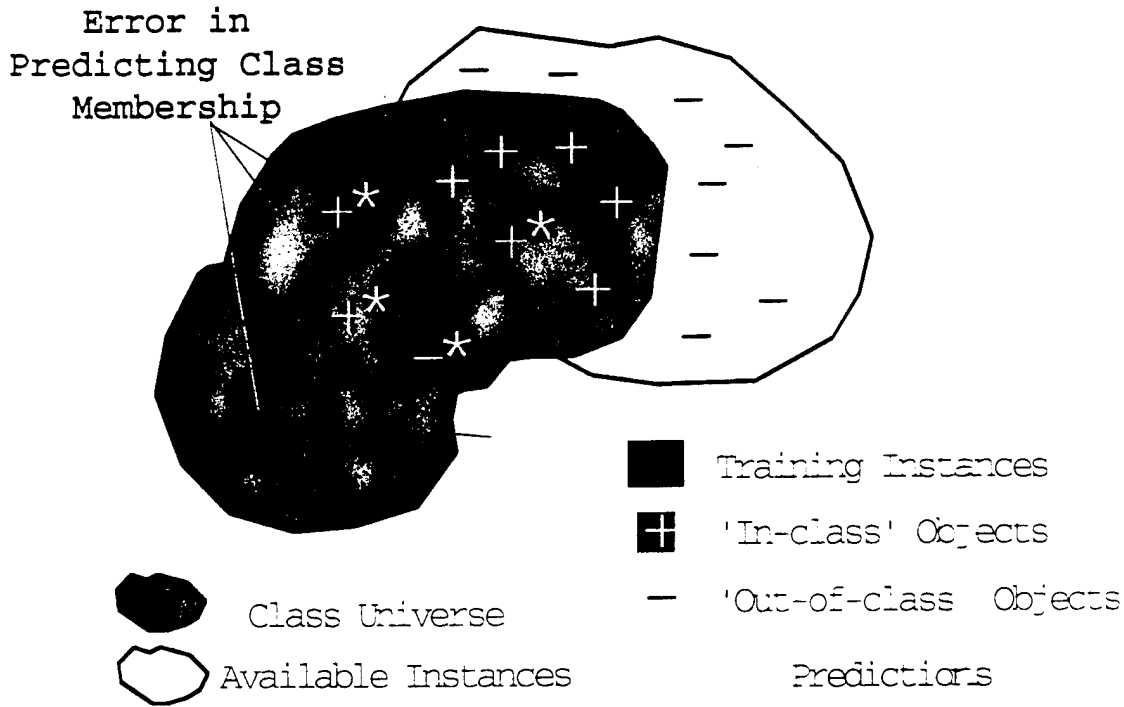
# Institute for Applied Informatics (Association of Developers & Users of Intelligent Systems)

## 1) Brief overview of the authors' perception of research in material/process discovery methods at the Institute for Applied Informatics

Dr. Victor P. Gladun & Dr. Nellia Vaschenko, of the Institute for Applied Informatics, are engaged in research of pattern recognition and concept generation methods. They have collaborated in the development of an acyclic-graph method referred to as the Gladun Algorithm, and have developed several software systems designed to organize empirical data into a hierarchical network referred to as a 'pyramidal-net'. One such software system, CONFOR (an acronym for 'concept formation'), is being applied to the area of Materials Design, by Dr. Nadya Kiselyova (discussed above), but more generally CONFOR is a tool for using empirical data to model a phenomenon. CONFOR has been applied to such real-world problems as control of Chemical Vapor Deposition of diamond films, prediction of solar flares relative to planned space flights, medical diagnosis, and recognition and prediction of geological formations.

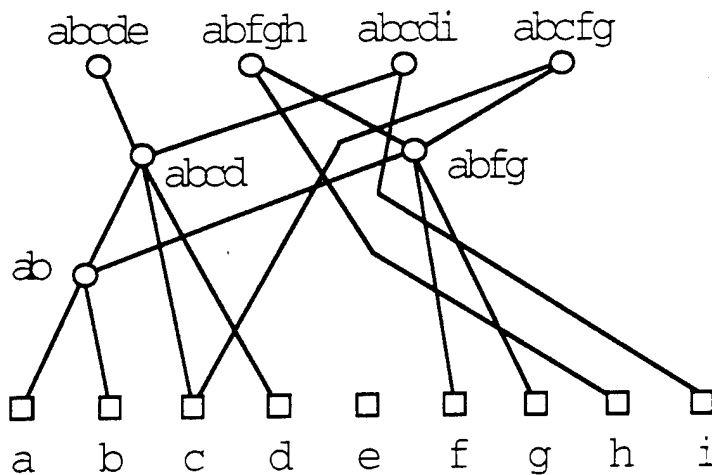
The Gladun Algorithm is a logic-based analog to an unsupervised Neural Net for modeling data (i.e., organizing data into classes or clusters). Both methods develop class membership empirically, but whereas a Neural Net uses 'Euclidean-distance' as a metric for membership, the Gladun Algorithm uses 'propositional-logic' (and, or, not) expressions. With either method, empirical data may be quantitative or qualitative and is usually coded. Typically, when using neural networks the coding is to normalize the data between 0 and 1, or to convert the data to a binary bit string. Contrary to neural networks, the Gladun Algorithm utilizes the existing data, whether they are numbers or symbols, as symbols.

As illustrated in Figure 3 below, the Gladun Algorithm is no less susceptible to error in predicting class membership than a neural net. If the set of objects used to train is not representative of the class, both methods fail to correctly establish class boundaries. Noteworthy in comparing the Gladun Algorithm with neural networks is the capability to self-organize the data set into classes. Both methods utilize a train-consult scenario to develop and then examine the ability of the network to correctly classify empirical data. But whereas a neural network uses no *a priori* knowledge of which class an object belongs, the Gladun Algorithm requires the user to establish whether an object is a member of a class prior to the training step. This *a priori* class assignment is an inherent weakness in the Gladun Algorithm because the user may not be capable of predetermining class membership if the object data set exceeds five (5) to seven (7) attributes.



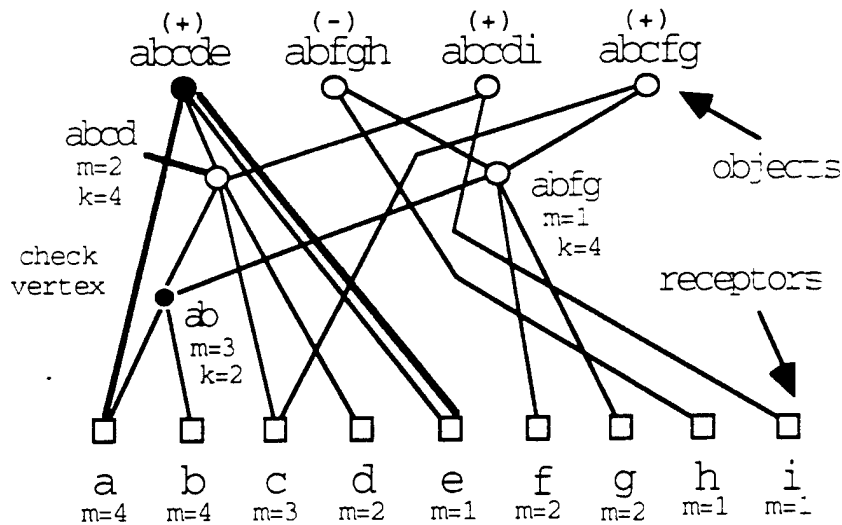
**Figure 3. Generating Class Membership Boundaries**

Although the predetermination of class membership is a weakness of the Gladun Algorithm for large data sets, this same characteristic is the basis for constructing concepts within a pyramidal-net. Concepts are established for purposes of prediction to determine if some new object is a member of a particular class, i.e. concepts are logical expressions (and, or & not) of attributes which establish the boundaries of a class. For example, consider the simple problem of four (4) objects: object 1 -> abcde, object 2 -> abfgh, object 3 -> abcdi, and object 4 -> abcfg. These objects constitute the 'training instances' referred to in Figure 3. At this point, we need not concern ourselves with objects we believe form a class, we merely must be able to form a pyramidal-net using the Gladun Algorithm. Without going through the details of exercising the Gladun Algorithm, the resulting pyramidal-net is illustrated in Figure 4.



**Figure 4. Pyramidal-Net of Example Problem**

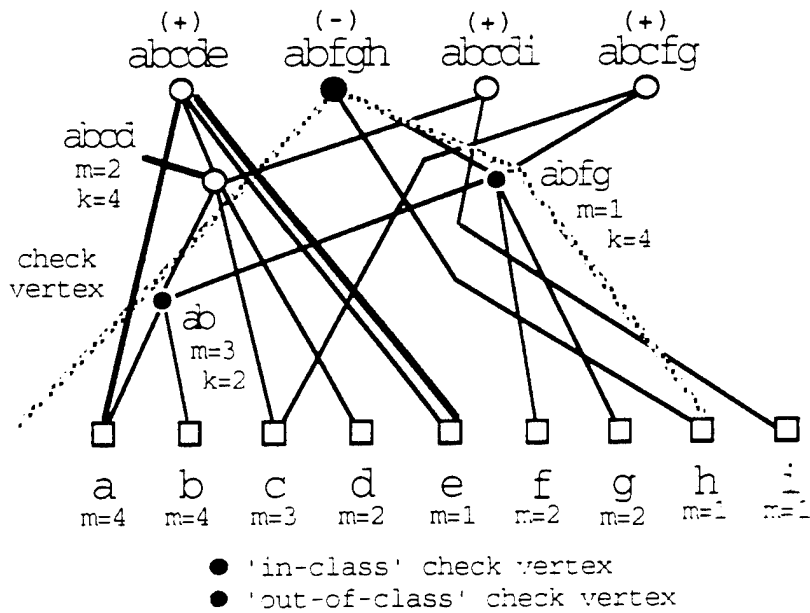
Let us assume that objects 1, 3, and 4 are predetermined to be an 'in-class' object (reference Figure 3), so designated as (+), and object 2 is predetermined to be an 'out-of-class' object, designated as (-). With these assumptions we are now ready to pursue what Dr. Gladun refers to as 'concept formation' which is depicted in Figure 5. Concept formation is necessary to establish 'in-class' boundaries to enable prediction of new objects. Next we must compute two values, 'm' and 'k'. The parameter 'm' is the number of positive objects (for positive check vertices) represented by (connected to) the node. The parameter 'k' is the number of attributes (receptors) in the conjunction formed by a node. Once we have computed 'm' and 'k', we need to consider their ratio 'm/k' to determine what Dr. Gladun refers to as 'check-vertices' for the concept for the particular class we have postulated.



**Figure 5. Pyramidal Net Concept Formation**

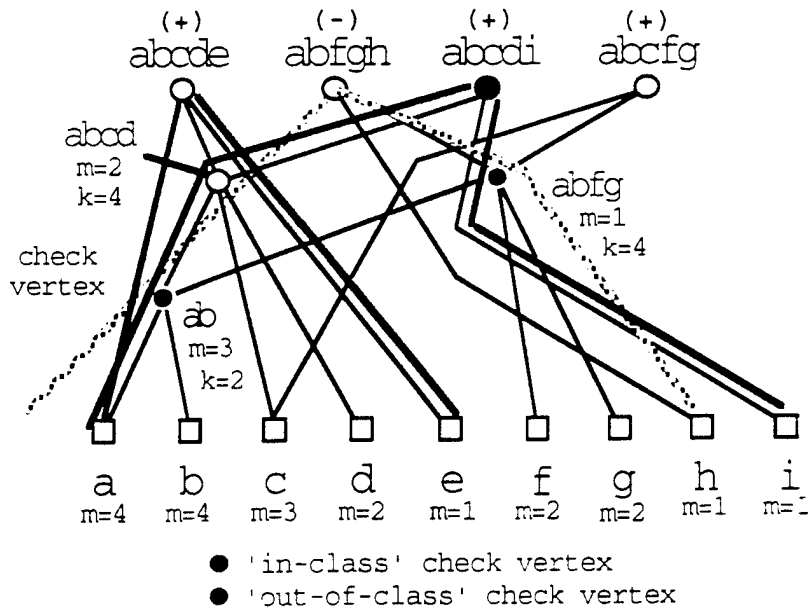
Beginning with object 1 -> abcde (with all nodes encompassed with dotted lines), we find the highest ratio of 'm/k' is node 'ab'. Note in the case of a tie for the highest ratio, an arbitrary selection is made between them. As a result node 'ab' is designated a 'check vertex' to denote that it is an element of the concept of the class. This designation may be temporary as we examine the remaining objects in Figure 6.

Next we consider object 2 -> abfgh which is an 'out-of-class' object. As with the previous 'in-class' object we must establish a 'check vertex' to further delineate the boundary between 'in-class' and 'out-of-class' objects. Note that the best ratio of 'm/k' is again 'ab'. When a 'check vertex' is shared by both an 'in-class' and 'out-of-class' object, we must find a new 'check vertex' for the 'out-of-class' object. The new 'check vertex' for the 'out-of-class' object is arrived at by following node connections to the next higher nodes but still within the scope of object 2. For each next higher node we must again select the highest 'm/k' ratio.



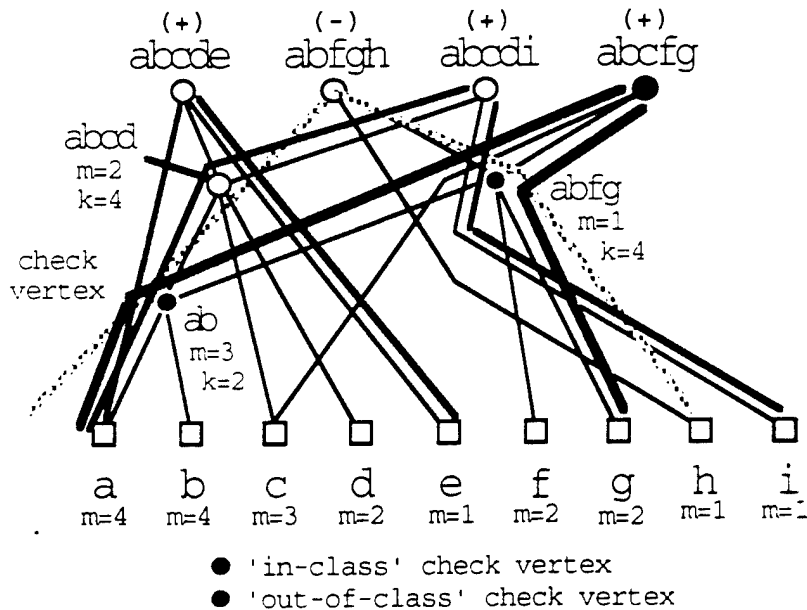
**Figure 6. Continued Concept Formation - 'Out-of-class' Object**

Subsequently, the next 'training instance' object (a new 'in-class' object) is introduced (reference Figure 7), and again the 'in-class' 'check vertex' must be examined to determine if it is suitable for all 'in-class' objects or a new 'in-class' check vertex must be found. It is clear that check vertex 'ab' remains the best selection for both 'in-class' objects, and thus no further evaluation is necessary.



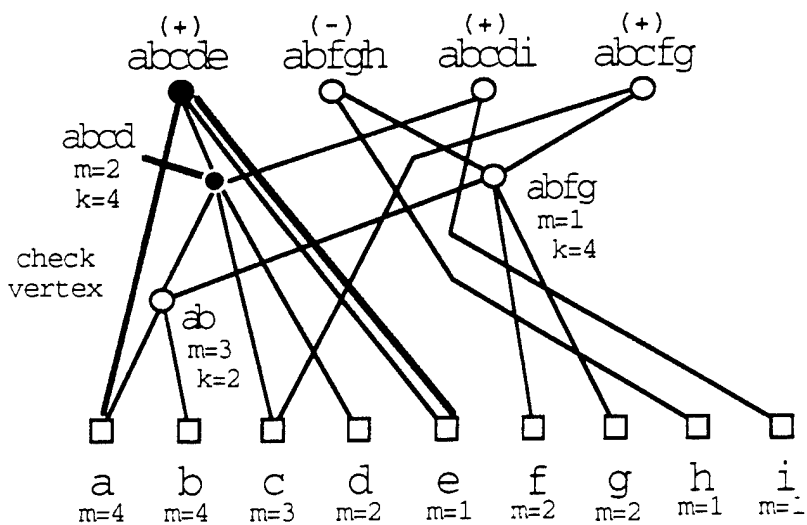
**Figure 7. Continued Concept Formation - New 'In-class' Object**

Finally, object 4 -> abcfg is examined as an 'in-class' object (reference Figure 8). This object has two (2) check vertices - 'ab' and 'abfg'. and in this case 'abfg' is a superset of 'ab'. Although this situation is similar to the introduction of object 2 -> abfgh, this case differs in that the highest level check vertex is for an 'out-of-class' object. Therefore, a new 'in-class' check vertex must be found for the object. This requires going back to the beginning object and selecting an alternative check vertex and iterate on the above steps to determine if a check vertex for object 4 can be found which distinguishes it from 'out-of-class' objects.



**Figure 8. Continued Concept Formation - Final 'In-class' Object**

As a result of iterating on the above steps (beginning with object 1), an alternate check vertex is found to be vertex 'abcd' as is illustrated below in Figure 9.



**Figure 9. New 'In-class' Check Vertex**

Now in Figure 10, we again need to establish the 'out-of-class' check vertex. It appears the 'out-of-class' can be upgraded (i.e.. in terms of the best m/k ratio) to check vertex 'ab'.

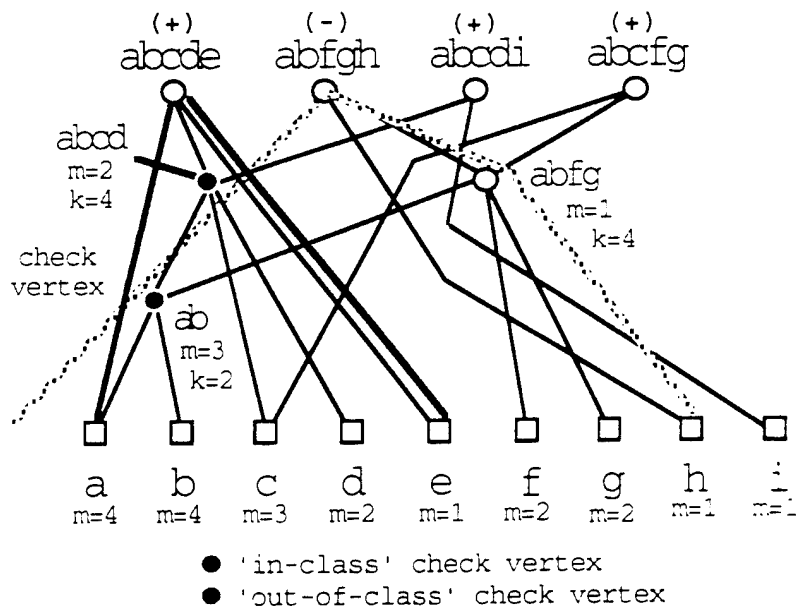


Figure 10. New Continued Concept Formation - 'Out-of-class' Object

As we continue, all appears well with object 3, in that the check vertex 'abcd' is well suited for both object 1 and 3 (reference Figure 11). Note that even though the check vertex 'ab' for the 'out-of-class' objects is within the scope of object 3, the 'in-class' check vertex is a superset of the 'out-of-class' check vertex. If the two were independent, then we would have to determine an alternate check vertex for object 3 because with independent 'in-class' and 'out-of-class' check vertices no class determination can be made.

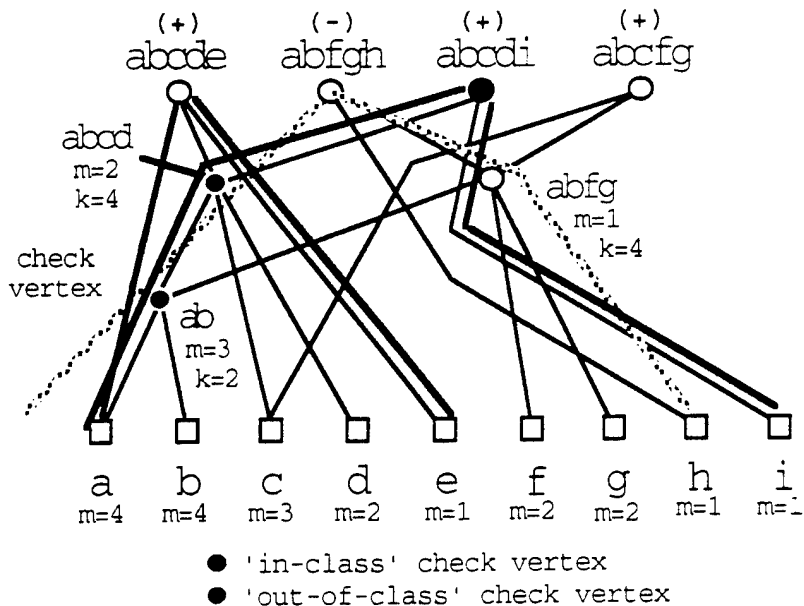
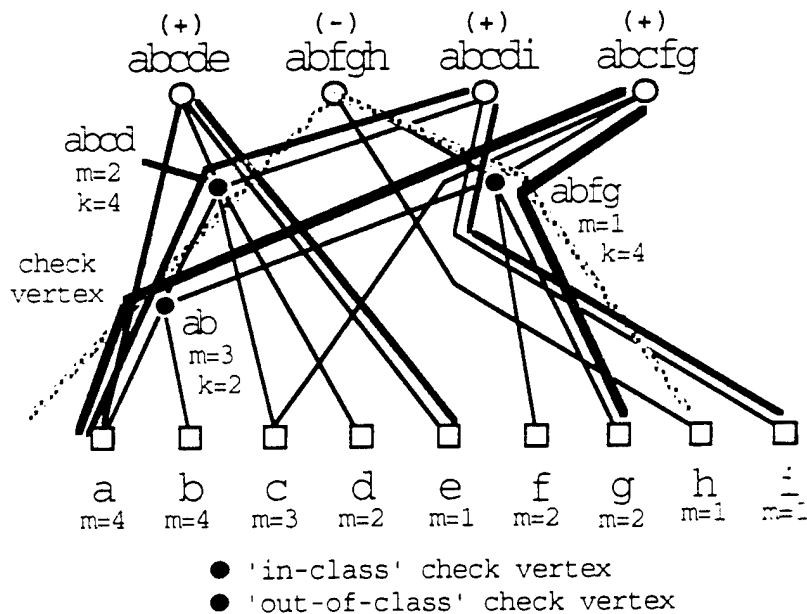


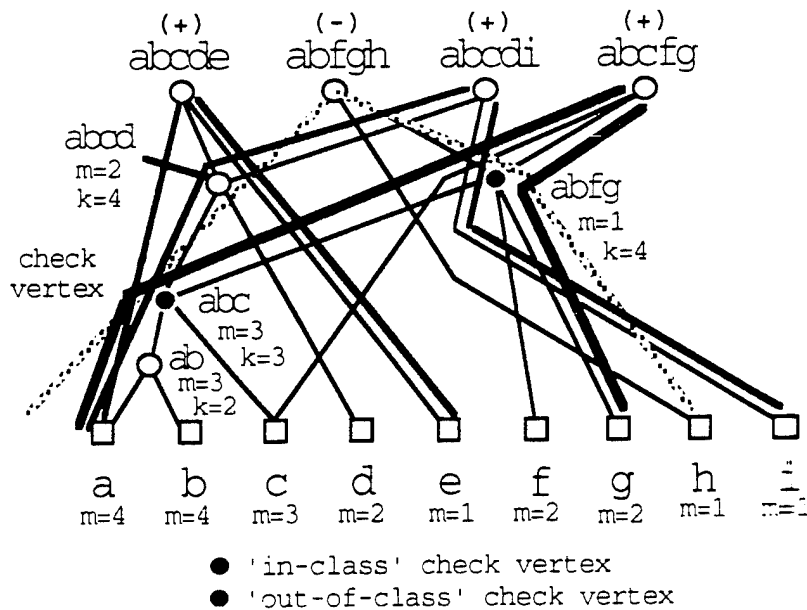
Figure 11. New Continued Concept Formation - New 'In-class' Object

It is clear that check vertex 'abcd' is not within the scope of object 4. Thus a new 'in-class' check vertex must be established and is illustrated in Figure 12 as check vertex 'abfg'. This finally resolves the concept formation task and the concept for the hypothetical class for objects 1, 3, and 4 can be expressed as: (**abcd** or **abfg**) and not(**ab**).



**Figure 12. New Continued Concept Formation - Final 'In-class' Object**

It should be noted that there is an alternative solution to this classification problem which is actually more succinct an expression of the hypothetical class for objects 1, 3, and 4. The alternate concept formation is illustrated in Figure 13 and left for the reader to verify. Note that for this alternative solution the hypothetical class model for objects 1, 3, and 4 is now expressed as: **abc** and not(**abfg**).



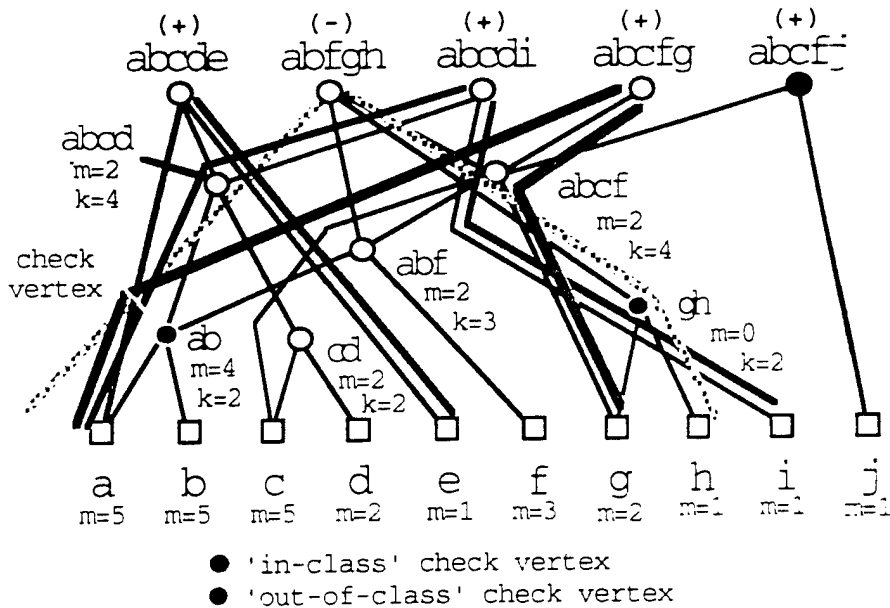
**Figure 13. Alternative Concept Formation**

Once the 'training-instances' have been exhausted, the result of the training (i.e., the logic expression) is available for consulting. What is evident from the above process involving the Gladun Algorithm is that unlike a neural net, we have a succinct expression or model of the class. And therein, the model defines very clearly the boundaries of the class. Furthermore, what is equally appealing about the resultant pyramidal-net, relative to neural nets is their adaptability, i.e., analogous to neural nets, any new training instance(s) can be added to the pyramidal-net to evolve the model.

Prediction is accomplished by comparing a new object to the logical expression to determine if it belongs to the class. For example from Figure 13, we have the following model:

**abc and not(abfg)**

If we have a new object (object->5 'abcfj'), using the expression we find that this new object is indeed a member of the above defined class, since 'abc' is contained in 'abcfj' and 'abfg' is not contained in 'abcfj'. This new object could also be added to the 'training-instances' to further define the boundaries of the class (reference Figure 14).



**Figure 14. Five (5) Object Concept Formation**

It appears that adding object 5 has a distinct effect on the concept which separates the 'in-class' and 'out-of-class' boundary. The new concept for these five objects is:

**ab and not(gh)**

**Note:** The significance of pyramidal nets (based upon the Gladun Algorithm) is as an alternative to neural nets for building a model based upon empirical data. The advantage of a pyramidal net over a neural net is that unlike a neural network, a pyramidal net not only predicts whether a new data instance is explained by the model, it also provides a 'logical' expression of the model.

## 2) A Description of Institute for Applied Informatics

A four story complex of three buildings in the center of old Kiev and of late 1940s to early 1950s construction. The Association of Developers and Users of Intelligent Systems (ADUIS) is affiliated with the Institute for Applied Informatics which was a division of the Institute of Cybernetics, Ukrainian Academy of Sciences. The Institute for Applied Informatics was comprised of 1500 personnel in the 1980s but with the breakup of the Soviet Union the staff was reduced to 600 personnel and more recently 200 personnel.

Of the remaining personnel in the Institute for Applied Informatics, a staff of approximately 100 is now led by Dr. Gladun, and of that staff, a group which appears to be no more than 20 people (mostly computer programmers and mathematicians with a mixture of professionals and students) are working on applications as part of the ADUIS. The Institute for Applied Informatics research budget has been effectively eliminated with the breakup of the USSR. Their funding for application development, which was largely working on specific problems from other countries (Bulgaria, Russia, Romania, etc.), has also been eliminated.

As with the Baikov Institute, it is obvious the Institute and, therein, the ADUIS complex suffers as a consequence of the breakup of the USSR - in terms of appearance and maintenance neglect. Researcher salaries appear worse in the Ukraine than in Russia, as we were told the salary is \$15/month. It is clear only the best personnel remain, but unlike the Baikov Institute, the ratio of men-to-women is not 1:4 but 4:1, i.e. for higher salary opportunities men appear to be staying in the Cybernetics research field, whereas they are leaving the Materials (Physics/Chemistry) research fields.

## 3) Facilities and Assistance

No specific facilities, except for the use of the phone, has been required or utilized. As with the hospitality we were shown in Russia, our Ukrainian hosts have been very hospitable and are eager to assist us in any way they can.

## 4) Research Objectives and Approach

The Group we visited within the Institute, and more specifically the ADUIS, is focused on empirical methods to solve various scientific and engineering problems. They have developed three software tools; 1) CODEX (A Complex of Tools for Decision Planning Systems Design), 2) MANAGER (Tools for Decision Support Systems Design), and 3) CONFOR (Tools for Regularities Revelation and Analysis).

CONFOR is of specific interest to our work in Materials Discovery, as it appears unique and complementary to the other approaches we have pursued. The basic functions of CONFOR are:

- > revealing regularities inherent in experimental data,
- > using the regularities for classification, diagnosis and prediction, and
- > display regularities in the form of both logical expressions (conjunctions, disjunctions and negations) and a hierarchical network (referred to as a Pyramidal Net).

The research objective of the ADUIS is to extend the theoretical framework of their tools, and to enhance the tools to satisfy end-user needs. Their approach to extending these tools is to apply them to various problems and to learn of potential enhancements which might improve both the capability to recognize regularities and therein classifications of objects.

## 5) Progress

After four days of interaction, we have acquired an improved perspective of the research objectives, approaches and customer needs which are guiding both experimental and empirical research at the ADUIS. We have also addressed potential areas of collaboration.

## 6) Continuing Activities

As a result of discussions with Dr. Gladun and his associate, Dr. Vaschenko, concerning the detailed application and structure of the Gladun algorithm and corresponding pyramidal networks, a proposal is being prepared by Dr. Gladun to test extensions of the Gladun Algorithm using example materials design problems. Of immediate interest to us is the study of 'diamond-like' crystal structures as a class of semiconductor materials with considerable interest to the Air Force (i.e., relative to their non-linear optical properties). The compounds in this diamond-like semiconductor materials group are distinguished by the sites occupied by the elements of the compounds, and, in some cases, sites which are unoccupied. Parameters associated with these compounds are available, but some important electro-optic parameters related to nonlinear behavior have not been measured.

The proposed research objective is to apply an enhanced implementation of the Gladun Algorithm to material design questions involving diamond-like materials. Issues of pre-processing of data are also to be addressed, particularly the discretization or binning of data. Previous work has already established that the results of various discovery methods (neural networks, rough sets, etc.) are sensitive to binning. Automation of the binning process using a self-organizing, but adaptive, algorithm is highly desirable.

## 7) Potential for Further Collaboration

The potential for further collaboration is tremendous. We are being exposed to a novel, radically different, approach to problem classification involving both static, unordered data (e.g., materials data base of structure-property mappings) as well as dynamic, ordered data such as materials processing data (e.g., sensed parameters from daily process experiments). Further collaboration with the Institute and ADUIS is expected as we become better organized to exchange ideas and identify potential opportunities for cooperation regarding research objectives. Some of the future dates and opportunities to explore collaboration are as follows:

**September 1995** Window on Science Visit - Dr. Victor P. Gladun

**August 1996** Co-organize Materials and Cybernetics Workshop - ~~St.~~ Petersburg, Russia

**Now through 2000** Workshop and Conference Sessions focused on developing an *International Information Highway* of collaborators in pursuit of advancing knowledge and methods associated with Integrated Materials-Process-Shape Design.

# Engineering Design Center, Cambridge University

## 1) Brief overview of the authors' perception of research in material/process discovery methods at the Engineering Design Center

Cambridge University has a population of 15,000 students. Founded in the 1200's, Cambridge University has established its' preeminence in the sciences (particularly Physics and Chemistry). Ironically, the youngest discipline at Cambridge is engineering. Within the engineering discipline are many departments, one of which is Mechanical Engineering. The Engineering Design Center (EDC) we visited is under the purview of the Mechanical Engineering Department. The EDC is led by Prof. Ken Wallace and Prof. Mike Ashby.

The EDC is involved in many different aspects of engineering design including the 1) the organized interaction of disciplines (Configuration Optimization), 2) automated coupling of shape and function (Function Modeling), and most notably 3) the automated coupling of shape, function and materials (Material Selection).

It is the automated coupling of shape, function and materials which is of most interest. Although limited to bulk materials (not thin-films), the Cambridge Material Selector (CMS) is an impressive organization of property data (thermal, mechanical, electrical and even cost and production methods) on structural materials ranging from metals, ceramics, polymers, foams, composites and natural materials such as leather and wood.

**Note:** The property data reflects British material manufacturer information only.

## 2) A Description of Engineering Design Center

The EDC, established in 1991, is a research center for the development of fundamental engineering design methods for mechanical systems. The EDC comprises a team of 20 researchers, and is centrally located in the Department of Mechanical Engineering.

The overall objective of the center is to develop, validate and disseminate fundamental design methods for the design of mechanical systems. In particular: to create the theory and methods for a flexible design support environment, to provide an integrated computer system structure, to develop and test prototypes of an Integrated Design Framework (IDF) and framework support modules, and to demonstrate and test the methods on a variety of design applications in collaboration with industry.

## 3) Facilities and Assistance

No specific facilities, except for the use of the phone, has been required or utilized. As with the hospitality we were shown in Russia, and the Ukraine, our Cambridge hosts have been very hospitable and are eager to assist us in any way they can.

## 4) Research Objectives and Approach

The Cambridge EDC research program, funded by a major (1 million pound) grant from the Science and Engineering Research Council, involves the following modules:

- Specification Builder - the development of formalized methods of task clarification and conceptual evaluation,
- Functional Synthesizer - the development of methods for combining solution principles to fulfill desired functions,
- Embodiment Generator - the development of methods for determining suitable preliminary layouts for working principles,

- Configuration Optimizer - the development of methods for optimizing concept variants and embodiment layouts,
- Electronic Guidebook - the development of a structured engineering design guidelines database,
- Materials Selector - the development of a method for optimal materials selection in mechanical engineering design,
- Manufacturing Assistant - the development of methods for providing timely information to design engineers for economic and efficient manufacture.

Of specific interest and discussed further is the materials selector research. The research objective is focused on maximizing some aspect of function (performance), e.g., minimum price for a given strength, minimum mass for a particular stiffness, maximum safety or working temperature, etc.. Current research is addressing the automation of material selection based upon not only function but shape as well.

The underlying concept to this work is that the design of a structural component is specified by functional requirements, geometry, and material properties. The performance (p) of the component is described by an equation of the form

$$p = f(\text{Funct. Reqmts } F), (\text{Geo. Parameters } G), (\text{Mat'l. Properties } M)]$$

wherein F, G, and M are assumed to be separable and thus the optimal choice of material is independent of F and G. Prof. Ashby argues that experience has shown that F, G, and M are usually separable and thus design problems can be treated as belonging to a particular class which is characterized by one or more performance indices.

Prof. Ashby's approach to selecting materials is to characterize a design problem in terms of performance indices which effectively associate F and G to appropriate materials. The process of selection begins by identifying properties which are of interest, e.g., Young's modulus, density, yield strength, ultimate strength, and/or other similar macro-parameters. Relationships, in terms of F and/or G, between these parameters are derived based on mechanical models and material supplier data. From these relationships log-log plots of one parameter against another are depicted upon which is drawn a line with a slope dependent on the relationship. The chart in Figure 1. guides selection of materials for light, stiff, components. The lines are based upon a loci of points which establish materials above the line formed by these points to be suitable for the F and/or G described. The following relationships together with Figure 1 exemplify the use of a modulus-density performance index.

- 1)  $E/r = C$  (minimum weight design of stiff ties; minimum deflection in centrifugal loading, etc.),
- 2)  $E^{1/2}/r = C$  (minimum weight design of stiff beams, shaft and columns), and
- 3)  $E^{1/3}/r = C$  (minimum weight design of stiff plates)

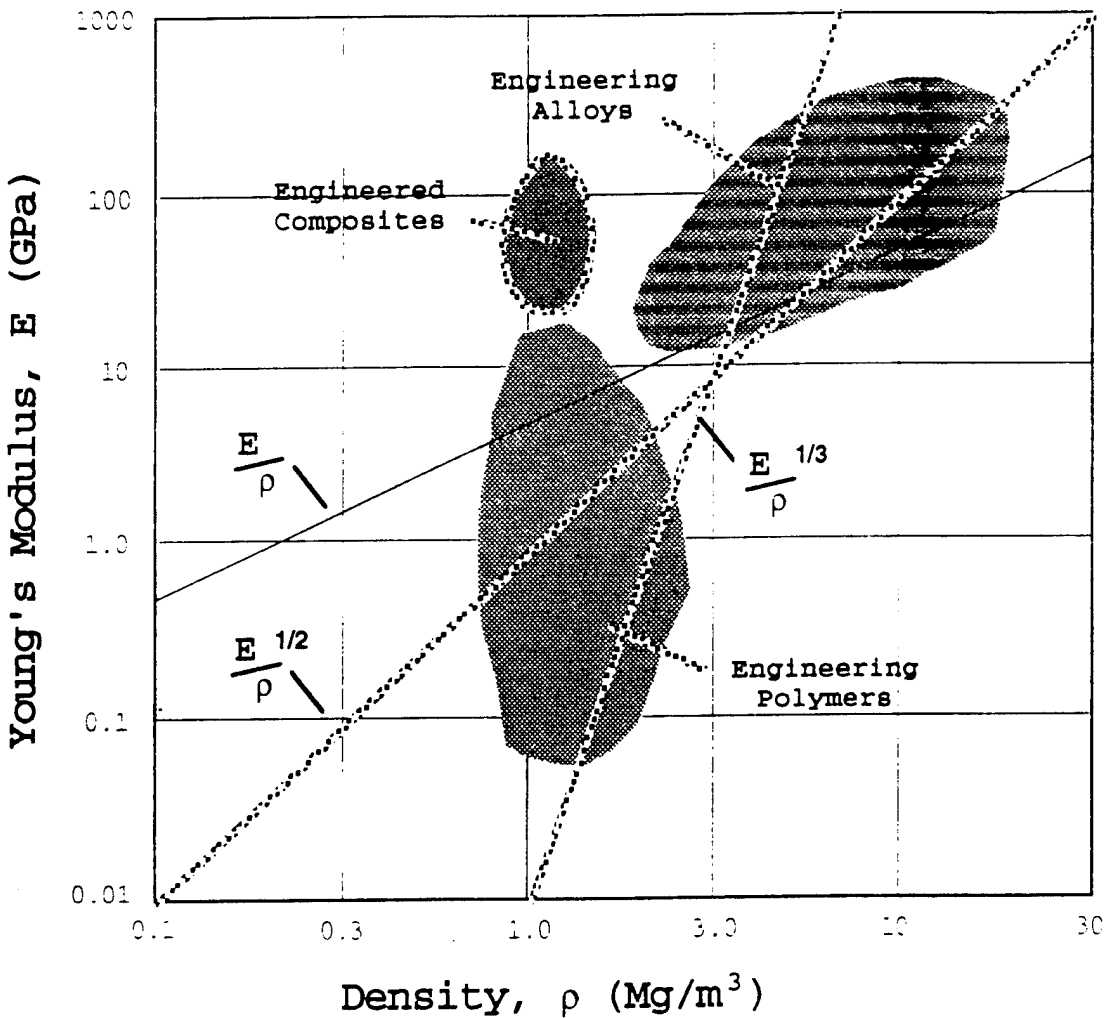


Figure 1. Modulus-Density Performance Indices

Various types of materials are represented by regions that enclose ranges of values typical for the class of material. The decision line is movable on the plot, and the display automatically highlights those groups that lie above or on the line. These materials satisfy the indices for the optimum behavior. Selection of materials is thereby reduced to choosing the group that appears to be best. This is the coarsest level of choice, and refinements are being generated to allow more detailed selection of materials. Current development is underway to combine shape factors with one or more of the indices, for example shape and strength for a beam structure. Such refinements to the indices reduce the number of materials options available, but they bring the materials selection aspect of design closer to real applications.

**Note:** Although it requires simplifying assumptions, Prof. Ashby's approach is indeed a major step forward in associating material knowledge with geometry and functional requirements. He has yet to associate processing information, except for averaged cost data, to assist in the design of process.

Additional databases containing detailed property data are also being prepared. A Copper alloy database was demonstrated that was created from a few hundred papers with data and some information from the British Copper Development Association. This exercise is rather labor intensive because data must be scanned, edited, and transferred to a CD. The Copper database took 8 months of effort to create.

The creation of successive levels of refinement follows the natural hierarchy of selection, and thus the approach being taken has merit in associating classes and specific materials and material property information. Implementation remains to be seen, of course, but based on past efforts, the materials selection system being developed may be of considerable value.

### 5) Progress

After one day of interaction, we have acquired an improved perspective of the research objectives and approaches which are guiding both experimental and empirical research at the Cambridge EDC.

### 6) Continuing Activities

As a result of discussions with Dr. Mike Ashby and Dr. Ken Wallace potential exists for future interaction toward the development of an international Materials and Process Information Highway.

### 7) Potential for Further Collaboration

Near term potential for further collaboration depends upon Prof. Ashby and his views toward an international information highway. At present, the Cambridge Engineering Design Center has restricted access to their material property data to CMS users only. This is peculiar because, although CMS may appear unique as a method to couple shape, function and material information, it is clear that academia (student practicum) and especially industry (promoting sales) will pursue similar methods.

Analogous to the need for world-wide exchange of product geometry, material property data exchange will also be desirable. To be commercially viable, material property data will need to be shared (possibly for a fee) between companies, nationally and internationally, between co-developers and customer(s)/supplier(s).

The smart, next step for Cambridge would be to couple their CMS tool to a computer aided design (CAD) system. It is our belief that this CMS-to-CAD coupling may be the best opportunity for collaboration and thus I have suggested the following to Prof. Ashby.

I would like to offer sending some of my people to Cambridge to give an overview, demonstration and training in the use of a feature-based design environment referred to as AML. This is a commercial product which we are grooming for the PowerPC but is available for use under UNIX, and soon WindowsNT, and Apple System 7.0. It is an object-oriented, open-architecture design environment involving a single non-manifold model (representation system) for design, meshing/analysis and manufacturing (materials and processing) which is compact (requires less than 15M bytes of storage and 3M bytes of RAM during use), tightly integrated (is directly linked to three (3) geometry engines: XOX, ACIS and ParaSolids), and provides open access to the representation system and user interface to modify/incorporate materials/processing data and knowledge bases.

My interest is to use the above design environment as the interface for a community of materials/processing suppliers and customers on an international information highway. My purpose in collaboration is to nurture

and support the development of this information highway. I believe your participation would be synergistic for both of us.

Now through 2000 Workshop and Conference Sessions focused on developing an *International Information Highway* of collaborators in pursuit of advancing knowledge and methods associated with Integrated Materials-Process-Shape Design.

# Artificial Intelligence Laboratory, University of Edinburgh

## 1) Brief overview of the authors' perception of research in material/process discovery methods at the Artificial Intelligence Laboratory

Although we learned of no materials processing applications, one noteworthy observation is the AI Department at the University of Edinburgh is possibly one of the best in the world, and yet I perceive that unless this department changes some of its precepts it may suffer the demise that other lesser AI departments have. AI must be more than symbolic computing, and even though some of the work at the University of Edinburgh involves robotics and computer aided design, it appears to remain isolated from the more traditional computational methods, i.e., mathematics and algorithmic approaches.

AI researchers must begin to realize that AI is but another approach to problem solving and does not necessarily replace more traditional methods. A research staff using the title - Artificial Intelligence Department - may become isolated in viewing all problems as solvable with only a subset of tools, when in fact the best solutions will require the combination of AI and other methods.

## 2) A Description of Artificial Intelligence Laboratory

The University of Edinburgh has about 15,000 students, about the same size as Cambridge University. The Artificial Intelligence (AI) Laboratory and Department has about 37 faculty and visiting research fellows, 55 PhD students, 42 MSc students, and 250 undergraduates. The AI Laboratory and Department is headed by Prof. James Howe who, after 30 years with the University of Edinburgh, will retire in 1996.

The size of the Department and the resources in terms of buildings and equipment is most impressive, particularly in light of the recent demise of AI in the academic arena. It was clear from the demonstrations provided us that this particular group of AI researchers are extremely talented and very ably led by Dr. Howe. As with all of the Universities in Great Britain, there is tremendous pressure to show near term payoff of research - which is the reason for the AI Applications Institute. But in addition to the 'near-term-payoff' pressure, there has been a 60% increase in student enrollment which has not been offset with additional staff. The combined effect is apparent - Dr. Howe is guiding his over-worked staff toward short-term development efforts to apply new ideas and exercise existing tools. The consequence of the above is that basic research has been reduced both for lack of time and funding.

## 3) Facilities and Assistance

No specific facilities have been required or utilized.

## 4) Research Objectives and Approach

We were briefed in the morning on activities within the Department by researchers currently active there. Interests were in assembly robotics (Prof. Malcolm), vision issues associated with 3-dimensional objects and representation visually (Dr. Fitzgibbon), and mobile robotics (Dr. Hallam). Overviews of work related to knowledge based systems (Dr. Robertson), genetic algorithms (Dr. Ross), and mathematical reasoning (Dr. Ireland) were presented. These presentations were concerned with the fundamentals of these areas of interest and were academic in perspective. The Genetic Algorithms presentation, however, did focus on some interesting applications in scheduling.

# General Observations Regarding Trip

## 1) Travel/Relocation Experiences

Travel in Russia has been surprisingly simple and efficient, but this has been due primarily to our being chaperoned. Without a chaperone, the language barrier would make travel near impossible as English is spoken by only a few people and the infrastructure (signs and directions) is very sparse. One specific, extremely positive, experience regarding travel has been the subway system.

The subway in Moscow is one of the most efficient transportation systems I have witnessed in all of my travels, in many ways comparable to the Tokyo, Japan subway system in that you can almost set your watch by the arrival of the scheduled train. On the other extreme lies the city-to-city train service. Our travel from Moscow, Russia to Kiev, Ukraine was over one-hour late and the overall accommodations and service were very poor.

Travel in Kiev is also best accomplished via the subway. Surface transportation generally suffers from road maintenance neglect. Noteworthy regarding our travel to the Ukraine was the hotel accommodations in Kiev. The hotel we stayed in was new and supposedly the best they had to offer in the city, yet it was obvious that it was poorly constructed and also generally without the proper services for the best hotel in a city of 3 million people.

Travel in London was again by subway with equally efficient service as in Moscow and Kiev.

## 2) Comments.

-> It is clear that our hosts, in Russia and the Ukraine, are most appreciative of our interest in their work. This is both from a technical and potential support perspective.

-> From the work we have witnessed and the discussions we have had, it is also clear that the potential synergy between groups in the US and in the former Soviet Republics holds great promise.

-> The former Soviet Union scientists appear to be much more interested in collaboration than I would have expected.

## 3) Acknowledgments

First, and foremost, to take an extended trip of this nature requires the back-up of a capable deputy, Captain Elizabeth Stark, to carry out a great many responsibilities for day-to-day operation of our research group. I, Dr. Steve LeClair, am indebted to Captain Stark for assuming all of my responsibilities while I have been out of the office - particularly for responding to all of the suspense's.

Secondly, we thank Dr. Osama El-Bayoumi (EOARD) for his support in arranging all of our visits and in rescheduling the Cambridge and Edinburgh visits due to our late receipt of official passports from the State Department. Upon our arrival in London, Dr. El-Bayoumi and Mr. Andy Davidson of EOARD provided support, even on the weekend (5-6 Nov 94), regarding phone/FAX and email access and further assisted us in using the London subway/train system. Dr. El-Bayoumi and Mr. Davidson have provided us excellent support on our Window-On-Europe visits and we express our appreciation.

Software systems developed by the Institute: PLINTH, HARDY and TOPKAT were demonstrated. Noteworthy regarding these tools is the emphasis on visualization for navigation through complex text systems such as building codes, system specifications and software manuals. TOPKAT was the highest level package and can serve as a tool for creating diagrams and maps required when creating an electronically based navigator of a complex process or set of rules and regulations.

#### 5) Progress

After one day of interaction, we have acquired an improved perspective of the Artificial Intelligence research objectives, approaches, and customer needs which are guiding both research within the Department and application development within the Institute.

#### 6) Continuing Activities

No near term collaboration is anticipated.

#### 7) Potential for Further Collaboration

The potential for further collaboration is in the area of genetic algorithms. Dr. Peter Ross clearly has several successful applications and of interest is to compare genetic algorithms with neural networks and pyramidal networks to classify materials and enable property prediction of new materials.

Another area of collaboration may be the 'information highway' and the use of so-called 'intelligent agents'. In addition to the above described demonstrations, Dr. Austin Tate of the AI Applications Institute gave us a demonstration of the new MOSAIC interface for the internet. One interesting part of the demonstration was the use of intelligent agents to autonomously search hosts worldwide, access their files and collect specific data. Until recently retrieval has been limited to whatever files were made available on the internet and search within the files for information of interest had to be performed by the requester (manually). This new autonomous retrieval capability could very well revolutionize an international materials and process information highway in terms of the gathering of information as a background, in lieu of a time consuming foreground activity.

**Note:** Here again is another example of the potential of a science 'information highway', which is slowly but surely under development and the use of 'intelligent agents' is clearly illustrative of how to use the highway to bridge academic and industrial interests with little if any additional workload on the users.