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NBS-Yugoslav Cooperative Research Program 1980-1984 US-Yugoslav Joint Board on Scientific and Technical Cooperation

Edited by:

Kurt F. J. Heinrich, Chief, Office of International Relations
Doris M. Bluebond, Program Analyst, Office of International Relations

A Record of Cooperative Scientific and Technological Projects Between the
National Bureau of Standards and Yugoslav Institutes During the Period
1980-1984.

January 1985

Issued May 1985



U.S. DEPARTMENT OF COMMERCE

NATIONAL BUREAU OF STANDARDS

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U.S. DEPARTMENT OF COMMERCE, Malcolm Baldrige, *Secretary*
NATIONAL BUREAU OF STANDARDS, Ernest Ambler, *Director*



FOREWORD

In this Publication we review the cooperative research program that the National Bureau of Standards has carried out with institutions in Yugoslavia during the period 1980-1984. NBS Technical Notes 753 and 986 cover the U.S.-Yugoslav program at NBS under the Special Foreign Currency Program for the period 1973-1978. The project descriptions presented here will provide scientists and scientific administrators with information on the program, and help the more general reader examine an example of successful international cooperation, aiming to contribute to the progress of the two countries involved and to improving international scientific relationships. The list of publications include some of the joint work performed previous to the formal establishment of this cooperative research program and are relevant to the project.

Grants from the U.S.-Yugoslav Joint Fund, to which the U.S. and Yugoslavia contribute equally, are made to finance cooperative projects of mutual interest and advantage. Projects are approved by the Yugoslav Federal Administration for International Scientific, Educational, Cultural and Technical Cooperation and by corresponding U.S. scientific and technological agencies under the egis of the Department of State. The NBS allocations from the Joint Fund have been fully committed and expended for the 1980-1984 period. Government-to-Government negotiations are now in progress to continue scientific and technological cooperation for an additional period of five years beginning in 1985. NBS plans to participate actively during that period.

ABSTRACT

An overview is given of cooperative projects conducted by the National Bureau of Standards and Yugoslav institutes under the U.S.-Yugoslav Joint Board on Scientific and Technical Cooperation. Each project is identified by title, principal investigator/s, institution in Yugoslavia, the NBS participants, and their organizational unit within NBS. The work is described briefly under the headings "Summary Description of Project Goals," "Results and Significance of Achievements to Date," and "List of Publications that Resulted from the Project." The NBS participants and the program manager judge that this grant program had a high benefit to cost ratio for NBS.

Key words: International scientific cooperation; physical science research; research planning; scientific research abstracts; U.S.-Yugoslav Joint Board on Scientific and Technological Cooperation.

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COOPERATIVE RESEARCH PROGRAM BETWEEN NBS AND YUGOSLAV INSTITUTES UNDER
THE U.S.-YUGOSLAV JOINT BOARD ON SCIENTIFIC AND TECHNICAL COOPERATION

1. INTRODUCTION

This report is intended to provide a summary review of the scientific and technological grants program that has enabled the National Bureau of Standards (NBS) to conduct joint research projects with Yugoslav Institutes under direction by the U.S.-Yugoslav Joint Board on Scientific and Technical Cooperation. Each project funded under the program is described briefly in terms of its initial project goals, its significant accomplishments, and its implications for science or technology at the cooperating institutions of both countries.

The NBS program has grown from 14 projects in the period 1973-1977 to 35 projects during the period 1980-1984. The projects are selected in accordance with the priorities by the Yugoslav side and complement current activities of NBS. They cover a wide range of scientific and technological areas, from the physics of subatomic particles to the protection of buildings against the effects of earthquakes and fires. The research proposals are reviewed by both sides to ensure that they have scientific merit and are relevant and mutually beneficial before being funded. Results of the research are being applied to practical needs and are usually published in journals of recognized international standing.

The NBS participants have been encouraged to communicate directly and continuously with the Yugoslav principal investigators. Visits by the NBS participants to Yugoslavia and of Yugoslav principal investigators to the U.S., aimed to broaden the basis of interaction, are considered an essential element of the program. These communications have promoted a

flow of scientific ideas and information and have often led to further important joint research, in addition to that performed within the projects.

Funding for the projects has been provided under the U.S.-Yugoslav Agreement for Scientific and Technological Cooperation. The two governments deposited into a Joint Fund in Belgrade the dinar equivalent of \$14 Million over a five-year period, on a 50-50 basis. Part of these funds provided NBS monitors with subsistence and international airfare for visits to Yugoslavia, but they were not used for research support of NBS. The Yugoslav side received limited dollar funds for per diem in the U.S. in addition to the dinar funds for salaries and equipment. However, the dollar funds were too modest to provide for long-term visits to NBS. With the available resources, the NBS policy has been to sustain as many channels of communication as possible rather than fund fully a few selected projects. Therefore, both sides had to contribute from their own resources for equipment and other expenditures.

Appreciation is expressed to the Yugoslav principal investigators and the NBS participants who provided the input for this report.

NBS expresses appreciation to the following for assistance and guidance for the S&T Cooperative Program:

Joint Board Members from the U.S. and Yugoslavia
Staff of the Yugoslav Federal Administration for International Scientific,
Educational, Cultural, and Technical Cooperation (FAISECTC)
Federal Republic Administrators in Yugoslavia
Bureau of Oceans and International Environmental and Scientific Affairs
Office of Cooperative Science and Technology (OES/SCT, State)
Foreign Currency Officers
Science Office and Staff of the Embassy of the United States of America,
Belgrade

Disclaimer:

Identification of commercial products does not imply recommendation or endorsement by NBS nor that the product is necessarily the best available for for the purpose.

Project Title: Organofunctional Derivatives of Inorganic Surfaces
(Project Page 313, NBS(G)-250)

Years and Funds: 1980-1984, Total Dinars 4,210,000

Principal Investigator: Dr. Velimir Pravdic

Yugoslav Institute: Rudjer Boskovic Institute

NBS Participant: Dr. Wolfgang Haller

NBS Laboratory, Center, Division: Center for Materials Science, Inorganic
Materials Division

Summary Description of Project Goals

Chemical surface modification of solids offers the unique possibility of combining desirable aspects of a material such as its mechanical and optical properties or the ability to be shaped into intricate shapes with a chemical resistivity or reactivity not obtainable from the base material. This well-known and widely used principle has penetrated almost every facet of modern materials technology. To give a few examples:

Surfaces are modified to increase the chemical resistance of structural materials and containers; surfaces are modified by chemical grafting, giving specific chemical reactivity to perform catalytically (e.g., immobilized enzymes), or to separate species by their affinity to the tailor-made surface (gas and liquid chromatography). While these technologies are presently practiced empirically, there remains the important question of how and why these effects do occur.

The stated principles are of great importance in producing composites such as glass fiber reinforced plastic, dental restorations made of polymer-bonded glass-spheres or reactive polymer fillers from inexpensive powders of mineral origin. In all these applications one can improve polymer penetration (wetting) and mechanical bonding by covalent grafting of organic molecules to the inorganic reinforcers.

Another area where chemical surface modifications play an important role is the interaction of solids and sediments with natural or man-made organic materials. Pollutant-cycling in natural waters (rivers, lakes, and in particular coastal waters) is largely controlled by the interaction of the water with particular solids. The latter are of mineral origin such as silica and silicates and exist in the natural medium with surfaces covered by organic substances of biological or detrital origin. Interpretation is difficult, unless one compares them with well-defined model systems. Glass and silica are not only highly suitable experimental materials, but are representing a larger class of natural non-swelling silicates.

The primary objective of this project was to investigate the adsorption behavior and energetics of surface-derivatized siliceous materials, in particular of surface derivatized silica glass of well-defined composition and properties, and to arrive at quantitative interpretations of the observed phenomena.

The methodologies and techniques used in this study were: precise manometric gas adsorption measurements, continuous flow and batch immersion colorimetry; interfacial charge distribution and density determination by streaming potential techniques, acidimetry, and electron-spin-resonance (ESR) techniques.

The project is a sequel of previous studies in which emphasis was put on correlating bulk and surface properties of glasses.

Results and Significance of Achievements to Date

Based on previous experiments of adsorption measurements by flow microcalorimetry, studies of the interaction of lower aliphatic alcohols with original and silicone treated surfaces of controlled pore glass were continued.

Results show that for the original surfaces of glass the average area per adsorbed molecule of alcohol (studied were: ethanol, propanol, n-butanol and n-pentanol) does not change significantly with the chain length ($0.28 \pm 0.02 \text{ nm}^2$), indicating an "upright" mode of adsorption at the surface.

In the same series of alcohols, however, the specific enthalpy of adsorption per unit surface area decreases (in $\mu\text{J cm}^{-2}$): 26, 18, 17 and 14. Thus, there is a quantitative measure of increased hydrophobicity of the adsorbate molecules.

For silicone oil treated surfaces (where the surface modifier is not covalently bound, but rather a layer held by adhesion forces) there is some steric repulsion observed with increasing chain length. The area per molecule is, at maximum adsorbed amount: 0.39, 0.82, 1.1 and 1.6 nm^2 . This is a significant, in the extreme case five-fold increase. That this is a typical steric hindrance effect is indicated by the observed reduction in the specific enthalpy of adsorption (in $\mu\text{J cm}^{-2}$): 7.1, 5.1, 3.2, and 3.4. These studies have thus revealed both steric factors and the energetics of interaction.

Functional group molecules, C_4 alcohol, acid, aldehyde, and nitropropane were used as adsorbates to probe into the specific properties of surface sites. In this case acidity or basicity is interpreted beyond the classical definition of Lewis acids. The specific enthalpies of adsorption were (in $\mu\text{J cm}^{-2}$): 30.5 for butylamine (relative basicity: +11.7); 5.4 for butyric acid; n-butanol (a molecule

with relative basicity of -0.26) yields 19.8; n-butyraldehyde (relative basicity -8.26) only 4.0. These data characterize the specific affinity of hydroxyl groups in the glass surface.

Another step in the research endeavors is the covalent binding of characteristic molecules to the surface: a process known as surface derivatization. Glass and silica are very convenient models to study, as indicated in the introductory part of this report. Suitable agents are found in bifunctional silanes which contain trichloro or triethoxy functionalities to form a covalent bond to the glass surface and selected other groups ("tails") to impart a different chemical functionality to the glass. These were expected, depending on the properties of the molecular "tail", to enhance the surface hydrophobicity, by exerting various degrees of hydrophobic shielding. Such derivatized samples have been used in various studies, at present in gas and water vapor adsorption experiments, and in ESR spectroscopy.

The ESR spin-label technique, with labels containing functional groups, allows for the identification of the number of spin-label molecules attached to typical sites to be quantitatively estimated. Acidity of a surface is indeed an excess of acid over basic sites, both of them co-existing in a sample. In adsorption the $-NH_2$ spin label molecule was expected to attach predominantly to acid sites. The ESR spectra recorded by comparison with a calibrated spin standard, yield the total number of spins of a sample accommodated within the cavity. Our experiments have indicated that the original glass surface shows a ratio of 78.22 percent in favor of acid sites. The result of surface derivatization indicates a reduction in acid sites down to a residual level of 0.1 OH-groups per nm^2 .

The next step in the research will require additional methodologies and/or techniques to estimate the distribution of sites at the surface. The question is whether grouping into patches occurs, or a statistically even distribution prevails. Such information would yield vital information with respect to the expected behavior of glass as adsorbent (carrier) for macromolecules, such as proteins or vira.

List of Publications or Other Input that Resulted from the Project

1. J. Jednacak-Biscan, V. Pravdic, "Adsorption Phenomena on Glass Surfaces. I. A Microcalorimetric Study of Adsorption of Alcohols on Controlled Pore Glass," J. Colloid Interf. Sci. 75 (1981) 322.
2. J. Jednacak-Biscan, V. Pravdic, "Adsorption Phenomena on Glass Surfaces II. Interaction of Small Organic Molecules with Porous Glass," J. Colloid Interf. Sci. 90 (1982) 44

3. J. Jednacak-Biscan, V. Pravdic, "Adsorption Phenomena in Glass Surfaces III. A Microcalorimetric Study of Adsorption of n-butanol on Heat Treated Surface of Controlled Pore Glass," *Thermochemica Acta* 53, (1982) 203.
4. J. Jednacak-Biscan, Doctoral Dissertation: "Physico-chemical Phenomena at Phase Boundaries: The Glass-liquid Interface," (in Croatian), University of Zagreb, Zagreb, June 1981.
5. D. Cukman, J. Jednacak-Biscan, Z. Veksli, W. Haller, "Characterization of Chemically Modified Glass Surfaces," *J. Colloid Interface Science* (to be submitted).

Guest Scientists who Visited NBS from Yugoslavia

1. Dr. J. Jednacak-Biscan, June 19-June 25, 1980
2. Dr. V. Pravdic, November 2-November 4, 1980
3. Dr. V. Pravdic, April 9-April 10, 1984
4. Dr. D. Cukman, June 14-June 18, 1984

Visits to Yugoslavia by NBS Participant

1. Dr. W. Haller, September 9-September 11, 1980
2. Dr. W. Haller, November 3-November 6, 1981
3. Dr. W. Haller, September 6-September 8, 1982
4. Dr. W. Haller, September 19-October 5, 1983
5. Dr. W. Haller, May 4-May 11, 1984

Project Title: Development of Reference Methodology for
Standardization at the Trace Level
(Project Page 314, NBS(G)-251)

Years and Funds: 1980-1984, Total Dinars 4,210,000

Principal Investigator: Professor Lado Kosta

Yugoslav Institute: Jozef Stefan Institute

NBS Participant: Dr. Harry L. Rook

NBS Laboratory, Center, Division: National Measurement Laboratory,
Center for Analytical Chemistry, Gas and Particulate Division

Summary Description of Project Goals

The objective of this project is to develop new nuclear analytical methods to help eliminate systematic errors and to determine elemental compositions of new NBS Standard Reference Materials (SRM's) using the developed methods.

The research and analytical measurements carried out by Dr. Kosta and his co-workers under this project have been an extremely valuable complement to work carried out in the Center for Analytical Chemistry on NBS SRM's. Data provided by Dr. Kosta have been included in certified values on seven NBS SRM's. These data are used worldwide in research on new analytical methodologies.

The analytical methods developed under this project are also of great value to scientists in Yugoslavia. Programs in environmental monitoring, health studies, and industrial quality control have available new trace analytical methods of verified accuracy. Data produced by the Jozef Stefan Institute for other studies have proven to be of the highest quality. In summary, the program is a model for future programs.

Results and Significance of Achievements to Date

During the past four years, research has been completed on new analytical methods for the determination of selenium, iodine, cadmium, molybdenum, arsenic, vanadium, and tungsten in reference materials. The research included the development of new highly selective radiochemical separations procedures, selective epithermal neutron irradiation procedures and a preirradiation separation procedure for short half-lived elements.

The methods have been tested on existing NBS SRM's and then applied to the certification analysis of minor and trace constituents in several new SRM's as well as selected IAEA reference materials. The following is a list of SRM's and elements for which data has been provided:

SRM 1577	Bovine Liver	(Se, Mo, W)
SRM 1577a	Bovine Liver	(As, Cd, Co, Cu, Mo, Sb, V, Zn)
SRM 1567	Wheat Liver	(As, Cd, Cu, Mn, Mo, Ni, Sb, V, Zn)
SRM 1568	Rice Flour	(As, Cd, Co, Cu, Mn, Ni, Sb, V, Zn)
SRM 1572	Citrus Leaves	(As, Cd, Co, Cu, Mn, Sb, V, Zn)
SRM 1549	Milk Powder	(As, Cu, Hg, I, Mn, Mo, Sb, Se, Zn)
SRM 1590	Stabilized Wine	(As, Cu, Mn, Zn)

List of Publications or Other Input Relevant to or Resulting from the Project

1. A. R. Byrne: "Extraction of some Trace Elements as Iodides with MIBK and Applications in NAA," Radioanal. Letters 40 (1979) 1-16.
2. I. Gvardjancic, L. Kosta, M. Dermelj, "Determination of Iodine in Reference Materials by Activation Analysis," J. Radioanal. Chem., 58 (1980) 359-365.
3. B. Pihlar, P. Valenta, H.W. Nurnberg, "New High Performance Analytical Procedure for the Voltammetric Determination of Nickel in Routine Analysis of Waters, Biological Materials and Food," Z. Anal. Chem., 307 (1981) 337-346.
4. L. Kosta, A.R. Byrne, "Analytical Evaluation of Comparative Data on Trace Elements in Biological Materials," J. Radioanal. Chem. 69 (1981) 117-129.
5. A. R. Byrne, "Simultaneous Radiochemical Neutron Activation Analysis of Vanadium Molybdenum and Arsenic in Biological Samples," Radiochem. Radioanal. Letters 52 (1982) 99-110.
6. K. Kosta, "Contamination as a Limiting Parameter in Trace Analysis," Talanta 29 (1982) 985-992.
7. H. Polkowska-Motrenko, M. Dermelj, A.R. Byrne, A. Fajgelj, P. Stegnar, L. Kosta, "Radiochemical NAA of Selenium Using Carbamate Extraction," Radiochem. Radioanal. Letters 53 (1982) 319-327.
8. J. J. M. de Goeij, L. Kosta, A. R. Byrne, J. Kucera, "Problems in Current Procedures for Establishing Recommended Values of Trace Element Levels in Biological Reference Materials," Anal. Chem. Acta 146 (1983) 161-169.
9. A. R. Byrne, L. Kosta, M. Dermelj, M. Tusek-Znidaric, "Trace Elements Analytical Chemistry in Medicine and Biology," Vol. 2 (P. Bratter, P Schramel Eds.), "Aspects of Some Trace Elements in Human Milk," W. de Gruyter, Berlin (1983) 21-25.
10. L. Kosta, A. R. Byrne, M. Dermelj, "Trace Element in Some Human Milk Samples by Radiochemical Neutron Activation Analysis," Sci. Total Environ. 29 (1983) 261-268.

11. B. Smodis, M. Dermelj, A. R. Byrne, "Rapid Nondestructive Determination of Sulphur and Vanadium in Petroleum Derivatives," Vestnik Slov. Kem. Drus. 30 (1983) 29-37.
12. A. R. Byrne, M. Dermelj, L. Kosta, M. Tusek-Snidaric, "Radiochemical NAA in Standardization of Trace Elements in Biological Reference Materials at the Nanogram Level," Mikrochem. Acta (1984) I, 119.

Guest Scientists who Visited NBS from Yugoslavia

1. Dr. Lado Kosta, 1981, one week.

Visits to Yugoslavia by NBS Participants

1. Dr. Harry Rook, 1979, one week
2. Dr. Harry Rook, 1982, 4 days
3. Dr. Harry Rook, 1984, 4 days
4. Dr. R. Zeisler, 1984, 2 days

Project Title: Standardization of Methods of Measurement of
Materials and Thermophysical Characterizations of
Standard Reference Materials
(Project Page 315, NBS(G)-252)

Years and Funds: 1980-1984, Total Dinars 4,811,500

Principal Investigator: Dr. Kosta Maglic

Yugoslav Institute: Boris Kidric Institute of Nuclear Sciences

NBS Participant: Dr. Ared Cezairliyan

NBS Laboratory, Center, Division: National Engineering Laboratory,
Center for Chemical Engineering, Thermophysics Division

Summary Description of Project Goals

The objectives are two-fold:

- Preparation of a Compendium, in two volumes, entitled "Thermophysical Properties Measurement Methods"

This Compendium will be unique of its kind and will serve investigators and students in the field of thermophysical properties. For the first time, it will bring together the methods and critical evaluation of the problems associated with the measurement of all the important thermophysical properties. The benefits will be global and will help not only those active in the field but will serve as a starting point for the newcomers in the field.

- Thermophysical characterization of selected standard reference materials.

Measurements by various investigators of selected thermophysical properties, such as specific heat and thermal diffusivity, of selected materials candidate to become reference materials, are essential in order to ascertain the reproducibility and reliability of the overall results. This work will lead to the establishment of reference materials above room temperature and up to about 3000 K.

By bringing together, for the first time, a comprehensive survey of all major techniques for measurements of thermophysical properties, the compendium will serve as a unique information source for the researchers in both industrial and developing countries. It will be an effective solution to problems faced in developing and operating thermophysical measurements systems. Accurate thermophysical data obtained through this program will help the establishment of international standards in thermophysics and will help increase the efficiency of industrial operations and improve industrial process control.

Results and Significance of Achievements to Date

A major output of the project will be the Compendium entitled "Thermophysical Properties Measurement Methods" which will consist of two volumes. Volume 1 will be on the general review of all measurement methods, and Volume 2 will be on selected standardized methods. As of this date, the preparation of Volume 1 is completed. It contains 20 chapters and is 780 pages long. The contributions represent a truly international effort in the field, including all major industrial countries. (Ed: this volume is now available.)

The preparations for Volume 2 have started and all authors have been identified and have been contacted. The preparations of the chapters are underway and it is expected that the first drafts of the manuscripts will be completed by the end of 1984.

With regard to the second objective, measurements of specific heat and electrical resistivity of iron in the temperature range 300 to 1400 K have been performed at the Boris Kidric Institute. The results were presented at the International Center for Heat and Mass Transfer Symposium in September 1983 in Yugoslavia and will be published in the Symposium Proceedings.

List of Publications or Other Input that Resulted from the Project

1. K. Maglic, et al., "Thermophysical Properties Measurement Methods," Volume 1, Plenum Publishing Corp., (1984) 780.
2. A. S. Dobrosavljevic, K. Maglic, "Pulse Heating Method for Specific Heat and Electrical Resistivity Measurements in the Range 300 to 1400 K," Proceedings of Heat and Mass Transfer Symposium (in press).

Guest Scientists who Visited NBS from Yugoslavia

1. Dr. Kosta Maglic, 1979, 3 days
2. Dr. Kosta Maglic, 1981, 5 days
3. Dr. Kosta Maglic, 1984, 3 days

Visits to Yugoslavia of NBS Participant

1. Dr. A. Cezairliyan, 1980, 3 days

(NOTE: On several other occasions, such as during national and international conferences, meetings were held between the principal investigators and other individuals related to the project.)

Project Title: Resonance Broadening of Spectral Lines and
Determination of Atomic and Molecular Parameters
(Project Page 316, NBS(G)-253)

Years and Funds: 1980-1984, Total Dinars 5,735,000

Principal Investigator: Dr. Goran Pichler

Yugoslav Institute: Institute of Physics, Zagreb University

NBS Participant: Dr. Wolfgang Wiese

NBS Laboratory, Center, Division: National Measurement Laboratory,
Center for Radiation Research, Atomic and Plasma Radiation Division

Summary Description of Project Goals

From the very beginning the main goal of the project was the study of the interaction of alkali atoms, of which at least one is in an excited state. Special emphasis was placed on the first excited state which usually produces strong resonance interaction between like alkali atoms. Once resonance interaction was well understood it was taken as the basis for studying short-range interatomic interactions. The experimental goal was to develop special heat-pipe ovens in order to measure the extended quasistatic wings of the self-broadened resonance lines of alkali atoms. In addition to far-line wing studies two kinds of structured continuum spectra were investigated in connection with higher excited molecular states. Besides homonuclear diatomic molecules some examples of heteronuclear diatomics were chosen to extend the basic knowledge on alkali interactions.

Another very important goal of the project was to carry out plasma spectroscopic studies of wall-stabilized arcs in argon, with additions of various gases, for the measurement of transition probabilities and Stark broadening parameters of a selected number of lines. The ultimate goal of these two parallel researches is to apply the alkali spectroscopy in neutral vapors to the spectroscopy of alkali plasmas created in various ways. This will be closely studied in the next five-year contract, although several elements of such studies were already attacked within the present project.

Results and Significance of Achievements to Date

Generally, the results of the investigations provide new basic knowledge about the interaction between alkali atoms, of which at least one is in the excited state. The large number of publications in selected international journals on physics shows steady activity within this field, which quite recently reached a very high level of understanding for the basic spectroscopic processes. Recent research in plasma spectroscopy of wall stabilized arcs has also provided a

number of new results published in international journals. These basic studies give rise to many interesting applications in different directions, especially some energy oriented applications.

In particular, increasing understanding of the interaction of alkali atoms was achieved. Starting from very basic calculations of the interaction potential curves and relevant oscillator strengths, the whole quasi-static line profile of self-broadened alkali resonance lines was generated. Several experiments confirmed these calculations in many ways, so that it was possible to apply them in different regions of internuclear separations. This led to the interpretation of broad satellite bands in the very far wings of sodium first resonance line (the other alkali examples are partially published or are still under investigations).

In the last two years the study of structured continuum spectra was intensified. The reason for this was that certain diffuse bands and interference continua can be used for tunable lasers. In a number of papers a model for the qualitative explanation of these structured continua was presented, which may help to attain the goal of laser action within alkali vapors.

All studies in alkalis were undertaken with pure or mixed alkali vapors, and sometimes in mixtures with noble gases. Different elements or mixtures require different experimental approaches which provide the driving force for the development of new experimental instrumentation.

The work in the last few months is continuing along the lines of the project goals, with special emphasis on understanding the basic processes that lead to the observed spectral phenomena. In connection with this, special interest is provided by a joint experiment at the National Bureau of Standards on the asymmetries and antisymmetries in neutral nitrogen spectral lines excited in a highly stabilized argon arc.

List of Publications or Other Input Relevant to or Resulting from the Project

1. M. Movre, G. Pichler, "Resonance Interaction and Self-broadening of Alkali Resonance Lines II. Quasi-static Wing Profiles," J. Phys. B: Atomic, Molec. Phys. 13 (1980) 697-707.
2. K. Kiemax, M. Movre, G. Pichler, "Near-wing Asymmetries of the Self-broadened First Rb and Cs Resonance Lines," J. Phys. B: Atom. Phys., Vol. 12, No. 21 (1979).
3. D. Veza, M. Movre, G. Pichler, "The shape of the Inner-wing Satellies of Self-broadened First Resonance Lines of Caesium and Rubidium," J. Phys. B: Atom. Molec. Phys. 13 (1980) 3605-3611.
4. D. Veza, J. Rukavina, M. Movre, V. Vujnovic, G. Pichler, "A Triplet Satellite Band in the very far blue wing of the Self-broadened Sodium D Lines," Optics Communications, Vol. 34, No., 1 (1980).

5. V. Lokner, M. Movre, "Determination of the true total line Intensity and the true Halfwidth of the Lorentz Components for the Class of Voigt Profiles from Graphical Analysis of Spectrum," *Fizika* Vol. 12, No. 1 (1980) 61-69.
6. G. Pichler, "Self-broadening in Metal Vapors, in Spectral Line Shapes," Ed., B. Wends, Walter de Gruyter & Co., Berlin (1981).
7. M. Movre, D. Veza, G. Pichler, K. Niemax, "Triplet Satellite Bands in the very far blue Wings of the Self-broadened Alkali D Lines, in Spectral Line Shapes," Ed., B. Wende, Walter de Gruyter & Co., Berlin (1981).
8. LD. Veza, G. Pichler, "Quasistatic Self-broadening of Li and Na first Resonance Lines, in "Spectral Line Shapes," Ed., B. Wende Walter de Gruyter & Co., Berlin (1981).
9. C. Vadla, R. Beuc, M. Movre, "Quasi-static Wings of K Spectral Lines Broadened by Cs, in Spectral Line Shapes," Ed., B. Wende, Walter de Gruyter & Co., Berlin (1981).
10. D. Veza, S. Milosevic, G. Pichler, "Triplet Satellite band in the very far blue wing of the Self-broadened Lithium Resonance Line," *Chem. Phys. Let.* 93 (1982) 401-405.
11. R. Beuc, S. Milosevic, M. Movre, G. Pichler, D. Veza, "Satellite Bands in the far blue wing of the Potassium First Resonance Doublet," *Fizika, Yugoslavia* 14 (1982) 345-349.
12. R. Duren, E. Hasselbrink, H. Tischer, S. Milosevic, G. Pichler, "On the Doublet Sigma Potentials for the Interaction of K(4P) and K(5P) with Argon," *Chem. Phys. Let.* 89 (1982) 218-222.
13. D. Veza, G. Pichler, "Peculiar Asymmetry in the Wings of Self-broadened Li and Na first Resonance Lines." Accepted for publication in *Optic Communication* (1982).
14. G. Pichler, S. Milosevic, D. Veza, S. Bosanac, "Peculiar Diffuse bands in Li , and K Absorption Spectra, Spectral Line Shapes," Ed., K. Burnett, Walter de Gruyter & Co., Berlin (1982 or 1983).
15. V. Vujnovic, C. Vadla, V. Lokner, M.S. Dimitrijevic, "Halfwidths of Neutral Fluorine Spectral Lines," *Astronom. Astrophys.* 123 (1983) 249-252.
16. V. Lokner, C. Vadla, V. Vujnovic, "Relative Transition Probabilities of F (I) Spectral Lines in the Visible," *J. Quant. Spectrosc. Radiat. Transfer* 30 (1983) 187-191.
17. D. Veza, G. Pichler, "Peculiar Asymmetry in the Wings of Self-broadening Li and Na first Resonance Lines," *Optics Communications* 45 (1983) 39-42.

18. D. Veza, S. Milosevic, G. Pichler, "Triplet Satellite Band in the very far blue wing of the Self-Broadened Lithium Resonance Line," Chem. Phys. Let. 93 (1982) 401-405, and "Spectral Line Shapes," Vol. 2, Walter de Gruyter and Company, Berlin (1983).
19. G. Pichler, S. Milosevic, D. Veza, S. Bosanac, "Peculiar Diffuse bands in Li_2 and K_2 Absorption Spectra, Spectral Line Shapes," Vol. 2, Walter de Gruyter and Co., Berlin (1983).
20. R. Beuc, S. Milosevic, G. Pichler, "New Diffused bands in KRb Molecule," J. Phys. B: Atom. Molec. Phys. 17 (1984) 739-745.
21. G. Pichler, S. Milosevic, D. Veza, D.D. Konowalow, "Observation and Interpretation of the Li Diffuse band in the Region of 420 nm," Chem. Phys. Let. 103 (1984) 352-356.

Guest Scientists who Visited NBS from Yugoslavia

1. Dr. G. Pichler, 1982, 2 weeks, Gaithersburg and Boulder Labs.
2. Dr. C. Vadla, 1982, 1 week, Boulder Labs.
3. Dr. G. Pichler, 1984, 6 weeks, Gaithersburg and Boulder Labs.

Visits to Yugoslavia of NBS Participant

1. Dr. W. L. Wiese, 1981, 3 days, University of Zagreb
2. Dr. W. L. Wiese, 1982, 1 week, Attendance at XI Symposium of Physics of Ionized Gases in Dubrovnik
3. Dr. W. L. Wiese, 1984, 2 days, University of Zagreb and 5 days, XII Symposium on the Physics of Ionized Gases in Sibenik
4. Dr. Daniel Kelleher, 1981, 10 days, University of Zagreb

Project Title: Phase Diagrams for Ceramists
(Project Page 317, NBS(G)-254)

Years and Funds: 1980-1984, Dinars 3,261,000

Principal Investigator: Prof. Drago Kolar

Yugoslav Institute: Jozef Stefan Institute

NBS Participant: Dr. R. S. Roth

NBS Laboratory, Division: Center for Materials Science, Inorganic
Materials Division

Summary Description of Project Goals

Development of new materials or materials with improved properties is a prerequisite for technical development in future years. Among the contemporary materials, inorganic high-temperature materials (ceramics) enjoy special attention. Continuous development in the recent ten-twenty years resulted in a large number of new products and materials with excellent properties for use in electronics, mechanical engineering, machining, energy production, etc. The basis for development of new inorganic materials is dependent on phase diagrams which enable understanding of chemical reactions and equilibria at manufacturing and operating conditions and thereby optimization of material properties. Therefore, the main goals in 1980-1984 projects were -

- To study and determine phase equilibria in binary and ternary oxide systems relevant to materials used in electronics
- To study kinetics and mechanisms of chemical reactions at increased temperature
- To evaluate reported phase equilibrium data and make them available to a broader scientific and technical community

Results and Significance of Achievements to Date

1. In the three-component systems $\text{BaO-TiO}_2\text{-Nd}_2\text{O}_3$ three new compounds and their crystal structures were determined, $\text{Nd}_4\text{Ti}_9\text{O}_{24}$, $\text{BaNd}_2\text{Ti}_3\text{O}_{10}$ and $\text{BaNd}_2\text{Ti}_5\text{O}_{14}$, respectively (Ref. 1). Moreover, a series of isomorphous compounds with other rare earth oxides (Pr, Sm, Eu, La) were synthesized and their crystal structure reported (Refs. 2, 3). The mechanism of chemical reactions in the system $\text{BaTiO}_3\text{-Nd}_2\text{O}_3$ and $\text{BaTiO}_3\text{-Nd}_2\text{Ti}_2\text{O}_7$ was investigated and model was proposed, which explains microstructure development during sintering of capacitor dielectrics based on these systems (Ref. 4). Electrical properties of ceramics in parts of the $\text{BaO-TiO}_2\text{-Nd}_2\text{O}_3$ ternary system were examined and two important regions

were defined. The region around the BaTiO₃ composition, enables the manufacture of class 2 dielectrics with high permittivity and reasonably high temperature stability, whereas the compositional region around BaNd₂Ti₃O₁₀ and BaNd₂Ti₅O₁₄ permits the manufacture of class 1 dielectrics with high temperature stability and extremely low dielectric losses (Ref. 5). In search for further improvement of electrical characteristics, preliminary investigations have been carried out in the quaternary system BaO-TiO₂-Nd₂O₃-SnO₂. The main reaction product in the system Ba(Ti,Sn)O₃Nd₂O₃ was found to be Nd₂Sn₂O₇, which is not ferroelectric and decreases the permittivity of BaTiO₃-based ceramics (Ref. 6).

2. Other phase equilibria and chemical reactivity studies within the project were concerned with the system Bi₂O₃-CdO and Al₂O₃ZrO₂PSZ (partially stabilized). In the system Bi₂O₃CdO, a new phase was identified CdBi₂O₄, stable up to 925K. Several other phases were identified and a revised phase diagram was proposed (Ref. 7). In the system Al₂O₃-partially stabilized ZrO₂, diffusion processes and solid state reactions were investigated, using diffusion couples. Among the systems investigated only yttrium-stabilized ZrO₂ was found to be stable in the presence of alumina, whereas Ca and Mg stabilized ZrO₂ were destabilized due to the formation of Mg and Ca aluminates (Ref. 8).

3. As a part of the project, the evaluation of published phase equilibrium data was carried out and some results were included in relevant publications of Am. Ceram. Soc. (Ref. 9).

List of Publications of Other Input that Resulted from the Project

1. D. Kolar, S. Gaberscek, V. Volavsek, H.S. Parker, R. S. Roth, "Synthesis and Crystal Chemistry of BaNd₂Ti₃O₁₀, BaNd₂Ti₅O₁₄ and Nd₄Ti₉O₂₄," J. Solid State Chem. 38 (1981) 158-166.
2. S. Gaberscek, D. Kolar, "Compounds in the BaO-Al₂O₃-TiO₂ Systems," J. Mat. Sci. Let. 1 (1982) 37-38.
3. J. P. Guha, D. Kolar, "Indexed X-ray Diffraction Data for Nd₄Ti₉O₂₁," J. Mat. Sci. Let. 1 (1982) 312-313.
4. D. Suvorov, S. Gaberscek, D. Kolar, "Reactions in the System BaTiO₃-Nd₂O₃-TiO₂," Proceedings 4th Internat'l. Joint Meeting on Elektro-and Magnetoceramics, DKG (1983) 87-97.
5. D. Kolar, D. Suvorov, S. Gaberscek, "Dielectric Ceramics in the System BaO-TiO₂-Nd₂O₃," Ferroelectrics (1981).
6. D. Suvorov, M. Trontelj, D. Kolar, "Reactions in the System BaO-TiO₂-Nd₂O₃-SnO₂," Science of Ceramics 12 (1983).
7. A. Jeger, D. Kolar, "Phase Relations in the System Bi₂O₃-CdO," J. Solid State Chem. (1984) in print.

8. T. Kosmec, D. Kolar, M. Trontelj, "Diffusion Processes and Solid State Reactions in the System Al_2O_3 - ZrO_2 -Stabilizing Oxides (Y_2O_3 , CaO and MgO)," Proceedings of Zirconia Conference, Stuttgart (1983) in print.
9. R. S. Roth, T. Negas, L. P. Cook (editors) D. Kolar, contributor, "Phase Diagrams for Ceramists," Vol. 4 (1981).
10. R.S. Roth, T. Negas, L.P. Cook (editors) D. Kolar, contributor, "Phase Diagrams for Ceramists," Vol. 5 (1984).

Guest Scientists who Visited NBS from Yugoslavia

1. Prof. Dr. M. Trontelj, 1982, 3 days
2. Prof. Dr. M. Drogenik, 1983, 2 days
3. Prof. Dr. D. Kolar, 1984, 2 days

Visits to Yugoslavia of NBS Participants

1. Dr. R. S. Roth, 1978, 6 days
2. Dr. R. S. Roth, 1981, 12 days
3. Dr. L. P. Cook, 1980, 6 days

Project Title: Investigation of Electron-atomic and Molecular
Binary Collision Excitation Processes
(Project Page 318, NBS(G)-255)

Years and Funds: 1980-1984, Dinars 3,259,500

Principal Investigator: Dr. Jelena Jovanovic-Kurepa

Yugoslav Institute: Institute of Physics, Belgrade University

NBS Participant: Dr. G. H. Dunn

NBS Laboratory, Division: National Measurement Laboratory, Center
for Basic Standards, Quantum Physics Division

Summary Description of Project Goals

This project is concerned with the investigation of electron-molecular dissociative excitation processes in medium electron energy interval (50-700 eV). In binary electron interactions with hydrogen containing molecular species, optical radiation is obtained and used in the analysis of dissociative molecular excitation processes. The emitted light in the visible and near IR spectral region, primarily Balmer radiations and some molecular fragment transitions, are detected. The measured data are presented as absolute line or band emission cross sections for the following molecules: H_2 , C_3H_6 (propene), C_3H_8 , $n-C_4H_{10}$, CH_3Cl and NH_3 . These results are of interest for atomic and molecular physics, plasma physics, radiation chemistry, and for better understanding of the processes in laser physics.

Results and Significance of Achievements to Date

The main achievements of this work are:

1. The first use of He benchmarks for apparatus calibration, i.e. for obtaining the absolute emission cross section data with improved accuracy. By this procedure the uncertainties in the use of radiometry standards as well as the possible errors due to imprecisely determined geometrical parameters of the apparatus are avoided.
2. The design and use a simple automatic spectroscopic photon counting detector system to eliminate the molecular continuum contribution in molecular fragment radiation.
3. The determination and analysis of the "escape factor" of light atomic (hydrogen) molecular fragments during the process of measurements, i.e. in evaluation of absolute line emission cross section data.

4. The investigation of the power law dependence of excitation cross sections and the principal quantum number n for the Balmer series which are investigated.

List of Publications of Other Input that Resulted from the Project

1. M. D. Tasic, J. M. Kurepa, "The Influence of High Velocity Excited Dissociated Fragments to their Absolute Emission Cross - Section Determination," Proc. X SPIG, Dubrovnik (1980) 52-54.
2. J.M. Kurepa, M. D. Tasic, "Analysis of Balmer Emission Cross-Sections Data Obtained in Dissociative Electron Excitation of Ammonia," Proc. X SPIG, Dubrovnik (1980) 46-48.
3. J.M. Kurepa, J. M. Marendic, "Optical Investigation of the Dissociative Electron Excitation Processes of High Rydberg and Superexcited States of CH_3Cl Molecules," Proc. V. ESCAMIG, Dubrovnik (1980) 75-76.
4. J. Jovanovic-Kurepa, "Opticko Ispitivanje Elektronskih Ekscitacionih Procesata Atoma i Molekula," Monograph, Savremena Istrazivanja u Fizici, Belgrade (1981) 138-157.
5. M.D. Tasic, J. M. Kurepa, "The Influence of Fast Excited "H" Fragments to Balmer Emission Cross Section in Ammonia," Proc. XII Int. Conf. Phys. Atomic Coll. Ed. Sh. Datz, Gatlinburg, U.S. Vol. I, (1981) 388-390.
6. J.M. Kurepa, J. M. Marendic, "Spectroscopic Investigation of Cl I Line Emission in Controlled Electron Impact," Proc. 9th Inter. Conf. Atom. Spectr. and XXII Colloc. Spectrosc. Internat., Tokyo, Japan (1981).
7. M. D. Tasic, J. Jovanovic-Kurepa, "O Kvantitativnom Merenju Emitovanog Optickog Zracenja iz Disocijativnih Molekularnih Procesata," Stublicke Toplice, Yugoslavia, II Jug. Simp. Fiz. Atom. Sud. Proces. (June 1981).
8. J.M. Marendic, J. Jovanovic-Kurepa, "Ispitivanje Elektronske Disocijativne Ekscitacije CH_3Cl ," Stublick Toplice, II Jug. Simp. Fiz., Atom. Sud. Proces. (June 1981).
9. J. M. Kurepa, J. M. Marendic, "Balmer Lines Emission Cross Sections Determination in Controlled Electron Impact with C_3H_8 and C_3H_6 Molecules," VI ESCAMPIG, Oxford, Book of Abstr. (1982) 57-60.
10. M. D. Tasic, J. M. Kurepa, "Emission Cross Sections from Electron Dissociative Excitation of Some Molecules," VIII ICAP, Gutheborg Book of Abstr. (1982) A101-A103.

11. J.M. Marendic, J. M. Kurepa, "Electron Impact Dissociative Excitation of C₃H₈ and C₃H₆ Molecules," XXI SPIG, Dubrovnik, Book of Extended Abstr. (1982) 87-91.
12. M. D. Tasic, J. M. Kurepa, "Emission Cross Section of Balmer Radiation from Electron Dissociative Excitation of H₂" XXI SPIG, Dubrovnik, Book of Extended Abstr., (1982) 91-93.
13. J. Jovanovic-Kurepa, "O Disocijativnim Procesima SiH Molekula," III Jugoslovenski Simpozium o Fizici Atomskih Sudarnih Procesaa, Donji Milanovac, godine (June 1983).
14. M. D. Tasic, J. M. Kurepa, J. M. Marendic, "Power Law Dependence of Excitation Cross Sections and the Principal Quantum Number in Some Molecules," 15th EGAS, Madrid (July 1983).
15. J. Jovanic-Kurepa, J. M. Marendic, "Investigation of H₂ Rotational Lines Intensity for (d³ a³ g⁺) Transition due to Electron Beam Bombardment," 6th Nat. Conf. Low Temp. Plasma Phys., Leningrad, Vol. I (1983) 51-54.
16. J. M. Marendic, M. D. Tasic, J. M. Kurepa, "Electron Impact Induced Balmer Lines Emission from Some Aliphatic Hydrocarbons." (Accepted for publication in Chem. Phys.)
17. J. M. Kurepa, J. M. Marendic, "Dissociative Excitation of CH₃ Cl by Electron Impact," (Submitted to "Physica")
18. J. M. Kurepa, M. D. Tasic, "Spectroscopic Investigation of Absolute Lines and Bands Emission Cross Sections of Ammonia in Controlled Electron Impact," (In preparation for Chem. Phys.)

Guest Scientist who Visited NBS from Yugoslavia

1. Dr. Jelena Jovanovic-Kurepa, 1981, one-month (JILA)

Visits to Yugoslavia of NBS Participants

1. Dr. Gordon H. Dunn, 1982, one week

Project Title: Theoretical Investigation of Physical Surfaces
(Project Page 319, NBS(G)-256)

Years and Funds: 1980-1984, Dinars 5,140,000

Principal Investigator: Prof. Dr. Marijan Sunjic

Yugoslav Institute: Department of Physics, Faculty of Science,
University of Zagreb

NBS Participant: Dr. J. William Gadzuk

NBS Laboratory, Center, Division: National Measurement Laboratory,
Center for Chemical Physics, Surface Science Division

Summary Description of Achievements to Date

Two of the most important aims in modern surface science research, exemplified by work within the Surface Science Division of NBS and the Department of Physics at the University of Zagreb, are the development of reliable surface characterization methods and the formulation of fundamental models and experiments focused on the microscopic basis of chemical dynamics at solid surfaces. The NBS/Zagreb project on surface theory is directed at both of these goals. The spectroscopic probes of surface excitations necessarily require an understanding of the dynamic response of the electronic, substrate lattice, and adsorbed atom/molecule excited states to an externally imposed perturbation. Over the recent past and for the foreseeable future, we have been using the full theoretical apparatus of modern many-body theory, inelastic scattering theory, and phenomenological modeling to build theories of line shapes, satellite distributions, and absolute intensities observed in valence and core level photoemission and Auger spectroscopy as well as in various vibrational spectroscopies.

Since the basic steps in elementary reactive chemical processes involve the motion of the constituent atoms under the influence of forces provided by possible electronic transitions (potential energy surface hopping) induced by the excess translational, vibrational, or rotational energy of an incident beam of reactants, many fundamental models can be formulated in terms of the same dynamic response functions developed in the spectroscopy research. We plan on continuing to work on time-dependent models which can describe the complex energy redistribution involved in reactive molecular events at both solid vacuum interfaces as well as solid-liquid interfaces of relevance in electrochemistry.

Results and Significance of Achievements to Date

The co-principal investigators have published extensively over the past decade, both jointly and with others, on research in many areas of surface theory, which research has been greatly facilitated by

funding under the PL-480 Program (since 1975), the Joint Board projects (since 1980) and other international assistance. Both the NBS monitor and the principal investigator have worked together at the International Center for Theoretical Physics, Trieste, Italy; Institute of Theoretical Physics at Chalmers University, Goteborg, Sweden as visiting NORDITA Professors; and most recently (July 1984) as group leaders of the 3rd Electrochemistry Study Group held at the Fritz Haber Institute, Berlin, West Germany. The results of this work will be reported in the Journal of Electro-analytical Chemistry. In addition to providing combined papers, they have coordinated international workshops on the topics of theoretical investigation of physical surfaces; such as, core level spectroscopy, chemisorption, and dynamics of surfaces. Much of the theoretical work carried out at each institution has symbiotically benefitted the regular contact between the investigators. A continuous and prolific sequence of papers on various aspects of surface spectroscopy and dynamics stands as the best testimony to the success of the project.

List of Most Current Publications (in press) Related to Project Goals

Prof. Dr. Marijan Sunjic and coworkers:

1. "Incoherent Low-Energy Atom Scattering from Adsorbates at Low Coverages."
2. "Surface Electronic Excitations in the Random Phase Approximation and Infinite Barrier Model: Surface Plasmons, Electron-hole Pairs and the Interaction with External Particles."
3. "Effects of Plasmon Dispersion and Damping on Strengths and Shapes of Plasmon Satellites in XPS Spectra of Metals."
4. "Dynamical Screening and Surface Excitation in the Planar, Spherical, and Cylindrical Solids."

Dr. J. William Gadzuk and coworkers:

1. "Resonance Vibrational Excitation in Electron Energy Loss Spectroscopy of Adsorbed Molecules."
2. "Excitation Mechanisms in Vibrational Spectroscopy of Molecules on Surfaces."
3. "Dynamics of Molecular Processes at Surfaces."
4. "Energy Redistribution and Dissociation in Molecule-Surface Collisions Involving Charge Transfer/Surface Hopping."

Project Title: Absolute Sputtering Yields for the Analysis of Surfaces

(Project Page 320, NBS(G)-257)

Years and Funds: 1980-1984, Dinars 4,930,000

Principal Investigator: Dr. Boris Navinsek

Yugoslav Institute: Jozef Stefan Institute

NBS Participant: Dr. Joseph Fine

NBS Laboratory, Center, Division: National Measurement Laboratory,
Center for Chemical Physics, Surface Science Division

Summary Description of Project Goals

- To determine absolute sputtering yields of well-characterized materials of high purity.
- To develop improved absolute sputtering yield measurement methods capable of higher accuracy and greater sensitivity than is now available.
- To characterize sputter depth profile processes at interfaces and their relation to preferential sputtering, surface topography change and diffusion.
- To develop well characterized Standard Reference Materials (SRM's) appropriate for calibrating sputter erosion rates, sputter-depth-profile composition, and interface width as a function of sputtered depth.

The growing application of surface analysis and sputter depth profiling techniques to many diverse problems associated with failure analysis, device development, and quality control has created a need for standards to ensure measurement reliability. The results of this collaborative project in both SRM development and sputtering yield data determination represent, at this time, a unique accomplishment in the area of standards for surface analysis. These standards will allow for improved depth profile measurements of importance to both Yugoslav and U.S. industries which include semiconductor, computer, electronics, thin film, coatings, metals, chemical, and automobile manufactures, amongst others.

Results and Significance of Achievements to Date

1. SRM Development

Three different designs of thin-film structures for sputter depth profile calibration in surface analysis are being developed. Prototype SRMs

were fabricated at the Jozef Stefan Institute for evaluation and characterization: a single layer of Ta₂O₅ on Si, Ni/Cr/Ni/Cr... and Ni/Ag/Ni/Ag... periodically modulated multilayered thin films, and a Cr/Cr₂O₃/Cr/Cr₂O₃... marker type multilayered structure. Development is now completed on the Ni/Cr materials and their characteristics have been shown to be outstanding for depth profile calibration: sharp well-defined interfaces, structural uniformity better than 3%, absolute film thickness accuracy better than 2%, and high structural stability.

Production quantities of the Ni/Cr material have been produced and characterized using N(E) Auger spectroscopy, Rutherford backscattering spectroscopy, secondary-ion mass spectroscopy, and neutron activation analysis. They will shortly be issued by the NBS-OSRM as SRM 2135 and we anticipate that this very precise material will find wide-spread use amongst the surface analysis community.

2. Absolute Sputtering Yields

A quartz crystal oscillator microbalance system has been built at the Jozeph Stefan Institute for the determination of absolute sputtering yields using the mass-loss method. This microbalance system is coupled to a mass-analyzed argon ion beam accelerator (4 to 12 keV) and is operational under UHV conditions.

Sputtering yields have been determined for thin films of Ni, Ag, and Au and ion dose dependence of the yield monitored. Yields have also been obtained on multilayered Ni/Ag, Ni/Au, and Ni/Cr structures similar to those produced for SRM use. These measurements demonstrate that accurate, reproducible yield data can be obtained with this microbalance method.

Methods have also been developed which use microbalance mass-loss techniques to monitor sputtered thin-film interface widths. Such measurements of Ni/Cr interfaces allow not only for accurate width determinations to be made but also can be used to characterize processes which contribute to width broadening.

List of Publications or Other Input that Resulted from the Project

1. A. Zabkar, P. Panjan, B. Navinsek, "Sputtering Yield Measurement of Nickel Using a Quartz Oscillator Microbalance," Proceedings of Contributed Papers of the Tenth Symposium on the Physics of Ionized Gases, edited by B. Cobic, Boris Kidric Institute, Belgrade (1980) 132.
2. J. Fine, "Absolute Sputtering Yield Measurement Methods - A Review," Proceedings of Invited Lectures of the Tenth Symposium on the Physics of Ionized Gases, edited by M. Matic, Boris Kidric Institute, Belgrade (1981) 379-420.

3. B. Navinsek, P. Panjan, M. Peternel, A. Zabkar, "Comparative Erosion Yields, Topographical Changes and Depth Profile Analysis of Ion Eroded Nickel Based Alloys," Nucl. Instr. Methods (1981).
4. J. Fine, B. Navinsek, F. Davarya, T. D. Andreadis, "Sputter Depth Profiles of Ni/Cr Thin-Film Structures Obtained from the Emission of Auger Electrons and X-Rays," J. Vac. Sci. Technol. 20 (3) (1982) 449.
5. B. Navinsek, P. Panjan, A. Zabkar, "Sputtering Yields of Nickel and Iconels," Proceedings of Contributed Papers, Eleventh Symposium on the Physics of Ionized Gases, ed. by G. Pichler, Institute of Physics, University of Zagreb, (1982) 163
6. B. Navinsek, P. Panjan, Z. Zabkar, J. Fine, "Depth Profiles of Ni/Ag Multilayer Structures using a Mass Analyzed Ion Beam," Proceedings of Contributed Papers, Symposium on the Physics of Ionized Gases, ed. by G. Pichler, Institute of Physics, University of Zagreb (1982) 187.
7. J. Fine, T. D. Andreadis, F. Davarya, "Measurement of Time-Dependent Sputter-Induced Silver Segregation at the Surface of a Ni-Ag Ion Beam Mixed Solid," Nucl. Instrum. Methods 209/210 (1982) 187.
8. F. Davarya, M. L. Roush, J. Fine, T. D. Andreadis, O.F. Goktepe, "Ni/Cr Interface Width Dependence on Sputtered Depth," J. Vac. Sci. Technol. A1(2) (1983) 467.
9. J. Fine, T. D. Andreadis, F. Davarya, "Summary Abstract: Kinetics of Sputter-Enhanced Surface Segregation at a Ni/Ag Interface," J. Vac. Sci. Technol. A1(2) (1983) 507.
10. J. Fine, B. Navinsek, "Thin Film Reference Materials for Sputter Depth Profile Calibration," Proceedings of Invited Lectures and Progress Reports, Eleventh Symposium on the Physics of Ionized Gases, ed. by G. Pichler, Institute of Physics, University of Zagreb, (1983) 223.
11. D.G. Simons, M.D. Brown, J. Fine, T.D. Andreadis, B. Navinsek, "Rutherford Backscattering Analysis of Multilayered Cr-Ni Structures to be used for Sputtering Standards," Nucl. Instr. Meth. 218 (1983) 585.
12. A. Zalar, B. Navinsek, "AES Depth Profile Analysis of Multilayer Cr/Ni Thin-Film Structures Deposited on Si Substrates of Two Different Roughness Degrees," Proceedings of Ninth Intl. Vacuum Congress and Fifth Intl. Conference on Solid Surfaces, Extended Abstracts, Madrid (1983) TF.P.25.A.

13. B. Navinsek, P. Panjan, A. Zabkar, J. Fine, "Depth Profiling of Low Energy Mass Analyzed Ion Beam and Quartz Crystal Oscillator Microbalance," Proceedings of Ninth Intl. Vacuum Congress and Fifth Intl. Conference on Solid Surfaces, Extended Abstracts, (1983) TF.P.41.A.
14. B. Navinsek, P. Panjan, A. Zabkar, J. Fine, "Determination of Sputtering Yields from a New Procedure for Depth Profiling of Multilayered Structures," Proceedings of Tenth Intl. Conference on Atomic Collisions in Solids (July 1983), Bielefeld, Germany, Nucl. Instr. Methods (1984) in press.
15. B. Navinsek, P. Panjan, A. Zabkar, "Interface Width Resolution of Ni/Cr Thin Films as Determined by Quartz Microbalance Techniques," Proceedings of Contributed Papers, 12th Symposium on the Physics of Ionized Gases (Sebinek, Yugoslavia, 1984) in press.

Guest Scientist who Visited NBS from Yugoslavia

1. Dr. Boris Navinsek, 1980, 1 week
2. Dr. Boris Navinsek, 1982, 1 week

Visits to Yugoslavia of NBS Participant

1. Dr. Joseph Fine, 1979, 3 days
2. Dr. Joseph Fine, 1980 (August) 1 week to attend 10th SPIG Conference (September) visit Institute
3. Dr. Joseph Fine, 1982, 1 week visit to attend 11th SPIF Conference and 2 weeks to visit Institute
4. Dr. Joseph Fine, 1984, 1 week

Project Title: Application of Plasma Line Broadening as a
Non-interfering Plasma Probe
(Project Page 321, NBS(G)-258)

Years and Funds: 1980-1984, Dinars 2,444,000

Principal Investigator: Dr. N. Konjevic

Yugoslav Institute: Institute of Physics, University of Belgrade

NBS Participant: Dr. Wolfgang L. Wiese

NBS Laboratory, Center, Division: National Measurement Laboratory,
Center for Radiation Research, Atomic and Plasma Radiation Division

Summary Description of Project Goals

To study the application of Stark broadening of spectral lines of neutral and ionized atomic lines as a non-interfering probe of plasma diagnostics and evaluate its usefulness and reliability over a large range of density and temperature.

To establish laws governing interrelations between Stark-broadened spectral lines of a single element and those of a group of elements.

To obtain data on the Stark constants of spectral lines for which no data are available so far.

Results and Significance of Achievements to Date

In accordance with the project goals, work was concentrated on the following tasks:

1. Critical evaluation of existing experimental Stark-broadening data for non-hydrogenic atoms and ions.
2. Theoretical calculations of Stark linewidths for ions and for neutral atoms for which theoretical results do not exist.
3. Examination of regularities and systematic trends of Stark widths of neutrals and ions as a function of atomic structure.
4. Experimental study of Stark broadening of prominent lines of singly and doubly ionized atoms.

As a result of the work on the critical evaluation of existing experimental data, two critical reviews ⁵⁻⁶ with tabulations of selected data for atomic and ionic lines for the period 1976-1982 have been completed and are now in press (see list of publications). These two reviews represent an extension of two preceding ones covering the period through 1976, which have been favorably accepted by the scientific community.

Previous comparisons of the selected experimental data for the Stark linewidths of isolated non-hydrogenic atomic lines with semiclassical results for helium through calcium and for cesium showed fairly good average agreement--typically within $\pm 20\%$. In order to test this theory for elements heavier than Ca, semiclassical calculations were performed for all lines for which experimental results existed. The comparison of our theoretical data with experiment showed large discrepancies previously undetected for lighter elements. Critical evaluation of experimental data indicated that in most cases the experiment must be blamed for this discrepancy.

For the evaluation of Stark widths and shifts of non-hydrogenic spectral lines of ionized atoms, various theoretical approaches have been used. Comprehensive semiclassical calculations of Stark-broadening parameters of spectral lines emitted by singly ionized atoms agreed well (within $\pm 20\%$) with the experiments. Improved agreement between the experiment and fully quantum mechanical calculations was observed in the case of alkaline-earth ions.

Both semiclassical and fully quantum mechanical methods can be used for the evaluation of widths of isolated lines of multiply charged ions. However, both approaches involve considerable labor, especially the quantum mechanical calculations. Furthermore, in some cases the lack of atomic energy-level data seriously limits the applications of sophisticated theoretical approaches.

Within this project, two approximate semiempirical methods were proposed for the calculation of electron-impact linewidths of multiply ionized atoms. Comparison with the experiments showed an average agreement of $\pm 30\%$.

The Stark-broadening theory and many experiments have proved the systematic dependence of Stark widths on plasma parameters. Until recently, however, it has not been clear as to which regularities in the broadening of spectral lines as a function of atomic structure are to be expected. Within this project, general foundations for these studies have been established for the first time, and numerous atomic structure-related similarities and regularities have been detected. Discovery and establishment of the systematic trends of Stark widths of spectral lines in plasmas have a considerable practical importance, because, on the basis of these trends, it is possible to predict widths of spectral lines of atoms and ions for which no experimental data are available. These data are important for the diagnosis of both high- and low-temperature plasmas.

Finally, in order to extend the investigations of regularities and similarities in spectral line widths and in order to obtain new, experimental Stark broadening data, two experiments were carried out; one at atmospheric pressure using a wall-stabilized continuous arc, and another with a pulsed Z-pinch discharge. The results of these experiments will be presented for the first time at the 7th International Line Shape Conference in Aussois, France.

List of Publications or Other Input that Resulted from the Project

1. M.S. Dimitrijevic, N. Konjevic, "Stark Widths of Doubly and Triply Ionized Atom Lines," J. Quant. Spectrosc. Radiat. Transfer 29 (1980) 451.
2. M.S. Dimitrijevic, N. Konjevic, "Semiempirical Stark Linewidths of Alkali Like Ions," Astron. Astrophys. 102 (1981) 73.
3. W. L. Wiese, N. Konjevic, "Regularities and Similarities in Plasma-broadened Spectral Line Widths (Stark Widths)," J. Quant. Spectrosc. Radiat. Transfer 28 (1982) 185.
4. M.S. Dimitrijevic, N. Konjevic, "Stark Broadening of Isolated Lines of Heavy Elements," J. Quant. Spectrosc. Radiat. Transfer 30 (1983) 95.
5. N. Konjevic, M.S. Dimitrijevic, W. L. Wiese, "Experimental Stark Widths and Shifts for Spectral Lines of Neutral Atoms (a critical review of selected data for the period 1976 to 1982)," J. Phys. Chem. Ref. Data, in press.
6. N. Konjevic, M.S. Dimitrijevic, W. L. Wiese, "Experimental Stark Widths and Shifts for Spectral Lines of Positive Ions (a critical review and tabulations of Selected Data for the Period 1976 to 1982)," J. Phys. Chem. Ref. Data, in press.

Guest Scientist who Visited NBS from Yugoslavia

1. Dr. Nikola Konjevic, 1982, 2 weeks
2. Dr. Nikola Konjevic, 1983, 10 weeks
3. Dr. Nikola Konjevic, 1984, 6 weeks

Visits to Yugoslavia of NBS Participants

1. Dr. Wolfgang L. Wiese, 1981, 1 week, Institute of Applied Physics, Belgrade
2. Dr. Wolfgang L. Wiese, 1982, 1 week, XI Symposium on the Physics of Ionized Gases in Dubrovnik, and 1 week, Institute of Applied Physics, Belgrade
4. Dr. Daniel Kelleher, 1981, 1 week, Institute of Applied Physics, Belgrade
5. Dr. Timothy Pittman, 1984, 2 weeks, Institute of Physics, Belgrade

Project Title: X-ray Diffraction, Electron-Microscopic Studies and the Investigation of Transport, Galvanometric and Magnetic Properties of Alloys Obtained by Rapid Quenching From the Melt
(Project Page 322, NBS(G)-259)

Years and Funds: 1980-1984, Dinars 5,655,000

Principal Investigator: Dr. A. Bonefacic

Yugoslav Institute: Institute of Physics, University of Zagreb

NBS Participant: Dr. M. B. Kasen

NBS Laboratory, Center, Division: Center for Materials Science, Fracture and Deformation Division

Summary Description of Project Goals

The overall project goal is to contribute to the fundamental understanding of the mechanical and electronic properties of metastable alloys produced by rapid quenching. The program addresses the following areas:

- Examination of the structural properties of supersaturated solid solutions directly after quenching and of the kinetics of decomposition of these solutions;
- Comparison of the structural and mechanical properties of alloys quenched from the liquid state with those of alloys quenched from the solid; and
- Electronic properties of metastable alloys.

Materials to be studied are aluminum-based supersaturated solid solutions and certain other systems such as Ag-Sn and Ag-In that may be included for investigation of differences in stacking fault formation in liquid and conventionally quenched alloys. Metastable alloys include amorphous alloys (metallic glasses) consisting of transition metals with some metalloids (TM-C) and transition alloys containing only metals (TM-M).

Techniques include x-ray diffraction, electron microscopy, hardness, electrical resistivity, magnetoresistivity, and magnetic susceptibility.

Results and Significance of Achievements to Date

The first case of terminal solid solubility being reduced by rapid quenching has been noted in the Ag-In system. It is attributed to the high concentration of defects introduced by quenching which serve

as nuclei for the fcc-hcp transformation. Stacking fault energy minima are shifted to lower electron concentrations with respect to the minima corresponding to equilibrium. The earlier hcp phase appearance is modeled as a consequence of enhanced interaction of the Fermi surface and contracted Brillouin zones due to quenched-in vacancies.

It has been found that the residual electrical resistivity of metastable transition metals with metalloids (TM-C, e.g. $\text{Fe}_x\text{Co}_{73-x}\text{B}_{12}\text{Si}_{10}$, etc.) always increases with x and that the resistivity curvature of ferromagnetic alloys is positive up to the Curie temperature. This indicates the magnetic contribution to the resistivity and suggests that magnetism plays a dominant role in resistivity variation. It is found that the magnetization of these alloys can be well fitted to a formula including both the spin waves and the Stoner excitations in a strong itinerant ferromagnet. This leads to an explanation of the difference between the spin wave stiffness constants as determined by magnetization measurements and from neutron diffraction, providing a better insight into the electronic structure of amorphous ferromagnets.

A comparison of observed resistivity values for nonmagnetic TM-M glasses (e.g. $\text{Zr}_{100-x}\text{Cu}_x$) with those calculations on the basis of an extended Ziman's model for liquid alloys using the experimental structure factor shows that the Ziman model is not suitable for such alloys. Results indicate that the electronic density of states at the Fermi level is dominated by the Zr d-electrons.

The proposed studies will make a significant contribution to the scientific principles underlying the emerging technology that is capitalizing on the unique properties attainable in metastable alloys. The work is therefore in the forefront of current materials research. Of special interest is the significant contribution this work will make to ongoing programs at NBS and in Yugoslavia on rapidly cooled metals and alloys.

List of Publications or Other Input that Resulted from the Project

1. V. Franetovic, D. Kunstelj, A. Bonefacic, "The Investigation of Metastable hcp Phase in the Ag-rich fcc Region of Ag-In Alloys Rapidly Quenched From the Melt," J. Mat. Sci. 17 (1982) 2771.
2. A. M. Tonejc, A. Tonejc, D. Kunstelj, "Electron Microscopic Determination of Structural Defects in Liquid-quenched Ag-Sn Alloys and their Dependence on Internal Residual Stresses," (to be published).
3. B. Leontic, J. Lukatela, M. Stubicar, "Investigation of Microhardness of Some Hydrogen Doped Zr-Ni Metallic Glasses," (accepted for publication, Journ. of Noncrystalline Solids).
4. E. Babic, M. Ocko, Z. Varohnic, H.A. Davies, I.W. Donald, "Electrical Resistivity of Amorphous $\text{Fe}_x\text{Co}_{78-x}\text{B}_{12}\text{Si}_{10}$ and $\text{Co}_x\text{Ni}_{78-x}\text{B}_{12}\text{Si}_{10}$ Alloys," Proceedings 4th Int. Conf. on Rapidly Quenched Metals (T. Masumoto and K. Suzuki, eds.) Japan: Institute of Metals, Sendai V. 1 (1982) 857.

5. E. Babic, Z. Marohnic, E. P. Wohlfarth, "Stoner Excitation in the Strong Itinerant Amorphous Ferromagnets $\text{Fe}_x\text{Ni}_8\text{O}_{-x}\text{B}_{18}\text{Si}_{12}$ and $\text{Fe}_{80}\text{B}_{20}$," (to be published).

Guest Scientists who Visited NBS from Yugoslavia

1. Dr. A. Bonefacic, 1979
2. Dr. B. Leontic, 1984

Visits to Yugoslavia of NBS Participants

1. Dr. M. Kasen, 1978
2. Dr. R. Reed, 1978
3. Dr. M. Kasen, 1984
4. Dr. R. Reed, 1984

Project Title: Measurement of the Differential Cross Sections for
Elastic and Inelastic Scattering of Electrons by
Metal Atoms
(Project Page 323, NBS(G)-260)

Years and Funds: 1980-1984, Dinars 3,300,000

Principal Investigator: Dr. Leposava Vuskovic

Yugoslav Institute: Institute of Physics, Belgrade University

NBS Participant: Dr. R. Celotta

NBS Laboratory, Center, Division: National Measurement Laboratory,
Center for Radiation Research, Radiation Physics Division

Summary Description of Project Goals

We planned to study the process of electron scattering by metal atoms. This remains the main goal of the experiments.

From these studies it became clear that for the differential cross section measurement for electrons scattered by atoms and molecules, a primary standard is needed, which would be proposed to all laboratories in the world as a basis for calibration of experimental devices in order to determine cross sections for scattering of electrons by atomic species. Five years ago this work was started at the Jet Propulsion Laboratory, U.S. and Dr. Vuskovic was a participant with the research team. In order to complete the standard for differential cross sections some additional measurements are needed, and they have been started under this project. This work is extremely important and the experiments must be done with the greatest care. This, however, required postponing slightly the other experiments planned with the apparatus.

For the measurements of electron scattering by metal atoms all preparations are completed including the construction of a special oven for the production of metal atom beams, so that the relevant measurements can be initiated as soon as the work with gaseous species is finished.

The measurement of electron-atom and electron-molecule collision cross sections is fundamental not only to furthering our understanding of the basic forces governing electron interactions but also provides us with much needed data in a variety of diverse fields. Cross sections are required to model and improve such processes as laser discharges, high voltage electrical switching gear, and fusion reactors. The focus of this project on electrons scattered from metal atoms is directed towards improving our knowledge of electrons scattered from solids. Very little information on electron-metal scattering is currently available

while many of the present needs in surface science depend on accurate cross sections for these species. Such information would be very beneficial in improving analytical techniques that could be used to further develop advanced electronics and other microscopic or surface-sensitive devices.

Results and Significance of Achievements to Date

The electron spectrometer has been assembled and tested to a residual magnetic field (less than 1mG) and vacuum ($1-2 \times 10^{-7}$ torr). A spherical monochromator and analyzer with cylindrical lenses are used. The insulators are made of Macor. Local heaters have been put on the spheres. Adequate voltage supplies for the monochromator and analyzer have been built. All power supplies are home-made except for the impact energy supply. A Faraday cup has been added for primary beam monitoring. The primary beam is produced readily in the range of 10 to 100 eV. Its current in the Faraday cup is of the order of 10^{-8} A. The second half has been tested by using inelastic features in nitrogen. The energy resolution is of the order of 50 meV. A channel electron multiplier is used as a detector for electrons. The electron multiplier pulses are amplified and stored by a multichannel analyzer. Distributions of electrons -30° to $+150^\circ$ can be measured.

The investigations were done on electron collisions with atomic particles which are in gaseous phase. The experiments on argon and xenon have the goal of obtaining absolute differential cross sections for elastic and inelastic electron scattering in the energy range 10 to 100 eV. Angular distributions for different processes were measured. Calibrations are in process to transfer data into an absolute scale.

Scattering from the H_2S and N_2O molecules was also measured. Our interest was to determine the absolute cross section of elastically scattered electrons, as well as to investigate electronically excited states of these molecules. All results obtained were compared with the results of other authors.

An oven for metal vapor production is built as well as the power supplies needed. Therefore, the system is ready for the investigation of alkali and alkali earth metals. At this moment, metals with a high melting point can not be the subject of investigation.

List of Publications or Other Input that Resulted from the Project

1. L. Vuskovic, D. Filipovic, V. Pejcev, "Electron Impact Excitation of Hydrogen Sulphide," VIIIth International Conference on Atomic Physics, Goteborg, Sweden (1982).
2. B. Marinkovic, D. Filipovic, V. Pejcev, L. Vuskovic, "Inelastic Electron Scattering by H_2S ," XI Yugoslav Summer School and International Symposium on the Physics of Ionized Gases, Dubrovnik, (1982).

3. D. Filipovic, V. Pejcev, B. Marinkovic, L. Vuskovic, "Angular Distribution of Electrons Scattered by Argon Atom," XI Yugoslav Summer School and International Symposium on the Physics of Ionized Gases, Dubrovnik.
4. D. Filipovic, V. Pejcev, L. Vuskovic, "Angular Distribution of Intermediate Energy Electrons Scattered by Xenon," XI Yugoslav Summer School and International Symposium on the Physics of Ionized Gases, Dubrovnik (1982).
5. B. Marinkovic, V. Pejcev, D. Filipovic, L. Vuskovic, "Differential Cross Sections for Elastic and Inelastic Scattering of Electrons by Xenon in the Energy Range of 15 to 80 eV," XIIIth International Conference on the Physics of Electronics and Atomic Collisions, Berlin (1983).
6. C. Smitkovski, D. Filipovic, M. Marinkovic, V. Pejcev, L. Vuskovic, "Differential Cross Sections for Elastic and Inelastic Scattering of Electrons by N_2O in the Range of 10 to 80 eV," (Submitted to J. Phys. B.)²
7. D. Filipovic, V. Pejcev, B. Marinkovic, L. Vuskovic, "Differential Cross Sections for Inelastic Scattering of Intermediate Energy Electrons by Argon Atoms," XII Yugoslav Summer School and International Symposium on the Physics of Ionized Gases, Sibenik, Yugoslavia (1984).
8. D. Filipovic, B. Marinkovic, V. Pejcev, L. Vuskovic, "Differential Cross Sections for Inelastic Scattering of Intermediate Energy Electrons by Xenon Atoms," XIII Yugoslav Summer School and International Symposium on the Physics of Ionized Gases, Sibenik, Yugoslavia (1984).
9. D. Filipovic, B. Marinkovic, V. Pejcev, L. Vuskovic, "Integral Cross Sections for Elastic and Inelastic Scattering of Electrons by Argon and Xenon Atoms," XII Yugoslav Summer School and International Symposium on the Physics of Ionized Gases, Sibenik, Yugoslavia (1984).
10. L. Vuskovic, Cz. Szmytowski, D. Filipovic, B. Marinkovic, "Differential Cross Sections for Elastic and Inelastic Scattering of Electrons by N_2O in the Range of 10 to 80 eV," (Submitted to J. Phys. B.).

Guest Scientist who Visited NBS from Yugoslavia

1. Dr. L. Vuskovic, 1981, 2 days

Visits to Yugoslavia of NBS Participants

1. Dr. R. Celotta, 1980, 3 days
2. Dr. R. Celotta, 1982, 7 days
3. Dr. Michael Kelly, 1984, 10 days

Project Title: Environmental Measurements - Electrochemical
Determination of Trace Elements and Surface
Active Substances
(Project Page 324, NBS(G)-261)

Years and Funds: 1980-1984, Dinars 3,784,000

Principal Investigator/s: Dr. Marko Branica and Dr. Bozena Cosovic

Yugoslav Institute: Rudjer Boskovic Center for Marine Research

NBS Participant: Dr. John K. Taylor

NBS Laboratory, Center, Division: National Measurement Laboratory,
Center for Analytical Chemistry

Summary Description of Project Goals

Electrochemical methods due to their simplicity and sensitivity, are especially convenient for the direct determination of trace metals in natural waters (rivers, lakes, seas) and industrial waste waters.

Various species of trace metals in samples of natural water adsorb on the walls of containers, thus changing the sample composition. The extent of adsorption on the walls and contamination from them depends on both chemical composition of the sample and chemical properties and the quality of the container.

Organic matter dissolved in natural and polluted waters comprises a complex mixture of various types of natural and compounds. A part of the organic compounds is surface-active and thus adsorbed and accumulated at interfaces (boundaries with atmosphere, sediment and dispersed particulate material and biota). Surfactants, both natural and pollutants, modify the structure of interboundary layers and effect the processes of mass and energy transfer through them, thus influencing biogeochemical cycles of natural micro and macro components and pollutants.

There are two fundamental approaches to the study of the organic content and composition of natural waters. Either analyses may be made of some feature related to the gross organic content or, alternatively, measurements may be made of a specific compound or class of compounds.

The main problems in the analysis of organic compounds in natural waters are their low concentration, the variety of types of substances, the lack of direct analytical techniques of sufficient sensitivity, and the changes which the components undergo during pretreatment.

Electroanalytical methods for the analysis of surface active substances in aquatic systems are based on the measurement of adsorption phenomena of organic molecules at the electrode/water interface. Adsorbed molecules change the charge and mass transfer processes at the electrode. The adsorption depends on the electrode potential and the nature of absorbable substances.

The aim of the work described here is to investigate and to find out the advantages, possibilities and limitations of direct electrochemical determination of some trace elements and surface active substances in:

- samples of natural and polluted waters (seawater, lake and river waters)
- effluents
- biodegradation test of detergents and speciation of trace metals

The electrochemical techniques used are: d.c. polarography, a.c. polarography and tensammetry, voltammetry with discontinuously changing potential (Kalousek commutator technique), differential pulse polarography, and anodic stripping voltammetry.

Special attention is paid to sampling procedures, storage and handling of samples and their treatment.

The work undertaken in this project closely parallels research efforts at NBS in inorganic and organic electrochemical analysis. The research outputs are thus not only of considerable interest to NBS, but have wide scientific interest and are contributing to a better understanding of the marine environment, with respect to both natural and polluted waters.

Results and Significance of Achievements to Date

The report describes research realized within the project during the period from December 1980 to May 1984. The results obtained have been published in a number of papers and theses listed and referred to under the list of publications.

Since the physico-chemical forms in which a certain metal ion occurs in the aquatic system and the possible interactions with organic matter significantly influence its biogeochemical pathways and cycles, efforts have been directed to a large extent to the development of methods suitable to the study of these processes at very low concentrations of both metal ions and organic ligands.

(1) Trace Elements

A new modified anodic stripping voltammetry method for the determination of the ionic form of trace metal ions, reported in our previous papers, has been evaluated experimentally and theoretically by the hanging mercury drop electrode and rotating disk electrode for lead and perchlorate medium (1,2).

A new experimental technique using differential pulse anodic stripping voltammetry with a thin film mercury electrode and efficient mixing of the electrolyte has been developed for the determination of the apparent copper complexing capacity of seawater (3).

The effect of some factors such as type of electrode and cell, pH of the solution, potential of deposition, time of equilibrium, and influence of a nonionic surface active agents on the measurement were examined in detail. The procedure proposed is an attempt to obtain results which are free from experimental artifacts because the electrode kinetics and adsorption phenomena are excluded.

The high sensitivity of the electrochemical determination of trace metals, which is very important for their speciation at the concentration levels actually present in seawater, can be achieved by a prior deposition of trace metals at the electrode surface followed by their anodic dissolution (ASV). However, this procedure is limited to the determination of reversibly or quasireversibly reducible species that have both cathodic and anodic polarographic waves in a suitable range of potentials. The speciation of irreversibly reducible cobalt (II) in seawater was realized by d.c. polarography and precipitation methods in a higher concentration range of the metal (10^{-4} mol dm⁻³) (5). The distribution of dissolved inorganic cobalt species in seawater was evaluated: free cobalt ion (hydrated) is the predominant species (about 45%), CoCl^+ and CoSO_4^0 are found in approximately equal amounts (about 22%), while the fractions of CoOH^+ , Co(OH)_2^0 and CoCO_3^0 are between 1% and 5%.

Polarographic and voltammetric methods have been used for characterization of uranium(VI) species in seawater (18). The world oceans contain considerable amounts of dissolved uranium and due to growing energy requirements, seawater is becoming an interesting potential source of this element. An understanding of the ionic species of uranium in seawater is essential for an evaluation of possible methods for its recovery from the ocean.

We have tried to experimentally identify the predominant uranium species under varying pH conditions, using sensitive polarographic and spectrophotometric methods.

Our results show that below pH 4, the hydrated uranyl ion is present in the "free" state (forming "labile" complexes). The monocarbonate complex is being formed in the pH region 4 - 4.5, between 4.5 and 5.3

the bicarbonate uranyl complex forms. Above pH 8, uranium is predominantly present as the tricarbonato and in a smaller degree as the trihydroxide complex.

Differential pulse anodic stripping voltammetry was applied for the determination of cadmium, lead, copper, and zinc in mineralized samples biomasses *Trichosporon fermentans*, *Saccharomyces cerevisiae* and of the alga *Scenedesmus obliquus*. The results obtained indicated high content of heavy metals in the investigated matrices (8).

A new type of vibrating dropping mercury electrode (VDME) with short drop-life time up to 200 drops per second was developed, which is more convenient and reliable than other kinds of electrodes for kinetic measurements and for analysis of samples which are highly polluted by organics (11). The electrode was tested on the $Cd^{2+}/CdNTA$ system in citrate buffer solution at pH=6, as a model for the effects of preceding homogeneous chemical reaction on the reversible charge transfer of free metal ions, as well as on the influence of Triton-X-100 on the Cd^{2+} polarographic wave as a good example of the surfactant interference with the metal ion charge transfer.

Attention has also been paid to development of the theory of electroanalytical techniques, especially pulse polarographic techniques (21). The common equation for differential pulse polarography of a simple redox couple on stationary, planar electrodes has been developed and used for the investigation of the influence of the ratio of pulse duration on density of current responses of reversible and irreversible redox reactions. Several differential pulse techniques have been compared and the dependence of their differences on the degree of reversibility of redox reactions has been analyzed. A new theoretical method for calculating normal and differential pulse polarograms which are under the influence of the adsorption of some electroactive species has been developed. The influence of the adsorption of the reactant, the product, or the intermediate of the reversible redox reaction on pulse and differential normal pulse polarographic waves has been analyzed. The results were compared with literature data.

The mechanisms of selenium(IV) electrochemical reduction in anodic solutions on dropping mercury and hanging mercury drop electrodes with d.c., a.c., pulse and differential pulse polarography as well as by voltammetry and potentiostatic electrolysis were studied (14).

(ii) Surface Active Substances

Surfactants, both natural and pollutants, modify the structure of inter boundary layers and affect the process of mass and energy transfer through them, thus influencing biogeochemical cycles or natural micro and macro components and pollutants. The application of electroanalytical methods to the analysis of surface active substances in aquatic systems, based on measurements of adsorption phenomena of organic molecules at the electrode/water interface, has many advantages,

because these methods are simple and sensitive enough for direct determination of trace amounts of surfactants. The fact that organic matter in natural and polluted water is comprised of a complex mixture of different naturally occurring substances and pollutants represents a special problem in the analytical determination of surfactants.

Adsorption of surface-active substances and their mixtures at the mercury electrode has been studied in more detail on the basis of the capacity current measurements by two polarographic techniques: the Kalousek commutator technique, and tensammetry (6,22). Model surfactants used in this work were synthetic and biogenic compounds representative of the composition of natural and polluted aquatic systems. Investigations were performed in a wide concentration range of surfactants. The study in the region of trace amounts, which is of great importance for understanding of adsorption processes in natural systems, was performed by the accumulation of surface-active substances at the hanging mercury drop electrode at the potential of maximum adsorption, -0.6 V vs. SCE, which is approximately the potential of the electrocapillary maximum. Special attention was paid to the influence of association and miscellaneous processes of surfactants in the bulk solution and at the interfaces on the adsorption effects at the electrode.

An electrochemical method based on measurement of the capacity current at the hanging mercury drop electrode by alternating-current polarography was developed and applied to the analysis of surface active substances in seawater and in the sea-surface microlayer samples. Surfactant activities of natural samples collected in the Adriatic Sea in 1978-1980 were compared with different model surfactants (Triton-X-100, albumin, fatty acids, humic acid, polysaccharide) and with parallel measurements by the polarographic maximum method. The advantages of comparative measurements by different methods of specific sensitiveness to different types of organic substances in natural and polluted waters were discussed (3,7,19).

A simple and fast numerical method for the simulation of linear scan voltammetric responses of the homogeneous catalytical reaction at the electroactive-monolayer-film rotating disc covered by an electrode has been developed (10). The linear relationship between the voltammetric peak current and the concentration of dissolved reactant ions has been predicted. The proportionality factor of this relationship is very similar to the one predicted for steady-state conditions. The voltammetric peak current, is also linearly proportional to the square root of scan rate and rotation rate of the disc electrode, but no cumulative relationship on these parameters is predicted.

Electrochemical determination was also applied to the biodegradation study of nonionic surfactants (9). The proposed method is simple, rapid, and applicable to direct determination of the loss of surfactant activity in biodegradation. Unlike many other methods, the electrochemical method is applicable to the determination of different types of non-ionic surfactants regardless of the number of ethylene

oxide groups including polyethylene glycols and biodegradation products of tert-octyl-phenol ethoxylates with a low degree of ethoxylation. The degree of biodegradation of nonionic surfactants obtained by the electrochemical method is lower than by the spectrophotometric Wickbold method because the latter method does not determine some active intermediates of biodegradation.

Electrochemical methods have been used in the study of the adsorption behaviour of different biogenic organic substances, constituents of biological membranes (12,15). Our investigations were concerned with the adsorption processes of different mixtures of lecithin and albumin at the mercury electrode and the influence of the adsorbed layer on the mass and charge transfer processes of cadmium, as a typical toxic pollutant. It was found that the adsorbed layers of different mixtures of albumin and lecithin are permeable to the transport of cadmium ions, while the degree of permeability depends on the ratio between the lipid and protein components in the mixture. A considerable effect of the presence of detergents was observed upon the structure and permeability of the adsorbed layers of biogenic organic substances.

List of Publications or Other Input that Resulted from the Project

1. M. Lovric, M. Branica, "Application of ASV for Trace Metal Speciation. II. Digital Simulation of Neopolarograms Using Hanging-Mercury-Drop Electrode," Croat. Chem. Acta 53 (1980) 447-483.
2. M. Lovric, M. Branica, "Application of ASV for Trace Metal Speciation. III. Simulated and Experimental Neopolarograms Using Rotating Disc Electrodes," Croat. Chem. Acta 53 (1980) (3) 485-501.
3. V. Vojvodic, N. Batina, Z. Kozarac, B. Cosovic, "The Application of Electrochemical Methods to the Determination of Surface Active Substances in Effluents," Kemija u industriji 30 (1981) (4) 169-176.
4. M. Plavsic, D. Krznaric, M. Branica, "Determination of the Apparent Copper Complexing Capacity of Seawater by Anodic Stripping Voltammetry," Mar. Chem. 11 (1982) 17-31.
5. B. Cosovic, D. Degobbis, H. Bilinski, M. Branica, "Inorganic Cobalt Species in Seawater," Geochem. Cosmochim. Acta 45 (1982) 151-158.
6. B. Cosovic, N. Batina, Z. Kozarac, "Adsorption of Some Mixtures of Surface Active Substances at the Mercury Electrode," J. Electroanal. Chem. 113 (1980) 239-249.
7. B. Cosovic, V. Vojvodic, "The Application of A.C. Polarography to the Determination of Surface Active Substances in Seawater," Limnol. Oceanogr., 27 (1982) (2) 361-369.

8. S. Kozar, J. Eder-Trifunovic, G. Zugcic, "Electrochemical Determination of Cadmium, Lead, Copper, and Zinc in the Yeast Biomasses *Trichosporon Fermentah*, *Saccharomyces Cerevisiae* and the Algae *Scenedesmus Obliquus*," *Kemija u industriji* 32 (1983) (5) 199-203.
9. Z. Kozarac, D. Hrsak, B. Cosovic, J. Vrzina, "Electroanalytical Determination of the Biodegradation of Monionic Surfactants," *Environ. Sci. Technol.* 17 (1983) 268-272.
10. M. Lovric, M. Branica, "The Simulation of the Homogeneous Catalytic Reaction at a Monolayer-Film Covered Rotating Disc Electrode," *Electrochem. Acta* 28 (1983) 1261-1267.
11. M. Lovric, T. Magjer, M. Branica, "Electrochemical Kinetic Measurements and Metal Speciation with Vibrating Dropping Mercury Electrode," *Croat. Chem. Acta* 57 (1984) 149-159.
12. Z. Kozarac, B. Cosovic, "Interactions of Cadmium with the Absorbed Layer of Biogenic Surface Active Substances at the Mercury Electrode," *Bioelectrochem. Bioenergetics* (in press).
13. B. Cosovic, V. Vojvodic, T. Plese, "Electrochemical Determination and Characterization of Surface Active Substances in Freshwaters, Water Research," (in press).
14. M. Zelic, L. Sipos, M. Branica, "Electrochemical Reduction of Selenium(+4) in Acidic Perchlorate Solutions," (submitted for publication).

(As an important collateral benefit of this project, many young researchers have completed higher education and training resulting in their obtaining 5 M.Sc. and 2 Ph.D. degrees. The titles of the thesis resulting wholly or in part from participation in this program follow:

1. Zlata Kozarac, "The Influence of Surface Active Substances on Electrochemical Processes of Cadmium(II) at the Mercury," Electrode, Ph.D. Thesis, University of Zagreb (1980).
2. Sonja Kozar, "Electroanalytical Determination of Trace Amounts of Cadmium, Lead and Copper in Seawater and in Some Marine Organisms in the North Adriatic," M.Sc. Thesis in Oceanology, University of Zagreb (1981).
3. Darko Martincic, "The Distribution of Trace Metals in the Lim Channel," M.Sc. Thesis in Oceanology, University of Zagreb (1981).
4. Renata Djogic, "Characterization of Uranium (VI) Species in Seawater," M.Sc. Thesis in Chemistry, University of Zagreb (1982).

5. Vjeročka Vojvodić, "Application of A.C. Polarography in Determination of Surface Active Substances in Natural and Polluted Water," M. Sc. Thesis in Ecological Engineering, University of Zagreb (1982).
6. Nikola Batina, "Adsorption of Surface Active Substances and Their Mixtures at the Mercury Electrode," M. Sc. Thesis in Oceanology, University of Zagreb (1982).
7. Milivoj Lovrić, "Contributions to the Theory of Differential Pulse Polarography," Ph.D. Thesis, University of Zagreb (1983).
8. Marina Skarić, "Interaction of Uranyl Ions with Phenylalanine Salicylic Acid and Phthalic Acids at Seawater Conditions," M.Sc. Thesis in Oceanology, University of Zagreb (1984).

Guest Scientists who Visited NBS from Yugoslavia

1. Dr. Marko Branica
2. Dr. Božena Cosović

The Yugoslav principal investigators have made a total of 3 visits to NBS during the previous project period and 2 visits during the current period. On each occasion, they have presented lectures at NBS and have participated in informal discussion groups with mutual benefit.

Visits to Yugoslavia of NBS Participants

1. Dr. John K. Taylor, July 1976, April 1978, March 1980, June 1982, and May 1984.

The NBS monitor has visited Rudjer Bosković Institute on five occasions during this and the previous project and has presented technical lectures on eight occasions. Three of these lectures have resulted in technical publications, as follows:

"Importance of Intercalibration in Marine Analysis," Thal. Jugosl. 14 (1978) 221-229.

"Quality Assurance Measures for Environmental Data" in "Lead in the Marine Environment," M. Branica and Z. Konrad, Eds., Pergamon Press (1980) 1-7.

"On Validation of Analytical Data," (to be published in Marine Chemistry, 1985).

Project Title: Interaction of Metal Ions with Bioligands; Development of Instruments and Methods in Action Microcalorimetry (Project Page 325, NBS(G)-262)

Years and Funds: 1980-1984, Dinars 3,660,000

Principal Investigator/s: Dr. O. Weber

Yugoslav Institute: University of Zagreb, Institute for Medical Research and Occupational Health

NBS Participant: Dr. E. J. Prosen

NBS Laboratory, Center, Division: National Engineering Laboratory
Center for Building Technology, Building Materials Division

Summary Description of Project Goals

The principal aim of the project is to develop a microcalorimeter for clinical purposes with the following properties:

- it must be possible to operate with small volumes of reagents (few hundredths of a mL),
- measure heat flow (temperature differential) with an accuracy of + one microkelvin, and
- total accuracy should be acceptable for a clinical calorimeter

Results and Significance of Achievements to Date

The electronic unit for the calorimeter has been completed and assembled. The unit contains an AC fed bridge with a 30 kohm thermistor and an AC fed amplifier. The performance is as follows:

Sensitivity: 30 mV/ μ K (max.)
Linear range: 9 V (at mx. sensitivity)
Noise: 20 mV (p-p)
Drift: 50 mV/h

The calorimeter testing started at the end of August 1984.

List of Publications or Other Input that Resulted from the Project

None.

Guest Scientists who Visited NBS from Yugoslavia

1. Dr. O. Weber
2. Dr. V. Simeon

Visits to Yugoslavia of NBS Monitor

1. Dr. E. J. Prosen, 1982 - 2 weeks

Project Title: Physico-chemical Aspects of Urinary Stone Formation
(Project Page 326, NBS(G)-263)

Years and Funds: 1980-1984, Dinars 4,160,000

Principal Investigator: Dr. Helga Fueredi-Milhofer

Yugoslav Institute: Rudjer Boskovic Institute

NBS Participant: Dr. W. E. Brown

NBS Laboratory, Center, Division: Center for Materials Science,
Polymers Division

Summary Description of Project Goals

A number of crystalline compounds are found as complex mixtures in renal stones. Most studies on the formation of renal stones are concerned with relatively simple systems in which only one of the stone-formation compounds is investigated at a time. One of the long-range objectives of the present cooperative program is to learn more about the interactions between the diverse components in urine. The kinetic aspects of the joint study are performed in Yugoslavia where experiments determine the range of solution compositions which yield precipitates. At NBS we carry out thermodynamic calculations which define the composition range where it is expected that precipitation can take place. The thermodynamic and kinetic results are then interpreted jointly.

The advantage to the Yugoslav side of the project is that NBS provides a theoretical base on which the Yugoslavs can test their kinetic data. The advantage to NBS is that NBS can test the equilibrium calculations on a relatively complex system. The advantage to society is basic information about the causes of renal stone-forming diseases.

Results and Significance of Achievements to Date

At this point progress has been made at both sides of the project. An extended abstract is available which describes progress that has been made in Yugoslavia. Precipitation boundaries for anhydrous uric acid and uric acid dihydrate at 25° and 37°C were established in one system. Conditions were established for the precipitation of monosodium urate monohydrate and of a compound that apparently contains one sodium for each urate ion, but its degree of hydration is not known. It may be a previously unidentified constituent in renal deposits. The calculations made at NBS reveal several very unusual features in the phase diagram that will require careful interpretation because they may affect crystallization processes in vivo because the slope of one of the isotherms approaches infinity.

List of Publications or Other Input that Resulted from the Project

None. (Plans are being made to prepare at least two manuscripts.)

Guest Scientist who Visited NBS from Yugoslavia

1. Dr. Helga Furedi-Milhofer, 1983, one week

Visits to Yugoslavia of NBS Participant

1. Dr. W. E. Brown, 1981, one week
2. Dr. W. E. Brown, 1982, one week
3. Dr. W. E. Brown, 1984, 10 days

Project Title: Radiochromic Dye Dosimeters for Radiation Research
and Technology
(Project Page 357, NBS(G)-264)

Years and Funds: 1980-1984, Dinars 3,370,000

Principal Investigator: Dr. Branislav B. Radak

Yugoslav Institute: Boris Kidric Institute of Nuclear Science

NBS Participant: Mr. William L. McLaughlin

NBS Laboratory, Center, Division: National Measurement Laboratory,
Center for Radiation Research, Radiation Physics Division

Summary Description of Project Goals

Industrial applications of ionizing radiation, especially of gamma rays and electron beams, have increased dramatically during the 1970's and 1980's. Part of these successes in both Yugoslavia and in the U.S. has been directly due to improved radiation measurement capability, which is vital to achieving quality control in radiation processing. The main project goal has been to improve the standardization of such measurements by designing and testing radiochromic dye dosimeters as both routine and reference measurement systems. Secondary goals have been to develop new measurement systems for practical industrial use in both countries.

Results and Significance of Achievements to Date

Several novel liquid and solid-phase dosimeters based on the radiochromic effect on dyes have been designed, developed, and tested to success under this project. In fact, these systems are presently the most successful in the world market for maintaining quality control in industrial radiation processing, in the U.S. and Yugoslavia as well as in other industrialized nations. They are sold by the millions per annum. The vitality and industrial growth of radiation processing are largely attributable to these advances in dosimetry. Moreover, the ability to standardize through continual dose intercomparisons between the NBS and the Boris Kidric Institute is largely responsible for the delivery of many safe commodities to the market place, (see attached list of radiation-sterilized products). Through this technical project, NBS has broadened its ability to satisfy measurement needs both at home and abroad, and Yugoslavia has gained high standing as one of the contributing members of an important International Atomic Energy Agency working groups in standardization of high-dose measurements in industrial radiation processing.

Table 1.1, Radiation Sterilized Products

Surgical sutures	Eye pads
Plastic and rubber medical devices	Gauze sponges
Blood handling equipment	Dental supplies
Anesthesiology kits	
Implant substances and tissues (heart valves, bone grafts, etc.)	Catheters
Hospital and surgical packs	Syringes and needles
Obstetrical supplies	Tubings and films
Transplant kits	Trays and containers
Wound and burn dressings	Surgical gloves
Inhalation equipment	Surgical utensils
Patient-care items (containers, masks, gowns)	Laboratory devices
	Animal serum
	Non-woven fabrics
Diets for immune-suppressed patients	
Diets for specific pathogen-free animals	Ointment tubes
Diets for Astronauts	
Hides and animal parts	

List of Publications or Other Input Relevant to or Resulting from the Project

1. W. L. McLaughlin, M. Kosanic, "The Gamma-Ray Response of Pararosaniline Cyanide Dosimeter Solutions," Int. J. App. Rad. & Isotopes, 25 (1974) 245-262
2. W. L. McLaughlin, "Solid-Phase Chemical Dosimeters," Sterilization by Radiation, Multiscience Publications, Ltd., Montreal (Eds: E.R.L. Gaughran and A.J. Goudie), International Conference, Vienna (1974) 219-324.
3. B.B. Radak, M.M. Kosanic, M.B. Sestic, W. L. McLaughlin, "A Calorimetric Approach to the Calibration of Liquid Dosimeters in High-Intensity Electron Beams," Biomedical Dosimetry, Vienna (1975) 633-641.
4. M.M. Kosanic, M.T. Nenadovic, B.B. Radak, V.M. Markovic, McLaughlin, "Liquid Radiochromic Dye Dosimetry for Continuous and Pulsed Radiation Fields Over a Wide Range of Energy Flux Densities," Int. J. Appl. Rad. & Isotopes, 28 (1977) 313-321.
5. W. L. McLaughlin, "Dosimetry Standards for Industrial Radiation Processing," National and International Standardization for Radiation Dosimetry, Vol. 1, International Atomic Energy Agency, Vienna (1978) 89-106.
6. W.L. McLaughlin, M. M. Kosanic, V. M. Markovic, M. T. Nenadovic, K. Sehested, J. Holcman, "The Kinetics of Dye Formation by Pulse Radiolysis of Pararosaniline Cyanide in Aqueous or Organic Solution," Riso Report M-2022, Riso National Laboratory, Roskilde, Denmark (1979).
7. W. L. McLaughlin, J. C. Humphreys, B. B. Radak, A. Miller, T. A. Olejnik, "The Response of Plastic Dosimeters to Gamma Rays and Electrons at High Absorbed Dose Rates," Radiat. Phys. Chem. 14 (Trans. 2nd Intern. Meeting on Radiation Processing, Miami, Oct. 1978, Ed: J. Silverman) (1979) 533-550.
8. B. B. Radak, V. M. Markovic, W. L. McLaughlin, "Dosimetry for the Commissioning of a Versatile Irradiation Plant," Radiat. Phys. Chem. 14 (Trans. 2nd Intern. Meeting on Radiation Processing, Miami, Oct. 1978, Ed: J. Silverman) (1979) 449-456.
9. W. L. McLaughlin, M. G. Simic, A. Miller, "Dosimetry by Means of the Radiation Reduction of Hemin in Aprotic Solvents," Proceedings of 3rd Symposium on Nuclear Chemistry, Radiochemistry, and Radiation Chemistry, Mexico, D.F., Dec. 8-10 (1980) 195-201.
10. W. L. McLaughlin, J. C. Humphreys, H. Levine, A. Miller, B. B. Radak N. Rativanich, "The Gamma-Ray Response of Radiochromic Dye Films at Different Absorbed Dose Rates," 3rd International Meeting on Radiation Processing, Tokyo, Oct. 1980, Radiat. Phys. Chem. 18 (1981) 987-999.

11. N. Rativanich, B.B. Radak, A. Miller, R.M. Uribe, W.L. McLaughlin, "Liquid Radiochromic Dosimetry," 3rd Int. Meeting on Radiation Processing, Tokyo, Oct. 1980 Radiat. Phys. Chem. (1981) 1011-1016.
12. K.V. Ettinger, J. W. Nam, W. L. McLaughlin, K. H. Cadwick, "Progress in High-dose Radiation Dosimetry," Biomedical Dosimetry, Int. Atomic Energy Agency, Vienna (1981) 405-431.
13. B. B. Radak, W. L. McLaughlin, "The Gamma-Ray Response of Opti-chromic Dosimeters," Radiat. Phys. Chem. 34 (1984) in press.

Guest Scientists who Visited NBS from Yugoslavia

1. Dr. Ivan G. Dragovic, 1976, 1980 and 1982
2. Dr. V. M. Markovic, 1977, 1979, 1982
3. Dr. B. B. Radak, 1983, and guest scientist for the period September 1984 - June 1985, at NBS.

Visits to Yugoslavia of NBS Participants

1. Mr. William L. McLaughlin, 1975, 1978, 1980
2. Mr. Michael Simic, 1983

Project Title: Mass Spectrometric Studies of High Temperature
Equilibria
(Project Page 358, NBS(G)-265)

Years and Funds: 1981-1984, Dinars 4,520,000

Principal Investigator: Dr. Kiro F. Zmbov

Yugoslav Institute: Boris Kidric Institute of Nuclear Sciences

NBS Participant: Dr. John W. Hastie

NBS Laboratory, Center, Division: Center for Materials Science,
Inorganic Materials Division

Summary Description of Project Goals

A detailed understanding of high temperature equilibria is important in many areas of modern technology, but particularly in materials processing and durability. The primary objective of this project is to develop (and apply) new, more accurate mass spectrometric techniques for the measurement of vapor-solid (or liquid) phase equilibria and of related thermochemical quantities, including bond dissociation energies and ionization potentials.

Combined thermodynamic and high resolution electron impact data will be obtained for selected high temperature systems by using a uniquely coupled system which contains a mass spectrometer, a Knudsen effusion cell and a trochoidal electron monochromator (TEM). Emphasis will be given to high temperature vapor systems of demonstrated importance in combustion, chemical transport and materials processing. Implementation of this coupled system will overcome many of the limitations associated with conventional high temperature mass spectrometry systems. The near-monochromatic nature of the TEM electron beam should reduce by an order of magnitude the uncertainties in bond energies and ionization potentials obtained with conventional ionization sources. TEM also has advantages over recently developed photoionization methods, principally in higher ion intensities, a wider energy range, and less restrictive selection rules for ionization.

Results and Significance of Achievements to Date

A systematic study of the formation of positive ions and the F^- ion from POF_3 molecule has been completed. The appearance potentials of all ions observed have been measured and the fine structure of the corresponding ionization efficiency curves has been analyzed to obtain the appearance energies of various excited states of the ions. The results have been reported at the 9th International Mass Spectrometry Conference in Vienna, September 1982, and published in the Internatl. J. Mass Spectrom. Ion Phys. (Ref. 1).

Singly and multiply charged ions formed by electron impact of the noble gases have been studied by the mass spectrometer. The ionization efficiency curves have been analyzed by various deconvolution methods and the excited states of various ions have been determined.

A new mathematical method for deconvolution of the ionization efficiency curves obtained by use of conventional Nier-type ion source has been developed. The method is based on application of the MONTE CARLO method for random selection of the ionization efficiency curve parameters. The results have been reported at the 9th International Mass Spectrometry Conference, Vienna.

A systematic study of the formation of positive and negative ions by electron impact from SO_2 and SO_3 has been undertaken. Two different approaches are being applied, e.g., use of a Nier-type ion source with subsequent application of a suitable deconvolution procedure, or use of a Trochoidal Electron Monochromator for obtaining precise data on the ionization and excitation energies of the ion formed.

The results of an experimental study of the vaporization of KCl and KOH by Transpiration Mass Spectrometry have been evaluated and prepared for publication.

List of Publications or Other Input that Resulted from the Project

1. D. Kovac, M. Veljkovic, M. Miletic, K.F. Zmbov, "The Ionization Potential of AuLi Molecule and the Heat of Formation of the AuL⁺ Ion," Bull. Soc. Chim. Beograd, 47 (1982) 217.
2. O. Neskovic, M. Veljkovic, D. Golobocanin, M. Miletic, K. F. Zmbov, "Bond Dissociation Energies of the CH₃CN Molecule from Mass Spectrometric Electron Impact Studies," Ibid., 47 (1982) 105.
3. O. Neskovic, M. Veljkovic, D. Golobocanin, M. Miletic, K.F. Zmbov, "Appearance Potentials of Positive Ions in the Mass Spectrum of CH₃CN," Internatl. J. Mass Spectrom. Ion Phys., 44 (1982) 61.
4. O. Neskovic, M. Veljkovic, M. Miletic, D. Golobocanin, K.F. Zmbov, "Ionization and Fragmentation of Phosphorus Oxyfluoride by Electron Impact," Ibid., 47 (1983) 141.
5. D. Golobocanin, M. Veljkovic, O. Neskovic, K. F. Zmbov, M. Miletic, "Application of Monte Carlo Method for Computation of the Ionization Efficiency Curve Parameters," Ibid., 48 (1983) 431.

6. J. W. Hastie, K.F. Zmbov, D. W. Bonnell, "Transpiration Mass Spectrometric Analysis of Liquid KOH Vaporization," Elect. Chem. Soc., (1983) in press.
7. K. F. Zmbov, J. W. Hastie, D. W. Bonnell, "Mass Spectrometric Study of KCl and KOH," (to be published).

Guest Scientist who Visited NBS from Yugoslavia

1. Dr. K. F. Zmbov, 1983, 1 month

Visits to Yugoslavia of NBS Participant

1. Dr. J. Hastie, 1982, 14 days

Project Title: Development of Monomolecular Layers for Preparation of Radioactivity Standards of Nuclides Emitting Low-energy Electrons
(Project Page 359, NBS(G)-266)

Years and Funds: 1981-1984, Dinars 2,770,000

Principal Investigator: Dj. N. Bek-Uzarov

Yugoslav Institute: Boris Kidric Institute of Nuclear Sciences, Vinca

NBS Participants: Dr. W. B. Mann and Dr. J.M.R. Hutchinson

NBS Laboratory, Center, Division: National Measurement Laboratory,
Center for Radiation Research, Nuclear Radiation Division

Summary Description of Project Goals

The project goals were (1) to develop the technology associated with the production of monomolecular layers, (2) to investigate the physical and chemical conditions that will optimize the formation of such layers, and (3) to apply the results to the development and production of radioactivity standards, particularly for the cases of low-energy beta-particle and x-ray emitting radionuclides.

It was originally estimated that, to be viable, this project would need to be financed at a level about five to ten times greater than that which was eventually found possible. In spite of the antiquity of the equipment with which Dr. Bj. Bek-Uzarov and Dr. Lj. Dobrilovic first started, their achievement as now reported using only limited funds is both encouraging and noteworthy.

Five years ago it was agreed that the electronic control did not have the stability required for the automatic torsion balance to maintain a uniform surface tension as the monomolecular film was being formed on the surface of the pool water. On NBS advice the Yugoslav investigators concentrated on updating this electronic equipment with the limited funds available. Drs. Bek-Uzarov and Dobrilovic reported that they are now able not only to produce monomolecular films of ^{55}Fe -ferric stearate with surface activities of $7.5 \text{ MBq}\cdot\text{m}^{-2}$, but they have also laid down as many as 120 monomolecular films onto metal and other substrates.

During the meetings of the International Standards Organization (ISO) at NBS last year, discussions took place on the draft of a new ISO standard on Radionuclide Surface Contamination. This standard was largely sponsored by the United Kingdom to meet their regulatory requirements, but if, as seems very likely it is adopted internationally, the monomolecular-film sources of low-energy photon and electron emitters are almost certain to be in demand. NBS has also gained knowledge from this research.

Results and Significance of Achievements to Date

In order to develop radioactive iron-55 sources of monomolecular thickness, the condition for existence of the ferric stearate layers and the physical properties of the layers were examined as a function of the pH of the solution.

The compressibility coefficients were determined and the ion adsorption times examined. As a result of these investigations, homogeneous iron-55 sources of mono- and multilayer thickness which had the activity of 7.5×10^6 Bq.m⁻² were obtained. Similar experiments were performed on calcium stearate layers.

Techniques for the transfer of monomolecular layers from a liquid substrate onto hard metallic and non-metallic supports were developed and up to 120 layers were formed in one experiment.

The old apparatus has been redesigned and a new apparatus will be constructed by the end of 1984.

List of Publications or Other Input that Resulted from the Project

1. Lj. Dobrilovic, M. Simovic, "Physical Properties of the Ferric Stearate Monomolecular Layer and Preparation of Radioactive Fe-55 Sources," Journal of Eng. Physics, No. XXIV (1982) 35-41.
2. Lj. Dobrilovic, M. Simic, Dj. Bek Uzarov, W.B. Mann, J.M.R. Hutchinson, "Physical Properties of the Calcium Stearate Monomolecular Layer," Internal Publication, Ibk-Fizika (to be published in 1984).
3. Dj. Bek-Uzarov, Lj. Papic, M. Simovic, Lj. Dobrilovic, W.B. Mann, J.M.R. Hutchinson, "Description of the Improved Construction of Automatic Torsion Balance for Investigation of Physical Characteristics of Insoluble Monomolecular Layers Existing on Boundary between Liquid and Gaseous Phases and their Transfer on the Solid Substrata," Internal Publication Ibk Fizika (to be published in 1984).

Guest Scientists who Visited NBS from Yugoslavia

None; scientists met at international conferences.

Visits to Yugoslavia of NBS Participants

None; scientists met at international conferences.

Project Title:

Part I: Electron Stimulated Desorption and Ion Scattering
Spectroscopy of Alkali Ions on Metal Surfaces

Part II: Ion Bombardment Induced Electron Emission from Surfaces
(Project Page 360, NBS(G)-267)

Years and Funds: PART I, 1981-1984
PART II, 1983-1984

Principal Investigator: Dr. J. Vukanic and Dr. Ilija Terzic

Yugoslav Institute: Boris Kidric Institute of Nuclear Science

NBS Participants: Dr. Theodore E. Madey, Part I
Dr. J. Fine, Part II

NBS Laboratory, Center, Division: National Measurement Laboratory,
Center for Chemical Physics, Surface Science Division

PART I

Summary Description of Project Goals

The project goals were (1) to develop theoretical models related to the electron stimulated desorption (ESD) of ions from surfaces; to describe the influence of the surface image potential and ion neutralization processes on the trajectories and survival probabilities of low energy ions leaving a surface, (2) to characterize experimentally the electronic excitation processes which cause electron stimulated desorption (ESD) of alkali ions from surfaces, and (3) to characterize low angle ion scattering from surfaces as a probe of the surface dipole field.

Surface science is a rapidly growing, exciting field offering many scientific and technological challenges. The characterization of surfaces and surface processes is an integral part of many industries, such as those related to catalysis, lubrication, semiconductor devices, corrosion, and metallurgical coatings.

The theoretical and experimental aspects of the present project provide important information relating to the characterization of surfaces, namely, the bonding structure of atoms and molecules adsorbed on surfaces of metals, semiconductors, and insulators.

The research performed by Dr. Terzic and his colleagues at the Boris Kidric Institute has brought direct and immediate benefits to our NBS program in determination of surface molecular structure using Electron Stimulated Desorption; we expect the joint project to continue being highly productive and mutually beneficial.

Results and Significance of Achievements to Date

Theoretical Calculations: The influence of the interaction between an ion and a conducting surface on ion desorption processes has been calculated semi-classically. For the first time, analytical solutions have been obtained for the trajectories of desorbing ions as well as the trajectories of ions trapped by the image field. The effects of both the image force and ion neutralization processes on the energy and angular distributions of desorbing ions have been obtained.

The objective in these studies has been to provide a guide for experimentalists to the surprisingly large changes in ion angular distributions due to image potential and neutralization effects. The results are highly useful in our NBS programs involving the use of ESDIAD (electron stimulated desorption ion angular distributions) for determining the structures of adsorbed molecules.

Experimental Program: There have been rather extensive materials shortages in Yugoslavia since the project began; this factor has hampered experimental progress. Despite such problems, Dr. Terzic has completely re-configured an ultrahigh vacuum system with an electron gun, silver, potassium effusion sources, cylindrical energy analyzer and magnetic sector mass spectrometer, all of which were fabricated skillfully at the Boris Kidric Institute. Parts of the apparatus are currently being tested, and appear to function as designed. Dr. Terzic and an experienced colleague, Dr. M. Tomic, anticipate accelerated progress now that the apparatus is nearly complete.

List of Publications or Other Input that Resulted from the Project

1. Z. Miskovic, J. Vukanic, T. E. Madey, "Influence of the Image Interaction on Ion Desorption Process," *Surface Sc.* 142 (1984) xxx.
2. Z. Miskovic, J. Vukanic, T. E. Madey, "Influence of the Image Interaction on Electron Stimulated Desorption Ion Angular Distribution," *Proceedings of Symposium on the Physics of Ionized Gases (SPIG), Dubrovnik (1984)* in press.
3. Z. Miskovic, J. Vukanic, T. E. Madey, "Effects of Neutralization Processes on Energy and Angular Distributions in Electron Stimulated Desorption of Ions," *Proceedings of Symposium on the Physics of Ionized Gases (SPIG), Dubrovnik (1984)* in press.
4. Z. Miskovic, J. Vukanic, T. E. Madey, "Neutralization Effects in Electron Stimulated Desorption Ion Angular Distributions," (to be submitted to *Surface Science*).

Guest Scientist who Visited NBS from Yugoslavia

1. Dr. Ilija Terzic, 1984, one week planned.

Visits to Yugoslavia of NBS Participant

1. Dr. Theodore E. Madey, 1981, one week
2. Dr. Theodore E. Madey, 1983, one week

PART II

Summary Description of Project Goals

The project goals were (1) to develop an increased understanding of collisional energy transfer and atomic excitation mechanisms that take place at ion bombarded surfaces, (2) to examine the effect of inner- and outer-shell excitation lifetimes on the collisional excitation mechanisms which led to electron emission both from the target and from ejected target atoms, (3) and to characterize electron energy distributions that result from bombardment with ions in the 20 to 80 keV range and to examine threshold dependence of Auger as well as total secondary electron emission.

We anticipate that the research in progress will contribute significantly to the rather limited understanding of collisional energy transfer and atomic excitation mechanisms at ion bombarded and sputtered surfaces. Even though these processes themselves are not well understood, there is now developing a keen interest in the use of sputter sources for various analytical measurement systems (e.g., mass spectroscopy, laser resonance ionization, laser fluorescence, etc.) In order to make proper use of such ion bombardment sources to analyze ejected ventral particles, it will be necessary to characterize and understand the excitation and energy transfer processes taking place. It is the purpose of this project to address such basic problems of atomic collisions. We believe that the answers also will find application in the development of new measurement systems that may be of great interest to many industrial users, both in Yugoslavia and in the U.S.

Results and Significance of Achievements to Date

Experimental research plans were made during Dr. Fine's February 1984 visit with Dr. Terzic and his group. In addition to developing a specific approach for investigating electron emission from gallium (Ga) surfaces bombarded with ions, the necessary apparatus design changes were made of Dr. Terzic's system for this Ga on Ga experiment. Modifications were planned so as to accommodate a Ga ion source which Dr. Fine will bring from NBS specifically for this work.

Modification of the ion accelerator and UHV electron energy analyzer is proceeding at Vinca and the equipment should be ready early in the fall of 1984, to begin our experiments. At that time, the U.S. monitor plans to work with Dr. Terzic in Vinca on the secondary electron yield measurement.

List of Publications or Other Input that Resulted from the Project

None.

Guest Scientist who Visited NBS from Yugoslavia

1. Dr. Ilija Terzic, 1984, (one week planned)

Visits to Yugoslavia of NBS Participant

1. Dr. Joseph Fine, 1979, 2 days
2. Dr. Joseph Fine, 1982, 1 day
3. Dr. Joseph Fine, 1984, one week

Project Title: Elastic and Inelastic Neutron Scattering from Liquid
Metals and Alloys
(Project Page 362, NBS(G)-269)

Years and Funds: 1981-1984, Dinars 2,770,000

Principal Investigator: Dr. Djordje Jovic

Yugoslav Institute: Boris Kidric Institute of Nuclear Sciences

NBS Participants: Dr. J. J. Rhyne

NBS Laboratory, Center, Division: Center for Materials Science,
Reactor Radiation Division

Summary Description of Project Goals

To develop a collaborative research program between the NBS Neutron Scattering Group and scientists at the Boris Kidric Institute in Belgrade. Both institutions have research reactors and instrumentation for making neutron diffraction measurements. In addition the NBS facility has state-of-the-art capabilities for inelastic scattering and small angle neutron scattering. The initial focus of this effort was in diffraction and time of flight studies of liquid metallic specimens. Within the last year, the scope of this project has been significantly broadened to include studies of amorphous metallic alloys and spin glasses. As originally proposed, neutron diffraction experiments on the amorphous systems will be carried out principally at Vinca, and the inelastic scattering studies will be done at NBS.

Results and Significance of Achievements to Date

In formulating an experimental study of liquid metals, plans for a series of diffraction experiments at an elevated temperature have been developed. A high temperature furnace for the diffraction studies has been designed at Vinca and recently completed and tested. Preparations have been made for a diffraction study of liquid germanium.

Extensive effort has been placed on enhancing and upgrading the data collection system at Vinca to make the experiments proceed more efficiently. Some sharing of equipment between the two laboratories is planned in this respect.

Preparations have been made for the transfer of the NBS powder profile refinement program to facilities at Vinca so that compatible data analysis procedures will be available at both laboratories.

The broadening of the program to include amorphous alloys and spin glasses offers considerable promise, since both institutions have scientists with significant expertise in these fields. It is clear that both laboratories will benefit from a mutual exploration of one of the forefront areas of research involving new high technology magnetic metallic materials. A series of diffraction studies on CrFe and MnAl spin glass alloys have been planned.

List of Publications or Other Input that Resulted from the Project

None

Guest Scientists who Visited NBS from Yugoslavia

1. Dr. Djordje Jovic
2. Dr. M. Davidovic, 1983, 2 weeks

Visits to Yugoslavia of NBS Participants

1. Dr. J. J. Rush, 1981, 3 days
2. Dr. J. M. Rowe, 1981, 3 days
3. Dr. J. J. Rhyne, 1983, 4 days
4. Dr. J. J. Rhyne, 1984, 1 week

Project Title: Development and Application of Ultrasensitive Magnetic Resonance Methods
(Project Page 363, NBS(G)-270)

Years and Funds: 1981-1984, Dinars 3,860,000

Principal Investigator: Prof. R. Blinc

Yugoslav Institute: Jozef Stefan

NBS Participant: Dr. D. H. Reneker

NBS Laboratory, Center, Division: Center for Materials Science

Summary Description of Project Goals

Nuclear-nuclear double resonance methods were developed more than a decade ago in order to detect nuclear magnetic resonance and nuclear quadruple resonance spectra that are too weak to be detected by conventional magnetic resonance techniques. Whereas some of these techniques are by now widely used in chemical, biological, and physical research, the full potential of this method is still not fully exploited and the method has not yet become a standard tool in the hands of materials scientists. The same is true for nuclear magnetic resonance techniques for the determination of self-diffusion coefficients in condensed matter.

The purpose of this research is to (1) develop new NMR techniques for double resonance and self-diffusion studies of condensed matter, and (2) to apply these techniques to problems in condensed matter physics and materials science which could not be solved by classical magnetic resonance methods. Among such problems is the characterization of disordered matter (such as incommensurate systems and spin glasses) by nuclear quadrupole resonance and the extension of classical NQR into the previously inaccessible region of 0.1 - 2 MHz. Still another problem is the determination of self-diffusion in polymer melts.

This work provides incisive new insights into the way polymer molecules move during melt processing into fibers and molded or extruded objects. These novel experiments provide a window to previously inaccessible information and replace empiricism with understanding. It complements the polymeric materials program at the National Bureau of Standards.

These and related magnetic resonance techniques not only establish a reputation for scientific excellence for Yugoslavia but also find application in improved understanding of the performance of concrete, ferroelectric crystals, liquid crystals and many other important and useful materials.

Results and Significance of Achievements to Date

New multiple-pulse NMR techniques for time-resolved self-diffusion measurements in condensed matter have been developed. These techniques allow for the determination of the self-diffusion coefficients as a function of the diffusion time in condensed matter where normal NMR spin-echo techniques cannot be applied because the spin-spin relaxation times are too short.

With the help of level crossing double resonance in the laboratory frame of reference and nuclear double resonance based on the solid effect, techniques have been developed which allow for a routine investigation of ^{14}N nuclear quadrupole resonance spectra in the previously inaccessible region 0.1 - 2 MHz in polycrystalline biological samples and disordered condensed matter as well as the determination of ^{17}O NQR spectra in natural abundance. These two techniques have the potential to become standard analytical tools in material science research.

With the help of NMR, spin-lattice relaxation of ^{87}Rb phason excitation in incommensurate systems was detected for the first time.

NMR techniques also allowed the first quantitative determination of the soliton density in incommensurate dielectrics. The above two achievements represent a verification of:

- The phason concept in incommensurate systems which exhibit perfect long range order but no translational symmetry (so that they are not crystals in a classical sense)
- A verification of the existence of phase solitons in incommensurate systems as predicted by McMillan.

The nature of the phase transitions in models of biological membranes was elucidated.

A new method has been developed for a determination of the spectrum of the velocity autocorrelation time of polymer melts with the help of time resolved self-diffusion measurements.

The newly developed techniques have thus allowed a better characterization of disordered condensed matter on a microscopic level and improved our understanding of phase transitions, incommensurate systems and polymer melts.

List of Publications or Other Input that Resulted from the Project

1. R. Blinc, S. Juznic, V. Rutar, J. Seliger, S. Zumer, " ^{87}Rb spin-lattice relaxation in the incommensurate phase of Rb_2ZnCl_4 ," Phys. Rev. Lett. 44 (1980) 609.

2. R. Blinc, V. Rutar, B. Topic, F. Milia, I.P. Aleksandrova, A. S. Chaves, R. Gassinelli, "Soliton density in structurally incommensurate systems," *Phys. Rev. Lett.* 46 (1981) 1406.
3. R. Blinc, "Magnetic Resonance and Relaxation in Structurally Incommensurate Systems," *Phys. Reports* 79 (1981) 332.
4. R. Blinc, F. Milia, V. Rutar, S. Zumer, "Spin Lattice Relaxation Via Phasons in a Multiresolution Lattice," *Phys. Rev. Lett.* 48 (1982) 47.
5. R. Blinc, "Phase Transitions in Incommensurate Ferroelectrics - Solitons and Phasons," *Physica Scripta* T1 (1982) 138.
6. R. Kind, R. Blinc, H. Arend, P. Muralt, J. Slak, G. Chapuis, K.J. Schenk, Be, Zeks, "Phase Transition from an Intercalated to a Nonintercalated Structure in a Lipid Bilayer," *Phys. Rev. A* 26 (1982) 1816.
7. V. Rutar, R. Blinc, L. Ehrenberg, "Protein Content Determination in Solid Organic Materials by Proton-enhanced Magic Angle Sample Spinning ^{13}C NMR," *J. Magn. Resonance* 40 (1980) 225.
8. V. Rutar, R. Blinc, Z. Naturforsch, "Nondestructive Determination of Protein Content of Viable Seeds by Proton Enhanced ^{13}C NMR," 35C (1980) 12.
9. L. Barbic, I. Kocuvan, R. Blinc, G. Lahajnar, P. Merljak, I. Zupancic, "The Determination of Surface Development in Cement Pastes by NMR," *J. of the Amer. Ceramic Soc.* 65 (1982) 25.
10. J. Selinger, V. Zagar, R. Blinc, " ^{17}O NQR Study of the Ferroelectric Phase Transition in PbHPO_4 ," *Physics Lett.* 93A (1983) 149.
11. R. Blinc, D.C. Ailion, P. Prelovsek, V. Rutar, "Floating of the Modulation Wave and Phase Pinning in Incommensurate Rb_2ZnBr_4 ," *Phys. Rev. Lett.* 50 (1983) 67.
12. V. Zagar, R. Blinc, H. Arend, G. Chapuis, " ^{14}N and ^{35}Cl Double Resonance Study of the Phase Transition in the Intercalated Bilayer Compound $\text{C}_{10}\text{H}_{21}\text{NH}_3\text{Cl}$," *J. Chem. Phys.* 78 (1983) 2661.
13. I. Zupancic, G. Lahajnar, R. Blinc, D. H. Reneker, D. L. Vanderhart, "NMR Self-Diffusion Study of Polyethylene and Paraffin Melts," *Hart Jour. of Polymer Science: Polymer Physics Ed.* (Submitted for publication).
14. I. Zupancic, G. Lahajnar, R. Blinc, A. Peterlin, D. H. Reneker, "Molecular Weight Dependence of NMR Line Shapes in Linear and Branched Polyethylenes in Melt," *Bull. Mag. Res.* 2 (1980) 342.
15. I. Zupancic, G. Lahajnar, A. Peterlin, D. H. Reneker, " ^{22}nd Microsymposium on Macromolecules," Prague (1981) M50-1.

16. R. Blinc, "NMR in Chaotic and Spin Glass State Ferroelectrics,"
Ferroelectrics 53 (1984) 83.

Guest Scientist who Visited NBS from Yugoslavia

Prof. R. Blinc, 1981, 1982, 1983, 1984, two days each visit

Visits to Yugoslavia of NBS Participant

1. Dr. D. Reneker, 1980, 1981

Project Title: The Role of Trace Elements in a Living Organism
(Project Page 365, NBS(G)-271)

Years and Funds: 1981-1984, Dinars 3,615,000

Principal Investigator: Dr. R. Draskovic

Yugoslav Institute: Boris Kidric Institute of Nuclear Sciences

NBS Participant: Dr. Rolf Zeisler

NBS Laboratory, Center, Division: National Measurement Laboratory,
Center for Analytical Chemistry, Inorganic Analytical Research
Division

Summary Description of Project Goals

Technological development is increasingly dependent on high quality analysis for monitoring and characterizing product and waste streams, and their impact on human and environmental health. Especially at trace levels in both relatively pure materials and complex geological, biological and environmental media, the analytical chemist faces an enormous challenge to meet the requirements of accurate analysis because of the range of concentrations (to less than 10^{-12} g/g) and complexity of matrices, as well as the importance of the results to the human subjects. This quest for high quality data is of global importance and international cooperation is required to achieve these goals.

The study utilizes neutron activation analysis (NAA) procedures that have been developed and evaluated for the accurate determination of critical trace elements in various healthy and diseased tissues. In addition, the NAA procedures are expanded to include the multielement analysis of living and non-living matter of river systems. The procedures provide sensitivity for the simultaneous determination of chromium, iron, cobalt, zinc, selenium, antimony and other trace elements in these media. Based on the analytical data the interrelationship of trace element distributions with pathological changes or ecological and other parameters is investigated. Research is conducted to explain the possible influence of biological and biogeochemical processes on the distribution of trace elements and the possible impact of these processes on human and environmental health.

Results and Significance of Achievements to Date

Distribution data of trace elements in normal and diseased human colon mucosa and liver tissues have been collected from a large number of

subjects. Computer programs including statistical treatment have been developed and used for the comparisons of normal and pathologically altered tissues. A dependency of the element distribution and the specific pathological state of some investigated human organs and tissues has been established from these data. This dependency may become important for the early diagnosis of specific diseases and corrective action via nutritional intake.

Data have been obtained for the distribution of trace elements in enamel, dentine, and pulp of teeth. The analytical results are used to study the influence of the ecological condition, the age of the patients and the number and kind of stomatological interventions.

Improvements in the quality of the data has been achieved in collaboration with NBS. Standard Reference Materials have been used to verify the analytical results. The ongoing exchange of experience in sampling and sample preparation between this project and the NBS Pilot Program for a National Environmental Specimen Bank will further enhance the quality of these results as well as aid the NBS program.

List of Publications or Other Input that Resulted from the Project

1. R.J. Draskovic, Lj. Jacimovic, M. Stojicevic, M. Pajic, V. Filipovic, "Investigations of Some Element Distributions in Dental Tissues by INAA as a Function of Ecological and Some Other Parameters," J. Radioanal. Chem. 69, Vol 1-2 (1982) 117-132.
2. K. Kostic, R. J. Draskovic, "Studies of Iron, Cobalt and Chromium Distribution in Some Continental Aquatic Ecosystems and Biological Materials," Ibid 69, No. 1-2 (1982) 417-426.
3. R.J. Draskovic, M. Bozanic, T. Bohus, "Computer Treatment of the Contents of Some Elements in the Normal and Pathologically Altered Human Colon Mucosa Tissues Obtained by INAA," Preprints der Vortrage and Posterbeitrage: "3. Tagung Nukleare Analysenverfahren", 11/15 04 1983 in Dresden, DDR, ZFK ISS. No. 135-2950 (1983) 388.
4. K. Kostic, R. J. Draskovic, M. Djordjevic, S. Stankovic, "Distribucija Zn, Fe, i Co u selektivno dobijenim uzorcima iz ciroticnog i kanceroznog tkiva humane jetre," Radiol. Jugosl. 16 (1982) 217-220 (Yugoslav publication).
5. R. J. Draskovic, K. Kostic, "Raspdela hroma, kobalta i gvozdja u nekim bioloskim materijalima," Ibid 16 (1982) 221-223.
6. M. Bozanic, R. J. Draskovic, "Odnosi sadrzaja nekih elemenata u tragovima u neizmenjenoj mukozni kolona dobijenih neutronsom aktivacionom analizom," Ibid 17 (1983) 461-465.

7. R. J. Draskovic, M. Bozanic, V. Bozanic, T. Bohus, "Kompjuterska analiza podataka o sadrzajima nekih elemenata u mukoznom tkivu normalnog i patoloski promenjenog humanog kolona," Ibid 17 (1983) 471-476.

Papers 1 and 2 were presented at the 6th Modern Trends Conference "Modern Trends in Activation Analysis," Toronto, Canada (Oct. 1981) 16/19.

Papers 4 and 5 were presented at the "III Yugoslav Congress on Nuclear Medicine," Skopje (1982) 3/6.

Papers 6 and 7 were presented at "XVIII Yugoslav Meeting on Nuclear Medicine," Donji Milanovac (1983) 21/24.

The following papers were accepted for oral presentation:

I. First International Conference on Elements in Health and Disease (February 1983) New Delhi, India:

1. K. Kostic, R. J. Draskovic, M. Djordjevic and S. Stankovic, "Distribution of Zinc, Iron and Cobalt in Selected Samples of Cirrhotic and Cancerous Liver."
2. M. Bozanic, R. J. Draskovic, K. Kostic, "Investigation of Some Element Distributions in Normal and Pathologically Changed Samples of Colonic Mucosa Tissues by Activation Analysis."

II. Twenty-first International Meeting of the Society of Nuclear Medicine in Europe (September 1983) Ulm/Neu Ulm, Germany.

K. Kostic, R. J. Draskovic, D. Ristanovic, M. Djordjevic, S. Stankovic, "Zn, Co, Fe, Sb and Sc Determinations in Cirrhotic and Tumorous Liver Tissues Studied by INAA."

III. XVIII Yugoslav Meeting on Nuclear Medicine (September 1983) Donji Milanovic.

K. Kostic, R. J. Draskovic, D. Ristanovic, M. Djordjevic, S. Stankovic, "Sadrizaj nekih oligo-elemenata u primarnom i sekundarnom karcinomu jetre odredjen neutronsom aktivacionom analizom."

Guest Scientists who Visited NBS from Yugoslavia

None

Visits to Yugoslavia of NBS Participant

1. Dr. Rolf Zeisler, 1982, one week
2. Dr. Rolf Zeisler, 1984, one week

Project Title: Thermal Degradation of Polymers
(Project Page 366, NBS(G)-272)

Years and Funds: 1981-1983, Dinars 2,120,000

Principal Investigator: Dr. Zoran Petrovic

Yugoslav Institute: Institute for Petrochemistry, Gas, Oil, and
Chemical Engineering, Faculty of Technology

NBS Participant: Dr. Joseph H. Flynn

NBS Laboratory, Center, Division: Center for Materials Science, Polymers
Division

Summary Description of Project Goals

Thermal degradation of polymers has become more and more important from the viewpoint of energy saving, environmental protection, as well as from the secondary raw material reclamation. The proposed area of research included investigation of mechanism and kinetics of thermal degradation of polymers and in particular polyurethanes. The principal investigator and his staff synthesized a series of eighteen polyurethanes in which the molecular weight and amount of polyether oligomeric soft segment have been varied in a systematic manner. These polymers have been extensively and carefully characterized and their thermal degradation has been monitored by thermogravimetry, thermo-mechanical analysis, infrared spectroscopy, dilatometry, X-ray diffraction and by other measurements of changes in chemical, physical, and mechanical properties. The project has reached a stage where attempts to mathematically model the kinetics and formulate mechanisms for these very complex degradation processes are desirable.

Results and Significance of Achievements to Date

A superior polyurethane sealant for high pressure values has been developed and the improvement of durability of polyurethanes by blockage of their surfaces with chemical groups to suppress diffusion processes is under investigation.

List of Publications or Other Input that Resulted from the Project

None to date.

Guest Scientists who Visited NBS from Yugoslavia

Dr. Zoran Petrovic, March 23-March 30, 1982.

Visits to Yugoslavia of NBS Participant

Dr. Joseph Flynn, September 1981, 8 days.

Dr. Joseph Flynn, October 1982, 7 days.

Project Title: Basic and Applied Studies on Dithiocarbamates and Related Compounds
(Project Page 367, NBS(G)-273)

Years and Funds: 1981-1984, Dinars 3,000,000

Principal Investigator: Dr. Sergej Gomiscek

Yugoslav Institute: Department of Chemistry and Chemical Technology
E. Kardelj University

NBS Participant: Dr. Richard A. Durst

NBS Laboratory, Center, Division: National Measurement Laboratory,
Center for Analytical Chemistry, Organic Analytical Research Division

Summary Description of Project Goals

The objective of this project is to study the electrochemical behavior of metal-dithiocarbamate complexes and related compounds as potential potentiometric and voltammetric sensors.

The electrochemical behavior of these compounds in aqueous and non-aqueous systems as well as the phenomena of thin layers at the surface of dithiocarbamate electrodes will be studied primarily by potentiometric, coulometric and voltammetric methods. For the more complete understanding of the mechanisms of reaction and characterization of thin layers of metal complexes other analytical methods will also be applied. Poly(dithiocarbamate) chelating resins will be included in the investigation.

If the electrochemical studies on these complexes indicate electrocatalytic behavior, their potential applications could range from analytical sensors to photoelectrochemical energy conversion devices. In the area of analytical chemistry, chemically modified electrodes may be developed which show greatly improved selectivity and sensitivity over conventional electrochemical sensors. This would result from the electrocatalytic enhancement of the redox reaction rate and reduction of the reaction overpotential. This development could lead to sensors for toxic environmental pollutants and biocomponents of clinical significance.

Results and Significance of Achievements to Date

This project was initiated in the 1981-1982 contract year; progress in achieving the research goals is still in the preliminary stages. Investigations carried out prior to funding under the Joint S&T Cooperative Program provided basic data on the properties of the dithiocarbamates and their metal complexes which were necessary for a better understanding of these systems and therefore an important requirement for the realization

of the goals of this project. This preliminary work included the determination of solubility product constants and their behavior in aqueous solutions under conditions of heterogeneous equilibrium.

Electrochemical studies are in progress and include the polarography of disubstituted dithiocarbamates and the investigation of poly-(dithiocarbamate) chelating resins. Resins based on cross-linked 4-vinylpyridine/styrene copolymers containing dithiocarbamate or a related active group may provide an electrode modification approach for the preconcentration of analytes by a chelation/sorption process. Further investigations are necessary to elucidate the sorption mechanism, to characterize the structural properties of the resin and its complexes, and to synthesize related compounds with improved sorption characteristics.

List of Publications or Other Input that Resulted from the Project

1. M. Meula-Zigon, J. R. Dias, S. Gomiscek, "Studies on Metal Dithiocarbamates and the Preparation and some Properties of Metal Tetramethylenedithiocarbamates," Vest. Slov. Kem. Drus., 29 (1982) 23
2. M. Veber, V. Francetic, M. Vranicar, S. Gomiscek, "Polarography of Disubstituted Dithiocarbamates," Proceedings of 8th Yugoslav Symp. on Electrochemistry, Dubrovnik (1983).
3. V. Francetic, M. Veber, S. Gomiscek, "Polarographic Determination of P_k value of Tetramethylenedithiocarbamic Acid," Ibid.
4. V. Francetic, M. Veber, S. Gomiscek, "The Behavior of Metal Disubstituted Dithiocarbamates in Solutions under Heterogeneous Equilibria," Anal. Chem. Acta. (will be published).
5. V. Francetic, M. Veber, S. Gomiscek, "Solubility Product Constants of Metal Dithiocarbamates," Vestm. Slov. Kem. Drus. (will be published).

Guest Scientist who Visited NBS from Yugoslavia

1. Prof. Sergej Gomiscek, 1982

Visit to Yugoslavia of NBS Participant

1. Dr. Richard Durst, 1984

Project Title: Local Computer Networking
(Project Page 396, NBS(G)-276)

Years and Funds: 1982-1984, Dinars 3,500,000

Principal Investigator: Dr. Marjan Spegel

Yugoslav Institute: Jozef Stefan Institute

NBS Participant: Dr. Robert P. Blanc

NBS Laboratory, Center, Division: Institute for Computer Systems and
Technology, Center for Computer Systems Engineering

Summary Description of Project Goals

1. Install NBS Class 4 transport protocol software and adopt test tools to run the existing set of test scenarios.
2. Modify existing code implementing some of the design alternatives outlined in Volume 5 of the NBS transport specification. The design alternatives would apply, for example, to the acknowledgment strategy, adaptive retransmission strategy, and multiple priorities associated with connections.

Under the cooperative project NBS and the Jozef Stefan Institute are working together on the development of prototype implementations and measurement methods for international networking standards. The results should further NBS's efforts to implement and test international protocol standards on different computers, using different operating systems and different languages. Testing will lead to the development of performance measures for those protocols, as opposed to the correctness measures which have been developed to date.

The Jozef Stefan Institute will benefit by having protocols that facilitate computer-to-computer communication in their laboratories and by having the test methods to develop performance oriented implementations. The Institute will have available the NBS correctness techniques to assist in their prototype implementations. They will work with NBS scientists in the development of performance techniques to assure that the networking standards work well in a variety of computer/communication environments.

Results and Significance of Achievements to Date

There has been little visible progress on the part of the Jozef Stefan Institute in preparing for testing transport protocol. This is attributed to several factors, soon to be remedied. First, the Institute has not been successful in obtaining a VAX interface for the Cambridge Ring. They expect to obtain one soon from Logica in the United Kingdom. Second, the transport software has not been installed in the microprocessor and the minicomputer due to personnel illnesses and other assignments. The Institute promises to staff the project adequately. Additionally, transport test tools must be developed and an agreed upon test plan developed and accepted before testing can take place.

Progress has been made in three areas of related work: Cambridge Ring, Teletex, and Transport Simulator. The Institute has purchased a master and two stations for the Cambridge Ring. The VAX DMA interface from Logica is expected to be installed in six months. They are attempting to get local industry support for teletex development. The transport protocol programmer assigned to the Jozef Stefan Institute-NBS project has implemented Class 0 transport for this period. They have been working on a transport simulator, but have experienced problems due to lack of UNIX documentation. They have decided to use the DEC VMS operating system. The transport simulator is expected to be completed in six months.

List of Publications or Other Input that Resulted from the Project

The Jozef Stefan Institute will have a summary of the protocol programmers work to date written and translated and will send this to NBS for prepublication review.

Guest Scientists who Visited NBS from Yugoslavia

1. Dr. Tomaz Kalin, 1983
2. Drs. Majan Spegel and Robert Reinhardt, 1983

Visits to Yugoslavia of NBS Participants

1. Drs. Robert Blanc and John Heafner, 1982
2. Drs. John Heafner and Kevin Mills, 1984

Project Title: Fracture Mechanics of Weldments
(Project Page 414, NBS(G)-278)

Years and Funds: 1982-1984, Dinars 10,620,000

Principal Investigator: Prof. S. Sedmak

Yugoslav Institute/s: Faculty of Technology and Metallurgy, University
of Belgrade
Technical High School, University of Maribor
Technical Sciences, Novi Sad University

NBS Participant: Dr. Richard Reed

NBS Laboratory, Center, Division: Center for Materials Science,
Fracture and Deformation Division

Summary Description of Project Goals

This program generally addresses fracture mechanics test methodology of weldments. The specific objectives of the program are to:

- evaluate the weldments quality of steels of different strength levels,
- introduce fracture mechanics test methods and analysis, as well as other modern testing methods in weldments assessment application; and
- compare the properties of weldable steels developed and produced in Yugoslavia with the steels of same properties, produced by well known steelmakers from abroad.

High-strength low-alloy and fine-grained structural steels have been selected for use. These steel classes are expected to be used extensively and have higher strengths than conventional alloy steels. Their ability to retain strength during welding currently restricts usage. The welding procedures to be evaluated include submerged arc, gas-shielded arc and manual arc; these are best suited for high-productivity structural welding.

The types of mechanical tests include: (1) tensile test; (2) instrumented impact tests (Charpy V); (3) drop weight test - ASTM E 208; (4) fracture toughness test - ASTM E 399; (5) crack opening displacement test British Standard 5762; (6) resistance curve determination - ASTM E 561; and (7) contour J integral tests - ASTM E 813T.

The determination of toughness of single and multi-pass weldments is a complex problem. Residual stress, under or over-matching weld strength, dendritic solidification and plastic anisotropy, coupled with the usual restricted through-thickness, combine to prevent single crack-opening-displacement J-integral and bend specimen tests from being completely meaningful. The program will explore these variables to establish reliable weldment toughness test methodology.

Radiography, ultrasonics or dye penetrant NDE techniques will be used to assess weldment integrity. Weldments containing controlled variables will be produced and the toughness evaluated, using various test methodologies, to assess the reliability of the tests. Weldment yield strength and work hardening characteristics will be varied to assess the role of material tensile behavior in affecting toughness measurements.

Results and Significance of Achievements to Date

Dr. B. Petrovski, Faculty of Technology and Metallurgy, Belgrade, was a guest worker at the NBS-Boulder Laboratories. The goal of joint research that he conducted during his stay at NBS was to clarify the effect of strength difference, between weld and base metal on the driving force for fracture for surface flaws in tensile panels. High strength low alloy (HSLA) steel was chosen as the specimen material system. Specimen materials were supplied by the Faculty of Technology and Metallurgy, University of Belgrade. Four types of specimen blanks, base plate, and under-, normal-, and over-matched weldments were used. For each type, three specimens were tested: no crack, small surface crack and large surface crack. The uncracked specimens were used to obtain strength data for the weldments; the cracked specimens allowed measurement of the interaction of weld strength matching with flaw size.

A recently developed technique for direct experimental evaluation of the J-contour integral, in which integrand quantities are measured using strain and displacement gages and J is obtained by numerical integration, was applied.

Results showed that for relatively large flaws, net section yielding and attendant large driving force for fracture occurred for all the specimens, including the over-matched weldments. For the smaller flaws, net section yielding occurred for the under-matching weldment but the over-matching weld exhibited gross section yielding, with an attendant smaller driving force for fracture.

These results provide an experimental benchmark for analysis techniques that seek to predict the interaction among weld strength matching, flaw size, and the fracture process; furthermore, they give an empirical demonstration of the effectiveness of over-matching weld strength in reducing the driving force for fracture.

Other achievements this year include the following:

J Contour Integral and J_R Curve Analysis

Three series of experiments were performed. The first was carried out on the welded joints, produced using the same consumable, but three different HSLA steels of the same nominal strength level (700 MPa for yield stress and 800 MPa for ultimate tensile strength). The steels chosen had been produced in Japan (SUMITEN 80P), in West Germany (N-A-XTRA 70 and in Yugoslavia (NIONICRAL 70), and the electrode for MAW was TENACITO 75 produced in Yugoslavia. The second series of experiments consisted of tests performed on specimens made of A516 or Gr 70 steel (produced in West Germany) and MAW and SAW weldments. In this experiment acoustic emission was monitored. In the third series, the specimens were machined from weldments with different degrees of undermatching strength. These experiments were carried out by the TMF and NBS collaboration. The specimens of SUMITEN 80P and SUMITEN 60 welded joints with the different degree of undermatching effect were prepared in Yugoslavia and tested in the U.S., by using the direct NBS J integral measurement method. The analysis of the results, obtained in the three series of experiments, will be continued in 1984.

Comparison of the Different Fracture Mechanics Parameters:

The first task is the geometric analysis of the effect of crack tip position on COD measurements. The differences in the integral value produced by modification of the normalized three point bend specimens were considered by numerical approaches. The finite element method was applied in this calculation, and it was shown that the 8% difference in the J integral for the modified shape results only in 1% difference of J value.

Low Cycle Fatigue Tests:

The three point bend specimens of N-A-XTRA 70 steel and its welded joints have been prepared for testing. The tests will be performed in 1984.

Experiments on the prototype:

The two first tests, performed in the low cycle fatigue region on the cylindrical pressure vessel welded prototype, made of 16 mm thick SUMITEN 80P steel plates, have shown that the behavior of pressurized prototype is in accordance with the expected linear elasticity below the yield stress. The notched test-piece was designed and machined with the notch positioned in the metal weld. The next step will be cutting of a window on the prototype cylindrical shell and welding the prepared test piece. After that, low cycle fatigue tests will be performed by pressurizing the prototype.

Further analysis of acoustic emission:

The application of acoustic emission in the sensing of crack growth during fracture tests has been encouraging. Therefore, a new device that enables the separation of different acoustic emission levels has been developed. The first tests, performed using the new device have shown that the separation of acoustic emission levels will be very useful information.

Comparison of the Fracture Mechanics Parameters of Three Differently Alloyed HSLA Steels:

The results, obtained in this experimental investigation, are summarized and were presented in a published paper at ICM 4. The same experiment will be continued with the welded joints of these steels, as is mentioned in (1).

Analysis of the Cracked Pressure Vessels:

The first part of this analysis was performed on the penstock model, that was experimentally tested some years ago, before the construction of "Bajina Basta" penstock had started. The second part is a numerical computer analysis, using the program for elastic behavior of cracked pressure vessel shell. FEM analysis for the same problem is under consideration and a decision on its application will be made in the near future.

List of Publications or Other Input that Resulted from the Project

1. S. Sedmak, Lj Nedeljkovic, A. Radovic, "Investigation of Mechanical and Structural Anisotropy of N-A-CTRA 70 MIG Weldments," 4th European Conference on Fracture, Proceedings, Vol. I Fracture and Fracture Toughness (1982) 228-235.

(Correlation of the properties of different park in MIG welded joints of N-A-XTRA 70 steel to the properties of heat treated samples, instrumented impact and three point bending tests.)

2. V. Radmilovic, Dj. Drobnjak, M. Rogulic, "Ductile Fracture in V/Nb Dual Phase Steel," 4th European Conference on Fracture, Proceedings Vol. I - Fracture and Fracture Toughness (1982) 322-327.

(The results of tensile testing and SEM of a V/Nb dual phase steel show that properties of martensite which coexists with ferrite in a dual phase structure play an important role in crack initiation and propagation. The fracture process of a soft low carbon and a hard high-carbon martensite is controlled by ferrite/martensite decohesion and martensite cracking, respectively.)

3. I. Rak, F. Vodopivec, V. Gliha, "Investigation of HAZ ductility by Using Vibration Microstress Relieving on Steels Susceptible to Reheat Cracking," IIW/IIS Doc. IX - 1249/82, IIW/IIS Doc. X - 1026/82, 35th Annual Assembly of International Institute of Welding, Ljubljana (1982).

(Three types of HSLA steels - NIOVAL 47 and NIONICRAL 40, produced by Jesenice - Yugoslavia, and SUMITEN SUM 80P, produced by Sumitomo Japan, were tested to evaluate the effect of vibration before stress-relief heat-treatment on reducing of microstresses around dislocations.)

4. S. Sedmak, B. Petrovski, "Stress and Strain Distribution on HSLA Steel Welded Pressure Vessel," International Meeting of Chemical Engineering ACHEMA 82, Frankfurt (1982).

(Using the results of experiments on a pressure vessel prototype, it was shown that the global safety of pressure vessel, welded with undermatched consumable, is questionable under stress concentrations. Undermatching effects produce weld metal of lower strength and toughness compared to the base metal, and post-yield fracture becomes inevitable when working stress locally reach yield point.)

5. I. Glavardanov, S. Sedmak, B. Petrovski, "Determination of crack Resistance Properties of HSLA Steel and its Welded Joint Using J Integral," 8th Congress on Material Testing in Budapest.

(The results of single-specimen partly unloaded tests, with different initial ligament length, are presented for base metal and SAW weld metal of SUMITEN 80P steel. The J curves for test results are plotted, following the Sumpter-Turner calculation method.)

6. A. Radovic, S. Sedmak, Lj. Nedeljkovic, "Effect of Local Plastic Deformation on the Safety of Welded Steel Penstock," International Symposium - Stresses and Deformation of Welded Construction, Zagreb (1982).

(This paper summarizes the results of an experimental investigation of a prototype, made of SM 80P HSLA steel 45-mm thick in the shape of the pressure vessel, corresponding to the most stressed part of the penstock for hydroelectric pumping up power plant "Bajina Basta", recently introduced in electric power in Yugoslavia.)

7. Lj. Nedeljkovic, A. Radovic, S. Sedmak, "Microstructural Analysis of the Cold Working Effect on the Fracture Toughness of Weld Metal in HSLA Steel Welds," 5th International Conference on Fracture (ICF5), Cannes, France - Advances in Fracture Research Vol. 3 (1981) 1193-1200.

(The analysis of stresses and strains in elastic and plastic regions of the prototype penstock was made, based on data measured by strain gages during pressurizing. From comparisons of data on specimens from deformed prototype and undeformed welded trial samples it was concluded that the safety of the penstock is satisfactory.

8. A. Radovic, S. Sedmak, Lj Nedeljkovic, "Comparative Study of Crack Resistance Properties of Three Differently Alloyed HSLA Steels," presented at ICM 4 (4th International Conference on Mechanical Behaviour of Materials) Stockholm, Sweden (1983).

(Alloy of three quenched and tempered HSLA steels (SUMITEN 80P, N-A-XTRA 70 and NIONICRAL 70, differently produced to 700 Mpa yield stress) are analyzed in terms of alloying, microalloying and cleanliness levels, and the effect of each on the crack resistance properties measured by Charpy V and J integral values is determined.)

9. I. Rak, V. Gliha, J. Kunder, "Pressure and Water Hammer Testing of Penstock Model," accepted for presentation at JOM-2 (International Conference on Metal Joining), Copenhagen, Denmark (1984).

(The paper summarizes experimental results, obtained on a welded SUMITEN 80P steel penstock model by pressuring and water hammer loading. The region of weldment in which artificial defects of design allowable sizes (from FM calculations) were introduced has been investigated.)

10. S. Sedmak, "Modern Aspects in Pressure Vessels and Penstocks Design and Construction," "Gosa" Institute and Faculty of Technology and Metallurgy, Belgrade (1983), in Serbo-Croatian.

(The monograph represents a collection of lectures and discussion from the Second International Fracture Mechanics Summer School, Velika Plana, Serbia (1982).)

11. A. Sedmak, "Finite Element Analysis of Fracture Mechanics Parameters using Rapid Mesh Refinement," accepted for presentation at ICF6 (6th International Conference on Fracture) to be held in New Delhi (December 1984).

(Rapid mesh refinement technique enables accurate modeling of cracked bodies response to the applied load. Simplex isoparameter triangular elements are applied in this analysis due to simplicity and generality in their formulation. A simple procedure based on the displacement field, is defined for the evaluation of stress intensity factor or J integral. The analysis of the errors enables

one to optimize the acting parameters. A final result is a possibility to use simple, commercially available program and simplex elements for accurate evaluation of fracture mechanics parameters with small number of freedom and without limitations on material properties.)

12. I. Potrc, A. Alujevic, J. Legat, P. Skrget, "Boundary Elements in Elasto-plasticity - BEPLAS Code Application," submitted to the Conference on Numerical Method Applications, Stubicke Toplice, (1983) in Slovenian.

(The paper presents the boundary elements application to non-linear problems (plasticity) part of continued study of boundary elements application in elasticity problems. Based on the theory of boundary elements in plasticity (PPPR-82) the computations by the BEPLAS code have been performed on VAX computer. Results of plastification evaluations for several components are presented, e.g. a "compound" tube, notched beam bending and an evolvent gear tooth.)

13. S. Sedmak, A. Radovic, "Analysis of Mechanical Properties of SAW Welded Joints of Fine-grained Steels of Different Strength Classes," presented at the International Symposium - Submerged Arc Welding and Electroslag Welding, Yugoslavia (1984) in Serbo-Croatian.

(The problem of cracking in SAW weldments of HSLA steels of 800 MPa strength class is overcome by using lower strength consumables. The introduced "undermatching" effect of weld metal was analyzed.

The SAW weldments of two fine-grained steels with "overmatched" and "undermatched" weld metals (A516 Gr 70 and SUMITEN 80P, respectively) were experimentally tested and the behavior of weld metals and weldments in tensile test and Charpy impact tests were compared with the base metal.)

14. Lj. Cvetkovic, Dj. Mitrovic, S. Sedmak, "The Comparison of Mechanical Properties and Acoustic Emission of Precracked Specimens of a Fine-grained Steel Thick Plate and its SAW Welded Joint," presented at the International Symposium - Submerged Arc Welding and Electroslag Welding, Yugoslavia (1984) in Serbo-Croatian.

(The paper presents SAW technology, applied to 120 mm thick A516 Gr 70 steel plate. The results of tensile tests, instrumented impact tests, guided bend tests and hardness determination have shown that welded joint, base metal and weld metal performances are satisfactory. The weld metal exhibits equal or better tensile properties compared to the base metal. Acoustic emission signals have shown different behavior of BM and Wm when the cracks develop in the plastic region.)

15. B. Gnjatovic, S. Sedmak, "The J Integral Application for Crack Resistance Evaluation of Fine-grained Steel Submerged-arc Welded Joint," presented at the International Symposium Submerged Arc Welding and Electroslag Welding, Yugoslavia (March 1984)

in Serbo-Croatian.

(Precracked specimens were tested using three-point bend tests to determine the crack resistance properties of the SAW weld metal and to compare with the behavior of the base metal under the same conditions. The 120 mm thick steel plates, of A516 Gr 70 were SAW welded using EPP3 wire and EP50 flux. The 25 x 50 x 220 mm specimens were cut from welded joint, and fatigue cracks were located in base metal and in weld metal. STM E813/81 standard method was used for determination of J_{IC} and K_{IC} values. The values of $J_{IC} = 283 \text{ kJ/m}^2$ and $K_{IC} = 241.45 \text{ MPa}\sqrt{\text{m}}$ for base metal and of $J_{IC} = 100.0 \text{ kJ/m}^2$ and $K_{IC} = 144.91 \text{ MPa}\sqrt{\text{m}}$ for weld metal are obtained.)

Guest Scientists who Visited NBS from Yugoslavia

1. S. Sedmak, L. Nedeljkovic, J. Legat, 1983
2. I. Glavardanov, 1984
3. B. Petrovski, guest scientist, July 1983-March 1984
4. S. Sedmak, I. Rak, July-August 1984

Visits to Yugoslavia of NBS Participants

1. R. Reed, 1981
2. E. Fuller, D. Read, 1981
3. R. Reed, M. Kasen, D. Read, 1984

Project Title: Experimental and Theoretical Investigations of Ion-atom Collision Processes (relevant to fusion research)
(Project Page 434, NBS(G)-279)

Years and Funds: 1983-1984, Dinars 2,800,000

Principal Investigator: Dr. Ratko K. Janev

Yugoslav Institute: Institute of Physics, University of Belgrade

NBS Participant: Dr. Gordon H. Dunn

NBS Laboratory, Center, Division: National Measurement Laboratory,
Center for Basic Standards, Quantum Physics Division

Summary Description of Project Goals

The project consists of two parts, theoretical and experimental, both aimed at generating quantitative information on atomic collision cross sections which are needed in the present-day fusion research (for plasma modelling and diagnostics, studies of energy loss, particle escape, etc). The main goals of theoretical investigations within the project were the advance of theoretical concepts and methods for describing the inelastic atomic processes occurring in collisions between ions and atoms (such as charge transfer, ionization, excitation, etc.) and on this basis to perform corresponding cross section calculations for collision partners and in energy regions which are of interest to magnetic fusion research. Particular attention is devoted to the processes involving multiply charged ions of impurity species in tokamak and mirror plasmas as they are connected with the energy balance and diagnostics of these plasmas.

The main goal of the experimental part of the project for this period was to make the necessary preparations for building an experimental set-up which would allow cross-section measurements for charge transfer and ionization in low-to intermediate-energy collisions of atoms with multiply charged ions. These preparations include: development of adequate ion sources able to produce high-charge-state ion fluxes of necessary intensity, and constructing a collision chamber with the associated detection techniques.

Results and Significance of Achievements to Date

The theoretical investigations within this project have been focussed on three topics:

(a) Total cross section calculation for charge transfer (δ_{cx}) and ionization (δ_{ion}) of hydrogen and helium atoms by medium and highly charged plasma impurity ions (C^{q+} , N^{q+} , O^{q+} , Fe^{q+}), (b) Creation of ionic excited states by electron capture in collisions of highly charged ions with atoms (in particular atomic hydrogen) and (c) Decay of atomic Rydberg states in collisions with ions.

Along the research line (a) a Monte-Carlo (CTMC) code has been used to calculate δ_{cx} and δ_{ion} which allows for arbitrary central-symmetric interactions of the active electron with the target ionic core and the projectile ion. Representing these interactions by suitable variable-charge pseudopotentials (constructed to account for the electronic structure of the cores), it was possible for the first time to treat capture and ionization by incompletely stripped multicharged ions within the CTMC methods. δ_{cx} and δ_{ion} cross sections have been calculated⁴ by this method for $H, He + C^{q+}, N^{q+}, O^{q+}$ collisions ($q = 3 - Z$, Z being the nuclear charge of the ion) in the energy range of 30 - 300 keV/amu. Similar calculations have been done for $He + Au^{q+}$ ($q = 5-25$), where the transfer-ionization channel has also been included. The results obtained are important for modelling of both central and periphery tokamak plasmas. Work is now in progress for $H, He^+, He + Fe^{q+}$ ($q = 3-26$) collisions.

Along the research line (b), cross sections for state-selective electron capture have been calculated³ by the CTMC method for $He + Au^{q+}$ ($q = 9-16$) collisions at $E = 100$ keV/amu, and similar calculations are in progress for $H, He + Fe^{q+}$ collisions at 50, 100 and 200 keV/amu. A model for population of angular momentum substates in hydrogen-fully stripped ion electron capture collisions has also been formulated⁵. The model has been tested on the $H + C^{6+} \rightarrow H^+ + C^{5+}$ (4 &) process and proved to be successful (results were compared with the 33-MO close coupling calculations of T. Green and associates). A review article on state-selective electron capture in atom-multicharged ion collisions has also been written.⁷

Within the theme (c) the decay of atomic Rydberg states in collisions with heavy charged particles was considered at adiabatic collision velocities². In this region, the charge transfer channel dominates. Specific calculations, based on both over-barrier and under-barrier electron transition mechanisms, have been performed for the $H^{**}(n) + p$ system¹, showing good agreement with the experiments of Koch and Bayfield ($n = 45-50$). Further work, involving more sophisticated description of decay dynamics, is now in process.

We have also generalized the adiabatic theory of two-electron capture in ion-atom collisions to the case of open-shell collision partners⁶ and to molecular collisions (to be published). The work on a low-energy model for the process of simultaneous capture and ionization in collisions of complex atoms with multicharged ions is now also in progress.

On the side of preparations for the experimental work within the project the following has been achieved:

(i) A detailed study of the physical and technical aspects of the experimental program has been performed, with definition of scientific priorities in the program and a detailed scheme of planned experiments. Capture into excited states by using the spectroscopic detection method has been chosen for one of the major immediate experiments. In the course of its preliminary stage total cross sections for charge exchange and ionization will also be measured.

(ii) A detailed technical plan for construction of an ECR ion source is now available (in collaboration with the Boris Kidric Institute for Nuclear Sciences in Belgrade), and a small part of the funds for its construction have been approved by the International Atomic Energy Agency. We expect work on the construction of the ion source may begin during 1984.

List of Publications or Other Output that Resulted from the Project

1. R. K. Janev, C.J. Joachain, N. N. Nedeljkovic, "Resonant Electron Transfer in Slow Collisions of Protons with Rydberg Hydrogen Atoms," Phys. Rev. A 29, No. 3 (1984) in press.
2. N. N. Nedeljkovic, C. J. Joachain, R. K. Janev, "Decay of Rydberg States in the Field of a Highly Charged Ion," Phys. Lett. A (1984) in press.
3. M.R.C. McDowell, R. K. Janev, "Electron Capture, Ionization and Transfer-ionization in fast $Au^{q+} + He$ Collisions," J. Phys. B (1984) in press.
4. R. K. Janev, M.R.C. McDowell, "Electron Removal from H and He Atoms in Collisions with C^{q+} , N^{q+} and O^{q+} Phys. Lett. A (1984) submitted.
5. T. P. Grozdanov, D. S. Belic, "A Model for Electron Capture into Specific Angular Momentum States in Collisions of Hydrogen Atoms with Fully Stripped Ions," Physica Scripta (1984) submitted.
6. T. P. Grozdanov, R. K. Janeve, V. Yu. Lazur, "Two-electron Exchange in Ion-atom Collisions at low Energies," J. Phys. B (1984) submitted.
7. R. K. Janev, H. Winter, "State-selective Electron Capture in Atom-highly Charged Ion Collisions," Phys. Reports (1984) submitted.
8. R. K. Janev, D. S. Belic, T. P. Grosdanov, D. Ciric, "Atomic Physics Experimental Program with the ECR Ion Source VINIS," Boris Kidric Institute Report, Belgrade (1984) in Serbo-Croatian.

(A few more publications are in a preparation stage. These and the work now in progress are likely to result in about 4-6 additional publications by September 1984.)

Guest Scientists who Visited NBS from Yugoslavia

Dr. D. S. Belic, 1984, 2-1/2 months

Visits to Yugoslavia of NBS Participant

None

Project Title: Bridge Columns Subjected to Reversed Cyclic Loading
(Project Page 445, NBS(G)-280)

Years and Funds: 1983-1984, Dinars 5,000,000

Principal Investigator/s: Prof. Jakim Petrovski
Prof. Vladimir Bickovski

Yugoslav Institute: Institute of Earthquake Engineering and Engineering Seismology, University of Kiril Metodij, Skopje

NBS Participants: Dr. William C. Stone

NBS Laboratory, Center, Division: National Engineering Laboratory,
Center for Building Technology, Structures Division

Summary Description of Project Goals

To determine the influence of size (scale factor) on the seismic performance of bridge columns and obtain performance data (strength and ductility) of full-scale bridge columns.

Results and Significance of Achievements to Date

The following activities have been completed relative to the full-test set up:

- Deep caisson foundation completed
- 14m high reaction wall completed. Vertical and lateral post-tensioning pending.
- Contract let for conversion of 12,000,000 UTM to computer control. High pressure/high volume servo-valves and service manifold have arrived.
- 1200 kip lateral actuator system has been received. Calibration now pending.
- Computer facility components have arrived and are undergoing shakedown
- Design and assembly of signal conditioning units for 100 data channels have been completed.
- Test specimens designed.

Specimen tests of 1/5 scale have been initiated.

Damage to bridge columns in the San Fernando earthquake of 1971 highlighted the need for reassessment of existing seismic design practice for bridges. During that event, a magnitude 6.5 on the Richter scale, five bridges collapsed, and 42 others were seriously damaged. Since that time column design requirements have been changed and now specify additional confinement steel to avoid compression buckling of longitudinal reinforcement and continuous steel at the footings and bent cap to avoid one of the more dramatic failure modes observed in the San Fernando event: complete pullout of the column reinforcement from the bridge foundation with a subsequent toppling of the bridge.

New column designs, despite predictions of being able to withstand a magnitude 8 quake (the equivalent of the one that destroyed San Francisco in 1906), have not been tested. Considerable controversy still exists as to the amount of confining reinforcement required to ensure adequate ductility (energy absorption capacity) without significant degradation in strength. The effect of the large scale reinforcement used in bridge columns was also considered to be of critical interest, since yield and bond characteristics change with size. The reinforcing bars used in most buildings are commonly three to six times smaller than those used in bridges. To answer these questions the National Bureau of Standards has undertaken a program to investigate the performance of large scale bridge columns subjected to simulated seismic loads.

List of Publications or Other Input that Resulted from the Project

The nature of the project would need a much longer lead time before any report can be prepared.

Guest Scientists who Visited NBS from Yugoslavia

None to date.

Visits to Yugoslavia of NBS Participant

Although the visit was not under the U.S.-Yugoslav Cooperative Program, Dr. Charles Culver took the opportunity of travel to Yugoslavia to visit and discuss the project.

Project Title: Determination of Liquefaction Potential of Level Sites by Cyclic Strain
(Project Page 446, NBS(G)-281)

Years and Funds: 1983-1984, Dinars 4,000,000

Principal Investigator: Prof. K. Talaganov

Yugoslav Institute: Institute of Earthquake Engineering and Engineering Seismology, University Kiril and Metodij, Skopje

NBS Participant: Dr. Riley M. Chung

NBS Laboratory, Center, Division: National Engineering Laboratory, Center for Building Technology, Structures Division

Summary Description of Project Goals

To determine the correlation between cyclic strain and pore water pressure build-up and volume change for sandy and silty soils, and to develop a new design approach based on these correlations.

Results and Significance of Achievements to Date

The following activities have been completed:

- The study of sample size effect on the results of cyclic shear tests.
- The study of effect of frequency on cyclic strength of saturated sands.
- Successfully conducted a comparison of energy measurements during Standard Penetration Testing using the cathead and rope method in the U.S. practice.
- Three basic questions associated with the problem of soil liquefaction were investigated:
 - behavior of sand under cyclic strain application - laboratory testing program
 - mathematical modeling - Davidenkov's model
 - development of two specific computer codes

Damages to structures, due to complete or partial liquefaction of supporting soils of these structures during earthquakes, have been a major concern of the design profession. An excellent example of these damages can be illustrated by the overturning of the apartment buildings during the 1964 Niigata, Japan Earthquake. These buildings were overturned like dominoes while the superstructures were still intact. Excessive settlement of buildings due to partial liquefaction of supporting soils also renders the buildings useless. Numerous cases can be cited for this type of permanent foundation damage.

We have recently proposed a new approach, the "cyclic strain method," to the liquefaction assessment. It has long been recognized that it is the magnitude of shear strain, not the shear stress, that causes the degradation of shear modulus of a soil mass, thus developing excess pore water pressure in the saturated soil. We have also postulated that there exists a threshold shear strain value, below which there should be no degradation of shear modulus; therefore, no excess pore water development and no liquefaction potential. This threshold strain concept has been verified analytically. For normally consolidated sandy soils, this value is at about 10-2%. Limited laboratory cyclic strain controlled tests conducted on sandy soils have also resulted in a threshold shear strain value at around the same value. The test results also indicate that the method of sample preparation is not a factor influencing the number of strain cycles to cause initial liquefaction.

A key soil property required for this approach is the in-situ soil shear modulus, G_{max} . Fortunately, G_{max} is probably one of the very few properties that can be quite reliably determined in the field. This certainly adds to the advantage of using this strain approach.

List of Publications or Other Input that Resulted from the Project

1. R. M. Chung, F.Y. Yokel, H. Wechler, "Pore Pressure Build-up in Resonant Column Tests," Journal of Geotechnical Engineering, ASCE (1984).
2. R. M. Chung, F.Y. Yokel, V.P. Drnevich, "Evaluation of Dynamic Properties of Sands by Resonant Column Testing," Geotechnical Testing Journal, ASTM (1984).
3. R. M. Chung, F.Y. Yokel, "Volume Change of San Deposits Subjected to Cyclic Shear," Proceedings, 8th WCEE (1984).
4. W. D. Kovacs, F.Y. Yokel, L.A. Salomone, R. Holtz, "Liquefaction and the International SPT," Proceedings, 8th WCEE (1984).
5. W. D. Kovacs, L.A. Salomone, F. Y. Yokel, "Comparison of Energy Measurements in the Standard Penetration Test Using the Cathead and Rope Method," NRC Report (1983).

6. K. Talaganov, J. Petrovski, V. Mihailov, "Soil Liquefaction Seismic Risk Analysis Based on Post 1979 Earthquake Observations in Montenegro."
7. K. Talaganov, V. Mihailov, T. Bogoevski, "Analysis of Soil Liquefaction During 1979 Montenegro Earthquake."
8. K. Talaganov, D. Aleksovski, "Soil Stability and Urban Design Case Study."

Guest Scientists who Visited NBS from Yugoslavia

1. Mr. Miha Tomazevic and Mr. Roko Zarnic, 1984, two days

Visits to Yugoslavia of NBS Monitor

Although the visit was not under the U.S.-Yugoslav Cooperative Program, Dr. Charles Culver took the opportunity of a travel to Yugoslavia to visit and discuss the project.

Project Title: The Development of Topography and the Erosion of
Metal Surfaces Under the Impact of Fast Ions
(Project Page 447, NBS(G)-282)

Years and Funds: 1983-1984, Dinars 3,3400,000

Principal Investigator: Drs. Lamija and Nenad Tanovic

Yugoslav Institute: Faculty for Electrical Engineering, University
of Sarajevo

NBS Participant: Dr. Joseph Fine

NBS Laboratory, Center, Division: National Measurement Laboratory,
Center for Chemical Physics, Surface Science Division

Summary Description of Project Goals

- To investigate mechanisms of surface topography change that result from bombardment with keV inert gas ions.
- To develop quantitative methods for characterizing and measuring surface microtopography in the few nanometer range.
- To characterize surface topography change as a function of sputtered depth for elemental and multicomponent solids and at solid/solid interfaces.

Results and Significance of Achievements to Date

Due to the rather limited laboratory research facilities available in Sarajevo and because of severe importation restrictions, initiating a new project at this time can be difficult. Nevertheless, the Yugoslav principal investigators have made arrangements to have access to a high resolution scanning electron microscope in Sarajevo and have access to facilities in other laboratories in Yugoslavia (at the Jozef Stefan Institute and at Boris Kidric Institute) to do some of their work.

They are presently constructing an apparatus for x-ray diffraction imaging of surface topography and also are building a system to measure total integrated scattered light from non-smooth surfaces. It is anticipated that some of these techniques will be capable of quantification; such measurements related directly to the NBS programs in surface standards, SRMs for surface analysis, and interface width measurement of thin-film SRM structures.

The role of microtopography in determining sputtered interface widths is not understood. At NBS we have made extensive interface width analyses of multilayered thin-film structures under various ion beam conditions. These same sputtered thin-film specimens will be used in Sarajevo to measure microtopography development and its relationship to interface width.

The development of new methods for surface microtopography characterization and measurement will have significant impact in surface science not only in areas related to ion bombardment sputtering but also in the study of epitaxy, thin films, and surface reactions. These areas are related to applied problems in semiconductor technology, corrosion, and surface modification of materials, to name a few. We believe that results of such a joint project will find specific application in many industries such as semiconductor, laser optics, corrosion, and surface treatment.

List of Publications or Other Input that Resulted from the Project

None

Guest Scientists who Visited NBS from Yugoslavia

1. Drs. Lamija and Nerad Tanovic (expected to visit for two weeks in 1985)

Visits to Yugoslavia of NBS Participant

1. Dr. Joseph Fine, 1979, 1 day
2. Dr. Joseph Fine, 1984, 1 week

Project Title: Evaluation of Aseismic Provisions in the U.S.
and Yugoslavia
(Project Page 448, NBS(G)-283)

Years and Funds: 1983-1984, Dinars 2,100,000

Principal Investigator: Prof. Peter Fajfar

Yugoslav Institute: Department of Civil Engineering, University E.
Kardelj, Institute of Structural and Earthquake Engineering

NBS Participant: Dr. E. V. Leyendecker

NBS Laboratory, Center, Division: National Engineering Laboratory,
Center for Building Technology, Structures Division

Summary Description of Project Goals

To compare and evaluate the aseismic design provisions in the ATC-3 documents in the U.S. and the 1982 aseismic code in Yugoslavia. Results of the evaluation will be used to revise and improve the Yugoslav code as well as the U.S. code to include the most up-to-date technology in the area of earthquake resistant design.

Results and Significance of Achievements to Date

The following activities have been completed:

- The comparison of the characteristics of the earthquakes in the U.S. and in Southern Europe.
- The study of the influence of the method of the analysis and of the vertical distribution of seismic forces on the design shear forces and overturning moments.
- The analysis and design of a 7-story RC building.

List of Publications or Other Input that Resulted from the Project

1. "Dynamic Response of Structural Systems Subjected to Horizontal Propagating Shear Waves," Proceedings, 8th WCEE (1984).
2. "Dynamic Stability of Structures Subjected to Shear Waves," Proceedings, Structural Stability Research Council Conf. (1984).

3. "Dynamic Eccentricity of Structures Subjected to S-H Waves,"
Journal of Earthquake Engineering and Structural Dynamics (1984).
4. "An Analytical Study of the Behavior of Unreinforced Masonry Walls
Subjected to Biaxial Stresses," NBSIR to be completed in 1984.
5. P. Fajfar, M. Fischinger, "Parametric Study of Inelastic Response
to Some Earthquakes Recorded in Southern Europe," Proceedings,
8th WCEE (1984).
6. P. Fajfar, M. Fischinger, "Comparison of Code Procedures for Seismic
Analysis of Buildings," presented at the Seminar Tall Structures and
Use of Prestressed Concrete in Hydraulic Structures, Indian National
Group of the JABSE, New Delhi (1984).
7. P. Fajfar, M. Fischinger, "Dynamic Analysis of RC Buildings - How
Much Sophistication is Justified," International Conference on
Computer-aided Analysis and Design of Concrete Structures, Split,
Yugoslavia (1984).

Guest Scientists who Visited NBS from Yugoslavia

1. Mr. Miha Tomazevic and Mr. Roko Zarnic, 1984, two days

Visits to Yugoslavia of NBS Participants

Although the visit was not under the U.S.-Yugoslav Cooperative Program, Dr. Charles Culver took the opportunity of travel to Yugoslavia to visit and discuss the project.

Project Title: Behavior of Horizontally Reinforced Masonry Shear Walls Subjected to Cyclic Lateral Loading
(Project Page 449, NBS(G)-284)

Years and Funds: 1983-1984, Dinars 2,670,000

Principal Investigator: Prof. Miha Tomazevic

Yugoslav Institute: Institute for Testing and Research in Materials and Structures, and Institute for Structures and Earthquake Engineering, Ljubljana

NBS Participant: Dr. Kyle Woodward

NBS Laboratory, Center, Division: National Engineering Laboratory, Center for Building Technology, Structures Division

Summary Description of Project Goals

To develop a rational procedure for determining the ultimate shear strength characteristics of reinforced and unreinforced masonry building shear walls for use in structural design.

Results and Significance of Achievements to Date

The following activities have been completed:

- Achieved fully operational status for the NBS Tri-directional Test Facility.
- Tests on 36 walls.
- A study of masonry infilled reinforced concrete frames subjected to cyclic lateral loading.
- A shaking table study of a 1/7-scale model modeling a four-story masonry building.
- The study of the effect of horizontal reinforcement on strength and ductility of masonry walls.

The data obtained from these research programs provide guidance to structural designers on the most effective method of resisting loads using the minimum material and/or cost.

List of Publications or Other Input that Resulted from the Project

1. The NBS Tri-directional Test Facility, NBSIR 84-2879.
2. Three NBSIR reports are currently under internal review:
"Influence of Vertical Compressive Strength on Shear Resistance of Concrete Block Masonry Walls,"
"Influence of Aspect Ratio on Shear Resistance of Concrete Block Masonry Walls,"
"Influence of Block and Mortar Strength on Shear Resistance of Concrete Block Masonry Walls."
3. Miha Tomazevic, Roko Zarnic, "Shaking Table Study of a Four-Story Masonry Building Model," Proceedings, 8th WCEE Conference (1984).
4. Roko Zarnic, Miha Tomazevic, "The Behavior of Masonry Infilled Reinforced Concrete Frames Subjected to Cyclic Lateral Loading," Proceedings, 8th WCEE Conference (1984).
5. Miha Tomazevic, Roko Zarnic, "The Effect of Horizontal Reinforcement on Strength and Ductility of Masonry Walls," CIB Symposium on Wall Structures, Warsaw (1984).
6. Miha Tomazevic, Roko Zarnic, "The Effect of Horizontal Reinforcement on Strength and Ductility of Masonry Walls - Part One," Institute of Testing and Research in Materials and Structures, Ljubljana, Yugoslavia (1984).

Guest Scientists who Visited NBS from Yugoslavia

1. Mr. Miha Tomazevic and Mr. Roko Zarnic, 1984, two days

Visits to Yugoslavia of NBS Participant

Although the visit was not under the U.S.-Yugoslav Cooperative Program, Dr. Charles Culver took the opportunity of travel to Yugoslavia to visit and discuss the project.

Project Title: Use of Silica Fume in Concrete
(Project Page 486, NBS(G)-285)

Years and Funds: 1984, Dinars 1,700,000

Principal Investigator: Dr. Kresimir Popovic

Yugoslav Institute: Civil Engineering Institute, University of
Zagreb

NBS Participant: Dr. James R. Clifton

NBS Laboratory, Center, Division: National Engineering Laboratory,
Building Materials Division, Center for Building Technology

Summary Description of Project Goals

The specific aims of the research are:

- Improving cement properties - strength development, ie. efficiency in concrete and durability of cement paste/concrete
- Environment protection through recycling waste material
- Reduction of concrete production costs

Results and Significance of Achievements to Date

The project was approved in the Oct. 1983 and funding received by the Yugoslav Institute in the Spring 1984 - no results achieved to date.

List of Publications or Other Input that Resulted from the Project

None to date.

Guest Scientists who Visited NBS from Yugoslavia

None to date.

Visits to Yugoslavia of NBS Participant

None to date.

Project Title: Chemical Aspects of Radiation Technology
(Project Page 496, NBS(G)-286)

Years and Funds: 1984, Dinars 3,000,000

Principal Investigator: Dr. Ljubica Josimovic

Yugoslav Institute: Boris Kidric Institute of Nuclear Sciences

NBS Participant: Dr. Michael G. Simic

NBS Laboratory, Center, Division: National Measurement Laboratory,
Radiation Physics Division, Center for Radiation Research

Summary Description of Project Goals

To provide measurements of radiolytic product yields, kinetic, and spectroscopic parameters of transient intermediates, and mechanisms of reactions in model systems. The proposed research is essential for the technological developments in immobilization of enzymes, irradiation processing of foods, FDA clearance of irradiated foods, sterilization of medical accessories, and a variety of other radiation processing activities.

Results and Significance of Achievements to Date

The project was approved in May 1984 and no research was performed to date.

List of Publications or Other Input that Resulted from the Project

None to date.

Guest Scientists who visited NBS from Yugoslavia

Dr. M. G. Simic, September 1985.

Visits to Yugoslavia of NBS Participant

Dr. Ljubica Josimovic, September 1985.

APPENDIX I

ALPHABETIC LIST OF PRINCIPAL INVESTIGATORS AND INSTITUTES IN YUGOSLAVIA

Principal Investigator	University, Institute or Laboratory	Page(s)
Bek-Uzarov, Dj. N.	Boris Kidric Institute of Nuclear Sciences, Vinca	63
Bickovski, Vladimir	Institute of Earthquake Engineering and Engineering Seismology, University of Kiril Metodij, Skopje.....	97
Blinc, R.	Jozef Stefan Institute, Ljubljana.....	71
Bonefacic, A.	Institute of Physics, University of Zagreb.....	35
Branica, M./Cosovic, B.	Rudjer Boskovic Center for Marine Research, Zagreb.....	43
Draskovic, R.	Boris Kidric Institute of Nuclear Sciences, Vinca.....	75
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Fueredi-Milhofer, H.	Rudjer Boskovic Institute, Zagreb.....	53
Gomiscek, S.	Department of Chemistry and Chemical Technology E. Kardelj University, Ljubljana.....	81
Janev, R. K.	Institute of Physics, University of Belgrade...	93
Josimovic, L.	Boris Kidric Institute of Nuclear Sciences, Vinca.....	111
Jovanic-Kurepa, J.	Institute of Physics, Belgrade University.....	21
Jovic, D.	Boris Kidric Institute of Nuclear Sciences, Vinca.....	69
Kolar, D.	Jozef Stefan Institute, Ljubljana.....	17
Konjevic, N.	Institute of Physics, Belgrade University.....	31
Kosta, L.	Jozef Stefan Institute, Ljubljana.....	7

Principal Investigator	University, Institute or Laboratory	Page(s)
Maglic, K.	Boris Kidric Institute of Nuclear Sciences Vinca.....	11
Navinsek, B.	Jozef Stefan Institute, Ljubljana.....	27
Petrovic, Z.	Institute of Petrochemistry, Gas, Oil, and Chemical Engineering, Faculty of Technology, University of Novi Sad, Novi Sad.....	79
Petrovski, J.	Institute of Earthquake Engineering and Engineering Seismology, University of Kiril Metodij, Skopje.....	97
Pichler, G.	Institute of Physics, University of Zagreb....	13
Popovic, K.	Civil Engineering Institute, University of Zagreb.....	109
Pravdic, V.	Rudjer Boskovic Institute, Zagreb.....	3
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Spegel, M.	Jozef Stefan Institute, Ljubljana.....	83
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Talganov, K.	Institute of Earthquake Engineering and and Engineering Seismology, University Kiril and Metodij, Skopje.....	99
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Tomazevic, M.	Institute for Testing and Research in Materials and Structures, and Institute for Structures and Earthquake Engineering, Ljubljana.....	107

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ALPHABETIC LIST OF NATIONAL BUREAU OF STANDARDS PARTICIPANTS AND DIVISION

NBS Participant	Division	Page(s)
Blanc, R. P.	650	83
Brown, W. E.	440	53
Celotta, R.	533	39
Cezairliyan, A.	774	11
Chung, R. M.	741	99
Clifton, J. R.	746	109
Dunn, G.	525	21, 93
Durst, R. A.	552	81
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Hastie, J. W.	420	59
Heafner, J. F.	651	83
Hutchinson, J. M. R.	532	63
Kasen, M.	562	35
Leyendecker, E. V.	741	105
Madey, T. E.	541	65
Mann, W.	532	63
McLaughlin, W. L.	533	55
Prosen, E. J.	746	51
Reed, R.	562	85
Reneker, D. H.	400	71
Rhyne, J. J.	460	69
Rook, H. L.	553	7
Roth, R. S.	420	17
Simic, M. G.	533	111
Stone, W. C.	741	97
Taylor, J. K.	550	43
Wiese, W. L.	531	13, 31
Woodward, K.	741	107
Zeisler, R. L.	551	

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11. ABSTRACT (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here) An overview is given of cooperative projects conducted by the National Bureau of Standards and Yugoslav Institutes under the U.S.-Yugoslav Joint Board on Scientific and Technical Cooperation. Each project is identified by title, principal investigator/s, institution in Yugoslavia, the NBS participants, and their organizational unit within NBS. The work is described briefly under the headings "Summary Description of Project Goals," "Results and Significance of Achievements to Date," and "List of Publications that Resulted from the Project." The NBS participants and the program manager judge that this grant program had a high benefit to cost ratio for NBS.			
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