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The objective of the research has been to identify how deleterious effects on bonding develop that can cause deterioration of mechanical properties of carbon-based ceramics in a high temperature environment and then to learn how to design modified ceramic systems that can better withstand such conditions. To do this, we have developed a coordinated computer modeling/experimental study concentrating on fracture and ductility behavior as affected by impurities and defects, high temperatures and bonding effects at material interfaces. We made and studied a variety of metal/carbon and silicon/carbon systems both in naturally occurring crystals and in superlattices. The results obtained in the coordinated study provide valuable information on the interface stability of superlattice systems and on their mechanical and structural properties as compared to systems in naturally occurring crystalline forms. This information is relevant to assessing the practicality of improved high-temperature performance for carbon-based structural ceramic systems by the use of superlattice geometries affording modified metallic/covant balance in bonding.

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AFOSR-87-0251. HIGH TEMPERATURE PROPERTIES OF CERAMIC/CARBON SYSTEMS IN AN OXIDIZING ENVIRONMENT

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Final Technical Report for Research Period (June 1,1987-September 30, 1990)

OBJECTIVE AND APPROACH

The objective of the research has been to identify how deleterious effects on bonding develop that can cause deterioration of mechanical properties of carbon-based ceramics in a high temperature environment and then to learn how to design modified ceramic systems that can better withstand such conditions. We have first made and studied samples in the naturally occurring crystalline form and then studied the potential benefits and problems of superlattice structures, presumably providing a modified balance of covalent and metallic bonding, as an alternative. To do this, we have fabricated such superlattices and developed a coordinated computer modeling/experimental study concentrating on fracture and ductility behavior as affected by impurities and defects, high temperatures and bonding effects at material interfaces.

The experimental methodology involves the use of x-ray diffraction techniques, and high resolution electron scattering in order to study the structure of metal/carbon interfaces. The techniques used in this research allow a complete characterization of the materials. In particular, we have used the elastic resonance scattering of alpha particles by oxygen-16 to measure the oxygen profile in carbon-based multilayer structures and in carbides.

For the computer modeling, new methodology has been developed that can model the opening up of structures going all the way from bulk behavior to the development of free surfaces, thereby allowing treatment of tensile cleavage. This modeling methodology has been designed to include all variations involving mixtures of covalent, metallic and ionic bonding. In the computational part of the work, in addition to modeling the bonding effects as related to physical structure at superlattice interfaces, we have concentrated (1) on modeling tensile fracture in brittle carbidic structural materials to obtain the cleavage energy as related to breaking of covalent bonds, (2) on modeling "rippling" surface relaxation effects at refractory transition metal carbide surfaces since this information serves as the basis for modeling interpenetration effects at interfaces in refractory metal/carbon superlattices.

1

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SUMMARY OF RESEARCH

The initial period of research was devoted to developing computational modeling capability and to initiating the fabrication of samples and the experimental measurements. These involved a variety of electron and x-ray diffraction and scattering techniques as well as resonance scattering of alpha particles. We then concentrated on understanding the bonding behavior at the titanium/carbon interface in Ti/C multilayer (superlattice) structures; and we found that our experimental measurements and total energy computational modeling theory of the interface were in agreement in predicting and identifying the bonding as being graphitic. Thus the interface appears to consist of a layer of graphite adjoining a titanium surface, i.e., not a strongly bonded interface. Next, we performed a comparable experimental study of the interface for the tungsten-carbon (W/C) system. Our experimental tools consisted of Auger Spectroscopy (AG), Electron Energy Loss Spectroscopy (EELS) including High Resolution EELS (HREELS), Reflection High Energy Electron Diffraction (RHEED), Angular Resolved EELS (AREELS), Spot Profile Low Energy Electron Diffraction (SPA-LEED, 1000 Å coherence width), X-ray Diffraction (XRD), Extended X-ray Absorption Fine Structure (EXAFS), and Surface Sensitive Electron Energy Loss Fine Structure (SEELFS). This large number of techniques was necessary in order to fully characterize the interfaces in these systems from room temperature up to high temperatures (up to 1300 C).

Experimentally, in contrast to the Ti/C multilayer structures, carbidic bonding is indicated in the W/C systems. On the other hand, our total energy modeling study indicated a preference for graphitic bonding. At first sight, this theoretical result is not surprising since the series IV transition metal carbides (including TiC) are least susceptible of the transition metal carbides to precipitation of graphite, i.e. from this general pattern our expectation would be for W/C to be more likely to have graphitic behavior at the interface than Ti/C. However, this does disagree with our experimental results, and we believe that the explanation can be found in the role played by oxygen at the interface.

We believe that oxygen affinity plays a crucial role in determining the departure of the experimental interface behavior from the ideal behavior predicted by the computational modeling. Modeling of ideal Ti/C and W/C gives graphitic carbon lying passively against the metal, while experiment gives an oxide layer between Ti and C and a carbidic interface for W/C. We believe that the source of this difference between the theoretical behavior for the ideal systems and experiment lies in the circumstance that the stable structure is that where carbon moves into the metal to form carbide, i.e. this gives the absolute minimum of total energy of the system. Allowing for this possibility goes beyond the initial computer modeling. For titanium the oxygen affinity is so strong that the oxide forms a barrier preventing carbon migration; but for tungsten, carbon migrates to form a carbidic interface.

2

Since we believe that reconstruction effects allowing the interpenetration of metal and carbon probably play a key role in practice for determining the bonding and stability of metal-carbon interfaces in multilayer structures, we initiated modeling studies to reproduce and understand the rippled reconstruction that occurs at refractory metal carbide surfaces. We indeed were able to accurately predict the experimental behavior and also, quite importantly, the modification of surface behavior as a function of density of carbon vacancies. We believe that the outward relaxation of the carbon and inward relaxation of the metal atoms by 4 or 5% provides a mechanism that enables us to understand the interpenetration at superlattice interfaces.

Since we want to understand how the detailed nature of bonding affects fracture mechanisms in carbon-based ceramic systems, we did a baseline modeling study of the fracture properties of perfect titanium carbide under tensile stress. While the determination of the elastic constants was in good agreement with experimental results, the determination of the stress at which fracture occurs, as expected, gave a value which is several times larger than obtained even under carefully controlled conditions. Rough estimates of ideal yield stress are often given in terms of the Young's modulus, with the ratio $_i a/E$ being estimated at about 10 or 20. Our calculations support these estimates in that we obtain a ratio $_i a/E$ of about 13.

Some further details of the computational modeling and experimental research follow.

COMPUTATIONAL MODELING

A. Development of Methodology

Our method for calculating electronic structures and total energies is a self-consistent implementation of the Kohn-Sham equations in the local density approximation. We employ a basis set which is a linear combination of "muffin-tin orbitals" and so the calculation is closely related to "LMTO" (linearized muffin-tin orbital) type calculations. While the LMTO method is generally regarded as efficient but relatively inaccurate, suited only to close packed materials in which the interstitial volume is kept to a minimum, this is not an inherent aspect of the basis set, but rather is related to various approximations which are usually associated with the method. Elimination of these approximations, as discussed briefly below, allows very accurate calculations.

LMTO calculations often employ either a muffin-tin approximation to the one-electron potential, or the atomic sphere approximation (ASA). Such approximations are clearly inadequate for structures with large interstitial regions or with low coordination symmetry, as in interface and surface calculations. We use here a completely general form for the potential and density in which space is divided into non-overlapping muffin-tin spheres (where the

potential is expressed as a linear combination of radial functions multiplied by spherical harmonics) and the remaining interstitial region (in which the potential is expressed as a Fourier series). A second approximation common in LMTO calculations is to fix the value of κ, the interstitial kinetic energy of the basis states at zero. This too is only adequate in close packed systems in which the interstitial potential is nearly constant and the interstitial volume small. We have implemented an increased basis set which includes multiple values of κ (in one "energy window") and optimize the values of these parameters. In a number of test calculations (largely for noble metal surfaces, and also for the TiC (001) surface), we have found that two values for κ in the basis set is adequate for surface calculations, as long as these values are chosen appropriately. We have found that the following method for choosing these parameters works well: A calculation of the bulk system is performed using one κ in the basis set, and this parameter is varied until the bulk total energy is minimized. This κ value is fixed in going to the repeated slab configuration we use in treating surfaces and interfaces, and a second set of basis functions are added, using a second value of κ. The total energy of the slab is then minimized with respect to this second κ parameter, a process which appears to be largely minimizing the surface energy. Application of this procedure in the test cases gave good values for surface properties, for example the calculated work functions agreed with the experimental values to within about 0.1 eV.

B. Modeling of Interfaces in Ti/C and W/C Multilayer (Superlattice) Structures

We used a Ti_2C_2 (or W_2C_2) four-layer slab superlattice structure to examine the competition between graphitic carbon-carbon bonding and carbidic titanium (or tungsten)-carbon bonding at the superlattice interface. With a small carbon-metal separation, the system approximates what one would expect for the interface structure if the carbon atoms are carbidically bound to the surface metals atoms. As the metal-carbon separation is increased, we effectively remove the carbon from the titanium surface and instead force two carbon layers closer together; and when the separation between the AB layers of carbon is reduced to zero, the carbon atoms then have the hexagonal structure of graphite. In this way, we are able to vary only one distance and move continuously from a carbidelike arrangement to a graphitelike interface arrangement. On calculating total energy as function of this distance, in both Ti/C and W/C we obtain two minima with the deeper minimum being at the larger distance in both cases, giving graphitic behavior.

C. Modeling of Rippling Surface Relaxation in Tantulum Carbide

4

LEED analysis of the TaC and Hfc (001) surfaces has shown that these surfaces undergo a significant rippling relaxation. TaC forms in the rocksalt structure, so the (001) surface contains equal numbers of Ta and C atoms arranged in a "checkerboard" pattern. The LEED studies on this surface indicate a rippled relaxation in which C atoms are displaced outward from their truncated bulk positions by 4.2% of an interlayer spacing, while the Ta atoms are displaced inward by 4.8%. What is of interest is the driving mechanism for such rippled relaxations, and in particular, the relationship of the relaxation to the bulk electronic structure, that is whether such relaxation behavior can be easily understood on the basis of the bulk properties alone. A related question is the extent to which it is possible to generalize results to obtain a qualitative understanding of rippled relaxations, at least of the most basic question--which atomic type is the one to relax outward relative to the other? In essence, we find that the relaxation of TaC is directly connected to the ionicity of the bulk material, along with the degree of covalent bonding present. Similar considerations also result in the surface core level shifts which we find to be relatively small.

Our LMTO, total energy repeated slab approach to surface calculations has given accurate results for the TaC surface. We find a relaxation of Ta inward by -3.7%, C outward by 5.8% of an interlayer spacing, in good agreement with the experimental results. The work function for the unrelaxed surface was calculated to be 3.86 eV (compared to the 4.59 eV we have found for the TiC (001) surface) and this work function increased to 4.24 eV upon relaxation. The relaxed surface energy was estimated to be 1.69 eV per surface atom, with a relaxation energy of 0.10 eV per surface atom.

It was determined that the truncated bulk electron density of TaC by itself implies the form of relaxation observed for this surface, and that the details of the calculated surface electron density did not change this effect, but merely gave a partial screening of these fields. Similarly, the truncated bulk density implied core level shifts such that the carbon core levels moved up relative to the Ta surface core levels, a result which again was reduced but not removed by the surface electron redistribution. The lack of radical modification of the truncated bulk approximation appears to be related to the fact that at the (001) surface, the net covalent bonding charge is little changed--a fact which is likely to be also related to the observation that the (001) surface is the preferred cleavage plane in the cubic carbides.

D. Modeling of Brittle Fracture in Titanium Carbide

Titanium carbide, and the other cubic carbides have (001) cleavage planes and fracture along these plane in a brittle manner up to relatively high temperatures, with a brittle to ductile transition occurring at about 800°C. Theoretical estimates of the tensile yield stress of

5

ideal crystals are often expressed in terms of the Young's modulus of the material, and common estimates run from E/20 to E/10, where E is the Young's modulus. For TiC, E/20 gives a yield stress of 2.3×10^{11} dyne/cm^2. In practice, however, cleavage under tensile stress is nucleated by preexisting cracks or other imperfections, and as a result, experimental values for the yield stress for most materials are typically tens or hundreds of times small than such estimates of the ideal yield stress. In addition, the carbides are commonly not stoichiometric, but contain a significant number of carbon vacancies, and these may also affect the fracture (and other) properties of the materials. For polycrystalline TiC, experimental results for the yield stress are generally 100-300 times smaller than E/20, although careful elimination of the surface defects on single crystal samples has succeeded in raising the yield stress to a value only four times small than this. Nonetheless, a more accurate theoretical determination of the yield stress of the perfect crystal is possible and worthwhile, since this provides an upper limit for the attainable yield stress, and is also related to the nature and propagation of cracks. Other matters of interest which can be investigated with electronic structure calculations include the relationship of the fracture properties of TiC to its electronic structure and factors determining the (001) plane as the cleavage plane. Our method of calculation is a full-potential variation of the standard LMTO electronic structure method. The method, is capable of dealing with very open systems, such as surfaces, while at the same time it is not constrained to surface situations, so that a continuous transition from a bulk, closely packed arrangement of atoms to an open arrangement, such as when a cleavage plane is created, it easily dealt with. The creation of a cleavage plane is achieved in this calculation by using a repeated slab arrangement of atoms, with four layers of TiC per slab.

The calculations have examined the cleavage of ideal TiC along (001) planes in a detailed manner and have arrived at a theoretical description of the behavior of TiC under tensile stress, examining both the elastic and inelastic behavior. While the determination of the elastic constants was in good agreement with experimental results, the determination of the stress at which fracture occurs, as expected, gives a value which is several times larger than obtained even under carefully controlled conditions. Rough estimates of ideal yield stress are often given in terms of the Young's modulus, with the ratio a/E being estimated at about 10 or 20. Our calculations support these estimates, in that we obtain a ratio a/E of about 13. We believe that these calculations actually represent the ideal yield stress of TiC, even though only one mode of failure has been considered, that of the simple separation along adjacent planes. One could imagine more complicated modes of failure, even those involving initiation of a crack at an ideal surface, however, it difficult to see why instability would be reached any sooner by any more complicated deformation of the crystal.

EXPERIMENTAL RESEARCH

The experimental program was directed towards the study of the surface properties of high temperature refractory carbides and the interface bonding in refractory metal superlattices of W/C and Ti/C. We also studied the structural and electronic properties of Si/C multilayers. Our objective was to investigate the thermal stability of the interface metal-bond of the artificial structures. The work on the pure carbides was carried out to obtain good and reliable standards for the analysis of our artificial structures. Some of the spectrocopic information did not existed in the literature or was of questionable accuracy.

We employed a large number of analytical tools in our studies. Auger spectroscopy (AS)was used as a routine technique for characterization of the elemental composition of the surface. The measurements of all the samples were performed in ultra high vacuum with a vacuum better than 10^{-10} Torr. The samples were characterized by x-ray scattering prior to their use in the UHV system. The samples were attached to a tungsten sample holder, and an electron beam heater was used to raise the sample temperature. The temperature was monitored and controlled using a proportional temperature controller. The chamber was equipped with a LEED system and a single pass cylindrical mirror analyzer(CMA) for AS and electron energy loss spectroscopy (EELS) measurements. The second derivative mode was used for the electron energy loss measurements using the CMA. The angular resolved AS and EELS measurements were performed in a UHV system equipped with a 50 mm hemispherical analyzer with a position sensitive electron detector. A high resolution electron gun was employed for the angular resolved EELS (AREELS) measurements (15 meV resolution at 25 eV).

A very powerful tool to investigate the local atomic structure is extended x-ray absorption fine structure (EXAFS). We have employed this techniques to study the variation in local structure around the carbon, tungsten and silicon atoms. We used electron energy loss fine structure in our studies because of the low threshold energies of the carbon K-edge and silicon L2,3-edge. The energy resolution for the SEELFS measurements was about 8 eV. A modulating voltage of 8 volts was used in the measurements. This is necessary in order to obtain good signal to noise in the second derivative detection mode. The incident electron energy used in this experiment was 1500eV.

The RBS and $^{16}O(\alpha,\alpha)^{16}O$ elastic scattering resonance measurements were performed using the Brooklyn College dynamitron. RBS is useful in obtaining concentration vs depth profiles of elements in the upper few microns of solids. It can provide fast and quantitative profiles, nondestructively and reliable. The ion beam was H or He, the scattering is simple Coulombic repulsion, and is accurately described by the Rutherford cross section. The resonance elastic scattering cross section (at 3.05 MeV) of α-particles on ^{16}O is very large compared to the RBS cross section. At the resonance energy is very sensitive to the presence of oxygen. We employed this technique to determine the oxygen content and depth profile in the samples. We also employed these tools to select our samples from different single crystal batches in order to have purest materials.

The multilayers were prepared by magnetron sputtering . The substrates were placed on a water cooled platform rotating below the targets. The base pressure of the in house system was around 10^{-9} Torr. The substrates used for -preparing the multilayers were α-Al_2O_3 (1120) and float glass for Si/C and Si(111) for W/C and Ti/C, the substrate temperature during growth was maintained around 300 K. The samples were characterized by low and wide angle x-ray scattering using an in house Rigaku diffractometer.

The x-ray specular reflectivity measurements were carried out at room temperature using beam line X-18B at the National Synchrotron Light Source facility at Brookhaven National Laboratory. A Si(220) double crystal monochromator was used for selecting the synchrotron radiation wavelength. All the multilayer were measured using this technique, but the full theoretical analysis (using the dynamic theory) has been completed only for all the Si/C multilayers. The Brillouin scattering measurements were performed at the Materials Science laboratories at ANL.

TIC. Titanium carbide is one of the most technologically important carbides . It has a simple cubic rock-salt structure.The electron energy loss (EEL) spectra of TiC (111) were measured over a wide range of electron primary energies . Laser annealing was employed to obtain oxygen free titanium carbide surfaces . The electron energy losses below 16 eV were analyzed using the theoretical band calculations. The volume and surface plasma excitations were identified from their electron primary energy dependence . Energy losses due to core electrons autoinization effects were identified above 35 eV . We observed a remarkable difference in the electronic structure of the surface vs the bulk of TiC . The temperature dependence of the EEL spectra was

studied between 300 to 1250 K .The reaction of the TiC surface with ethylene and oxygen was also investigated. The ethylene bonding to the TiC surface was found to be very weak and the hydrocarbons were easily removed from the surface after mild thermal annealing . We found from reflectivity measurements evidence of the formation of surface defects on the TiC (111) surface at high temperatures. The reaction with oxygen was studied over a wide range of temperatures , the formation of a surface oxide was detected by Auger and EEL spectroscopies.

α-SIC. We report a study of the surface composition of α-SiC between room temperature and 1273 K. Electron energy loss spectroscopy was employed to detect the changes in surface structure of silicon carbide as a function of temperature. The electron energy loss spectra were analyzed using the bulk and surface dielectric functions of α-SiC. Auger spectroscopy, RBS, elastic resonance scattering of a-particles from ^{16}O, and surface reflected electron energy loss fine structure were employed to characterize the sample. We observed the formation at rather low temperatures (around 570 K) of a graphitic surface layer on the silicon carbide. We attribute the formation of this layer to carbon migration to the surface. This migration creates carbon vacancies in the bulk. We also found evidence of internal oxidation of the silicon carbide at temperatures of 823 K and above.

Multilayers.

TI/C. We performed a systematic study of the electronic and crystallographic structure of Ti/C multilayers. The samples were characterized by low and wide angle x-ray diffraction and Microcleavage transmission Electron Microscopy. It was observed that the Ti/C interface is isolated by a thin titanium oxide layer. The center of the Ti layer gives a characteristic EELS spectrum of the metal. The oxide phase exists at all Si-C interfaces as shown by a-particles elastic resonance scattering from ^{16}O.The carbon shows graphitic characteristics.

W/C. We have studied the structure of W/C multilayers using a diverse numbers of techniques. The samples titanium thicknesses varied between 20 to 38 Å and the carbon between 5 to 41 Å. The samples were prepared by plasma rf sputtering techniques and the modulation and lattice structure were determined by x-ray diffraction and electron microscopy. Electron energy loss spectroscopy was used to obtain a non destructive composition depth profile of the material by changing the impinging electron energy. The measurements were carried out under UHV conditions. All the major electron energy loss peaks of the multilayers were identified. The measurements were performed as a function of temperature, between 293 and 973 K. Auger spectroscopy and Rutherford back scattering measurements were also performed in all the

9

samples. We found EELS to be very sensitive to the structural modifications in the samples. We observed the formation of a carbide at the W/C interface. The structure of the interface was identified using surface electron energy loss fine structure and x-ray scattering. We investigated the stability of the multilayers in an oxidizing environment and at high temperatures. Brillouin scattering measurements were also indicative of the formation of a strong interface bonding in the multilayers at high temperatures.

Si/C. We have studied using angular resolved electron energy loss spectroscopy the structure of silicon/carbon multilayers. The samples were characterized by low and wide angle x-ray scattering using an in house facility. The total thickness of the samples were between 900 to about 2000 Å. The carbon layer thicknesses were between 10 to 35 Å, and the silicon layer between 5 to 35 Å thick. The modulation wavelength of the samples was determined to be from 14 to 62 Å. The major electron energy loss peaks were identified. We inferred from the electron energy loss measurements that a carbidic interface is present at the silicon-carbon interface. The electron energy loss measurements of the multilayers were also carried out at high temperatures, up to 873 K. The x-ray specular reflectivity measurements were carried out at room temperature using beam line X-18B at the National Synchrotron Light Source facility at Brookhaven National Laboratory. The measurements were analyzed using Fresnel laws of optics and assuming Gaussian roughness at the interfaces. We found from the analysis of the data that a carbidic phase forms at the silicon-carbon interface for samples heated in vacuum to 873 K. These results are in very good agreement with the electron energy loss measurements.

PUBLICATIONS AND PRESENTATIONS

Publications (Reprints and preprints enclosed.)

1. "Interface Structure and Stability in Ti/C Superlattices" N. Thangprasert, P.A. Montano, D.L. Price, B.R. Cooper, E. Ziegler, I.K. Schuller, Y.Chan, H.S. Jin, D. Yan and P. Lesser, Materials Research Society Symposium Proceedings, Vol. 122, p 589 (1988).

2. "Total Energies and Bonding for Crystallographic Structures in Titanium-Carbon and Tungsten-Carbon Systems", D.L. Price and B.R. Cooper, Physical Review B, Vol. 39, p 4945 (1989).

3. "Full Potential Linear Muffin-Tin Orbital Study of Interface Behavior in Ti-C Superlattices", D.L. Price and B.R. Cooper, Journal of Vacuum Science and Technology A, Vol. 7 p 2049 (1989).

4. "Full Potential, Total Energy LMTO Calculation of Interface Structure in Ti-C and W-C Superlattices", D.L. Price and B.R. Cooper, Materials Research Society Symposium Proceedings, Vol. 141, p 393 (1989).

5. "LMTO Calculation of TaC (001) Surface Relaxation", D.L. Price and B.R. Cooper, to be published in Physical Review B.

6. "Full-Potential LMTO Study of Brittle Fracture in Titanium Carbide", D.L. Price and B.R Cooper, to be published in Physical Review B.

7. "Electron Energy Loss Study of TiC [111]", Y. Chan, D. Liao, S.W. Lee, B. R. Cooper and P. A. Montano, submitted for publication.

8. "Surface Study of α- SiC (0001) at High Temperatures", Y. Chan and P.A. Montano, submitted for publication.

9. "Study of the Electronic and Interface Structure of W/C Multilayers",Y. Chan, P. A. Montano, E. Ziegler, I. K. Schuller, Y. Cao, S. S. Kumar, M. Grimsditch, H. S. Jin, D. Yan, and P. Lesser, submitted for publication.

10. "Electron Energy Loss Study of Si/C Multilayers", Y. Chan, H. Homma, M. Kentjana, and P.A. Montano, submitted for publication.

11. " X-Ray Reflectivity Study of Si/C Multilayers", J. Bai, Y. Chan, H. Homma, M. Kentjana, and P. A. Montano (to be submitted).

Conference Presentations

1. "Full Potential LMTO Calculations of Interface Energies in Titanium-Carbon Systems", American Physical Society Meeting, New Orleans, March, 1988.

2. "Oxygen Effects in Ti/C Multilayers", American Physical Society Meeting, New Orleans, March, 1988.

3. "Interface Structure and Stability in Ti/C Superlattices", Materials Research Society Meeting, Reno, April, 1988.

4. "Full Potential LMTO Study of Interface Behavior in Ti-C Superlattices", National Symposium of the American Vacuum Society, Atlanta, October, 1988.

5. "Ion Beam Analysis of Ti/C and W/C Superlattices", 10th Conference on the Application of Accelerators in Research and Industry, Denton, Texas, November, 1988.

6. "Characterization of the Interface in Ti/C and W/C Superlattices", Materials Research Society Meeting, Boston, November, 1988.

7. "Full Potential, Total Energy LMTO Calculation of Interface Structure in Ti-C Superlattices", Materials Research Society Meeting, Boston, November, 1988.

8. "Full-Potential LMTO Study of TiC (100) Cleavage, American Physical Society Meeting, St. Louis, March, 1989.

9. "Electron Energy Loss Study of SiC Single Crystals", American Physical Society Meeting, St. Louis, March, 1989.

10. "Full-Potential, LMTO Calculation of TiC Fracture", Materials Research Society Meeting, November, 1989.

11. "Effect of Carbon Vacancies on the Work Function of TaC", American Physical Society Meeting, Anaheim, March, 1990.

12. "Electron Energy Loss Study of W/C Multilayers at High Temperature" American Physical Society National Meeting,Anaheim (1990).

13. " Electron Energy Loss Study of The Electronic Structure of Titanium Carbide", Materials Research Society Meeting, Boston, November, 1990.

14. " Crystallographic and Electronic Structure of Si/C Multilayers", Materials Research Society Meeting, Boston, November, 1990.

15. " Applications of Synchrotron Radiation Techniques to Materials Sciences", Academia de Ciencias de Materiales, Mexico City, April, 1991.