

AD-A211 550

REPORT DOCUMENTATION PAGE

2

1a. REPORT SECURITY CLASSIFICATION UNCLASSIFIED			1b. RESTRICTIVE MARKINGS FILE		
2a. SECURITY CLASSIFICATION AUTHORITY			3. DISTRIBUTION / AVAILABILITY OF REPORT Approved for public release; distribution unlimited		
2b. DECLASSIFICATION / DOWNGRADING SCHEDULE					
4. PERFORMING ORGANIZATION REPORT NUMBER(S) Final Report			5. MONITORING ORGANIZATION REPORT NUMBER(S)		
5a. NAME OF PERFORMING ORGANIZATION Dept. of Chemistry George Washington Univ.		6a. OFFICE SYMBOL (If applicable)	7a. NAME OF MONITORING ORGANIZATION Office of Naval Research (Code 413)		
5c. ADDRESS (City, State, and ZIP Code) Washington, DC 20052		7b. ADDRESS (City, State, and ZIP Code) Chemistry Program 800 N. Quincy Street; Arlington, VA 22217			
3a. NAME OF FUNDING / SPONSORING ORGANIZATION Office of Naval Research		8b. OFFICE SYMBOL (If applicable)	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER Contract N00014-80-K-0852		
3c. ADDRESS (City, State, and ZIP Code) Chemistry Program 800 Nth Quincy, Arlington, VA 22217		10. SOURCE OF FUNDING NUMBERS			
		PROGRAM ELEMENT NO. 61153 N	PROJECT NO. RR013-08	TASK NO. PP013- 08-01	WORK UNIT ACCESSION NO. NR056-681
11. TITLE (Include Security Classification) Quantitative Interpretation of Auger Lineshapes and Electron/Photon Stimulated Desorption					
12. PERSONAL AUTHOR(S) D.E. Ramaker					
13a. TYPE OF REPORT Final		13b. TIME COVERED FROM 80/7/1 TO 89/3/31		14. DATE OF REPORT (Year, Month, Day) 89/8/18	
15. PAGE COUNT 15					
16. SUPPLEMENTARY NOTATION					
17. COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)		
FIELD	GROUP	SUB-GROUP	Auger Spectroscopy, Electron Stimulated Desorption Photon Stimulated Desorption		
19. ABSTRACT (Continue on reverse if necessary and identify by block number)					
This project has involved a quantitative theoretical interpretation of electron spectroscopic data with a view toward elucidating the chemical environment and electronic structure of atoms in the bulk and adsorbed on solid surfaces. Many-body effects, such as shake satellites, initial core hole screening, and final state hole-hole correlation, etc. have been examined and found to have significant effects on the spectral lineshapes. We have more recently examined electron spectroscopic data for the high temperature superconductors, and for chemisorbed species on metals. Electron/photon stimulated desorption (ESD/PSD) was also of interest. Here, an interpretation of spectroscopic data and comparison with PSD spectral yields was very helpful in obtaining an understanding of the image charge, surface resonances, polarization, and the role of many-body interactions in the desorption mechanism itself.					
20. DISTRIBUTION / AVAILABILITY OF ABSTRACT ☒ UNCLASSIFIED/UNLIMITED ☐ SAME AS RPT. ☐ DTIC USERS			21. ABSTRACT SECURITY CLASSIFICATION UNCLASSIFIED		
22a. NAME OF RESPONSIBLE INDIVIDUAL Dr. David L. Nelson			22b. TELEPHONE (Include Area Code) (202) 696-4410		22c. OFFICE SYMBOL

DTIC
UNCLASSIFIED
89/8/18

OFFICE OF NAVAL RESEARCH
FINAL REPORT

1 July 1980 through March 31, 1989
for
Contract N00014-80-K-0852

R&T Code: 413e022

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Dist	Avail. and/or Special
A-1	

QUANTITATIVE INTERPRETATION OF AUGER LINESHAPES
AND ELECTRON/PHOTON STIMULATED DESORPTION

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- c. Telephone: 202-994-6934
- d. Description of Project

This project has involved a quantitative theoretical interpretation of electron spectroscopic data with a view toward elucidating the chemical environment and electronic structure of atoms in the bulk and adsorbed on solid surfaces. Many-body effects, such as shake satellites, initial core hole screening, and final state hole-hole correlation, etc. have been examined and found to have significant effects on the spectral lineshapes. We have more recently examined electron spectroscopic data for the high temperature superconductors, and for chemisorbed species on metals. Electron/photon stimulated desorption (ESD/PSD) was also of interest. Here, an interpretation of spectroscopic data and comparison with PSD spectral yields was very helpful in obtaining an understanding of the image charge, surface resonances, polarization, and the role of many-body interactions in the desorption mechanism itself.

- e. Significant Results

Table 1 summarizes our significant accomplishments in Auger spectroscopy, and Table 2 that in ESD/PSD. In each case, the tables indicate the system studied, the significance of the work, and the numerical sequence (as indicated below) of the papers (P) and technical reports (TR) published.

In summary we have shown that a very complex "many-body" experimental Auger spectroscopy can be used in a straightforward and simple manner to obtain important information on the electronic structure. On the other hand, we have shown that very complex "many-body" states are the primary actors in the ESD/PSD process, where previously very simple-minded one-body states were assumed to be the primary actor. By studying AES and ESD/PSD in the same context, we have shown that AES can be used to map the states responsible for the ESD/PSD process.

TABLE 1 - Review of Significant Accomplishments in AES

	SYSTEM	SIGNIFICANCE	PRODUCTIVITY (TR, P)*
1.	NO ₃ ⁻ , SO ₄ ²⁻ SiO ₂	Proposed intermediate localization model. First det'm. of theo. shake/Auger lineshapes.	P- 1,2,6 TR- 1,4,7,14
2.	O ₂ gas	First ab-initio determination of experimental Auger widths	P- 3,23 TR- 6,30
3.	NO ₃ ⁻	Effect of Mulliken vs. local populations on Auger intensity.	P- 4 TR- 5
4.	NO ₃ ⁻ , O ₂ , C ₂ H ₃ , Cu, Be,	Proposed final state rule for Auger lineshapes.	P- 5,8,12 TR- 8
5.	C ₆ Li, C ₈ Cs	Proposed orthogonalized final state rule to account for enhanced intercalant peak	P- 7,9
6.	N ₂ , CO, O ₂ , NO	Systematic and consistent interpretation of spectra for diatomic molecules	P- 13,25,28,29 TR- 11,21,26,27,28
7.	Graphite	Established first case of localization in extended covalent system; first obs. of shakedown satellite.	P- 14,20,24,27 TR- 13,19,22,24
8.	Atoms with atomic # = 8-54	Det'm. of semi-empirical KVV and L ₂₃ VV atomic Auger matrix elements.	P- 16
9.	TM carbides nitrides, oxides, SiC	Related Auger lineshapes to ionic bonding effects	P- 19 TR- 17
10.	Si	First quantitative interpretation of CCV Auger lineshapes;	P- 21 TR- 15
11.	Benzene Cyclohexane Polyethylene	Consistent interpretation and comparison of DU's in molecules and solids	P- 26,34,41 TR- 25,33,39,48
12.	Diamond	Established evidence for antiferromagnetic ordering on surface	P- 30 TR- 29

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| 13. | Polyethylene,
diamond | Established the role of
excitation and shakeoff
in AES processes. | P= 31
TR- 30 |
| 14. | Benzene,
Transition
metals | Interpretation of Auger
line shapes for systems with
less than 1/2 filled VB. | P- 32
TR -31 |
| 15. | Y-BA-Cu-O
La-Sr-Cu-O | Interpretation of AES and XPS
data indicates the Cu-O bond
covalency correlates with T_c ,
and that no Cu^{3+} is present. | P- 37,43,44,45,46
TR- 37,43,44,
45,46,47 |
| 16. | C_2H_6/Ni ,
C_2H_4/Ni ,
CH/Ni | First quantitative interpreta-
tion of Auger line shapes for
chemisorbed systems. | TR- 41 |

*P and TR indicate sequence numbers of publications and ONR technical reports as listed below.

TABLE 2 Summary of significant accomplishments in ESD/PSD.

	SYSTEM	SIGNIFICANCE	PRODUCTIVITY (TR, P)*
1.	CO,N ₂ ,H ₂ O	Established role of 2h1e type states in PSD of chemisorbed systems.	P- 10,11,15 TR- 9,10,12
2.	OH/Ti, Cr, Cu, O/Cr	Established the Auger induced desorption mechanism for non-maximal valency systems.	P- 19 TR- 18
3.	H ₂ O,OH/TiO ₂ O/W,O/Mo	Resonant dissociative attachment mechanism found to be active for OH* and O ⁻ .	P- 22 TR- 23
4.	NH ₃ /Ru mixed N ₂ ,O ₂	Role of secondary electrons in desorption yields.	P- 18,38,40 TR- 16,36
5.	O ₂ /Ar/Pt	Elucidated the role of image charge effects in PSD.	P- 33,39 TR- 32
6.	O ₂ /Ar/Pt	Established the role of coherent scattering effects in the enhancement of ESD cross-section.	P- 35,42 TR- 34,40
7.	O ₂ /Pt,W	Elucidated the role of symmetry and its breakdown at surfaces in ESD	P-36 TR- 35,38,42

*P and TR indicate sequence numbers of publications and ONR technical reports as listed below.

f. Personnel who Worked on Project.

1. Dr. Hideo Sambe - Research Associate Professor
Period worked: 11/1/81 - 3/15/89
Understanding the nature of dissociation/desorption of small molecules and negative ion desorption.
2. Mr. Fred Hutson - Research Associate, part time
Period worked 1/1/81 - 3/15/89
Applications of electron spectroscopic data.
3. Mr. Hengxiang Yang - Graduate Student, partial summer support
Period worked: 7/1/88-8/31/88
Experimental study of thin films.
4. Dr. Wai-Ning Mei - Research Scientist
Period worked: 5/19/81 - 3/31/82
5. Dr. Arnold Wahl - Research Professor
Period worked: 11/01/81 - 12/31/81

g. Publications emanating from contract.

1. "Final State Correlation Effects in Auger Lineshapes, Application to Silicon Dioxide", D.E. Ramaker, Phys. Rev. B21, 6408 (1980).
2. "Auger Lineshapes of Solid Surfaces - Atomic, Bandlike, or Something Else?", B.I. Dunlap, F.L. Hutson, and D.E. Ramaker, J. Vac. Soc. Technol. 18, 556 (1981).
3. "A Semiempirical X_{α} Calculation of the KVV Auger Line Shape of O_2 ", B.I. Dunlap, P.A. Mills, and D.E. Ramaker, J. Chem. Phys. 75, 300 (1981).
4. "Interpretation of the N KVV Auger Lineshapes for Alkali Metal Nitrates", F.L. Hutson, D.E. Ramaker, B.I. Dunlap, J.D. Ganjei, and J.S. Murday, J. Chem. Phys. 76, 2181 (1982).
5. "A Final State Rule for Auger Lineshapes", D.E. Ramaker, Phys. Rev. B 25, 7341 (1982).
6. "Auger Spectroscopy as a Probe of Valence Bonds and Bands", D.E. Ramaker, Published in "Chemistry and Physics of Solid Surfaces IV, Ed. by R. Vanselow and R. Howe, Springer Series in Chemical Physics Vol. 20, (Springer-Verlag, Heidelberg, 1982), p. 19.
7. "Effect of Screening on the Carbon KVV Auger Lineshape of Alkali Intercalated Graphite", B.I. Dunlap, D.E. Ramaker, and J.S. Murday, Phys. Rev. B25, 6439 (1982).
8. "Initial and Final State Screening Effects in Auger Lineshapes", D.E. Ramaker, N.H. Turner, and W. N. Mei, J. Vac. Soc. Technol. 20, 563 (1982).
9. "Evidence for Screening Effects in the KVV Auger Lineshape of Intercalated Graphite", B.I. Dunlap, D.E. Ramaker, and J.S. Murday, J. Vac. Soc. Technol. 20, 900 (1982).
10. "Models for Desorption in Covalent Systems", D.E. Ramaker, published in "Desorption Induced by Electronic Transitions", ed. by N.H. Tolk, M.M. Traum, J.C. Tully, and T.E. Madey (Springer, Berlin, 1982) p. 70.
11. "Covalent Interaction Effects in Electron/Photon Stimulated Desorption", D.E. Ramaker, J. Vac. Soc. Technol. A1, 1137 (1983).
12. "Evidence for Core Hole Screening by 3d Electrons in Third Row Oxyanions", N.H. Turner and D.E. Ramaker, J. Vac. Soc. Technol. A1, 1229 (1983).

13. "Comparison of Autoionization and Photoemission Spectra for CO", M. Yousif, D.E. Ramaker, and H. Sambe, Chem. Phys. Letters. 101, 472 (1983).
14. "Understanding Localized Behavior in the Auger Spectra of Covalent Systems such as Graphite", D.E. Ramaker, F.L. Hutson, R.R. Rye, J.B. Houston, and J.W. Rogers, J. Vac. Soc. Technol. A2, 1146 (1984).
15. "Photon-Stimulated Ion Desorption from Condensed N₂ and CO", H. Sambe, M. Yousif, and D.E. Ramaker, J. Vac. Soc. Technol. A2, 1011 (1984).
16. "Bonding Information from Auger Spectroscopy", D.E. Ramaker, Appl. Surface Science 21, 243 (1985).
17. "Mechanisms for Excited Neutral, and Negative and Positive Ion Desorption from Surfaces", D.E. Ramaker, published in "Desorption Induced by Electronic Transitions", ed. by W. Brenig and D. Menzel, Springer Ser. Surf. Sci. 4, 10 (1985).
18. "Electron Stimulated Desorption and the Role of Backscattered Electrons", F.L. Hutson, D.E. Ramaker, V.M. Bermudez, and M.A. Hoffbauer, J. Vac. Soc. Technol. A3, 1657 (1985).
19. "Chemical and Localization Effects in the Auger Lineshapes of Transition Metal Compounds", P.E. Pehrsson and D.E. Ramaker, J. Vac. Soc. Technol. A3, 1315 (1985).
20. "Relationship Between the Auger Lineshape and the Electronic Properties of Graphite", J.E. Houston, R.R. Rye, J.W. Rogers, F.L. Hutson, D.E. Ramaker, and J.S. Murday, Phys. Rev. B34, 1215 (1986).
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22. "Desorption of Excited Neutrals from Surfaces via an Electron Attachment Mechanism", D.E. Ramaker, Nuclear Instruments and Methods in Physical Research B13, 545 (1986).
23. "An Interpretation of the O₂ Auger Electron Spectrum", H. Sambe and D.E. Ramaker, Chem. Phys. 104, 331 (1986).
24. "Dynamical Core Hole Screening Effects in the C KVV Auger Lineshape of Graphite", J.E. Houston, D.E. Ramaker, R.R. Rye, J.W. Rogers, Jr. and F.L. Hutson, Phys. Rev. Letters 56, 1302 (1986).
25. "An Interpretation of the N₂ Photoelectron Spectrum", H. Sambe and D.E. Ramaker, Chem. Phys. Lett. 124, 420 (1986).

26. "A Consistent Quantitative Interpretation of the Auger Lineshapes of Carbon in Molecules and Solids", D.E. Ramaker and F.L. Hutson, J. Vac. Sci. Technol. A4, 1600 (1986).
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28. "Rydberg States Converging to the N_2^{++} Ionized States", H. Sambe and D.E. Ramaker, Chem. Phys. 107, 351 (1986).
29. "Identification of Resonantly Excited Auger Electron Spectra for N_2^+ ", H. Sambe and D.E. Ramaker, Chem. Phys. Letters 128, 113 (1986).
30. "Direct Experimental Evidence for Antiferromagnetic Spin Ordering on the (111) - (2 x 1) Surface of Diamond", D.E. Ramaker and F.L. Hutson, Solid State Communications 63, 335 (1987).
31. "Identification of Satellites due to Resonant Excitation and Shakeoff in the C KVV Auger Lineshape of Polyethylene", F.L. Hutson and D.E. Ramaker, Phys. Rev. B35, 9799 (1987).
32. "Interpretation of Auger Lineshapes on Systems with Half-Filled Valence Bands", D.E. Ramaker and F.L. Hutson, Journal Vac. Sci. Technol. A5, 630 (1987).
33. "Image Charge Effects in Electron Stimulated Desorption: O^- from O_2 condensed on Ar Films Grown on Pt", H. Sambe, D.E. Ramaker, L. Parenteau and L. Sanche, Phys. Rev. Letters 59, 236 (1987).
34. "Identification of Resonant Excitation and Shakeoff Contributions to the C KVV Auger Lineshapes of Several Gas Phase Hydrocarbons", F. Hutson and D.E. Ramaker, J. Chem. Phys. 87, 6821 (1987).
35. "Electron Stimulated Desorption Enhanced by Coherent Scattering: O^- from O_2 condensed on Ar Films Grown on Pt", H. Sambe, D.E. Ramaker, L. Parenteau and L. Sanche, Phys. Rev. Letters 59, 505 (1987).
36. "The s- Selection Rule in Electron Attachment and Autoionization of Diatomic Molecules", H. Sambe and D.E. Ramaker, Chem. Phys. Letters 139, 386 (1987).
37. "Observed Trends in the X-ray Photoelectron and Auger Spectra of High Temperature Superconductors", D.E. Ramaker, N.H. Turner, J.S. Murday, L.E. Toth, M. Osofsky, and F.L. Hutson, Phys. Rev. B36, 5672 (1987).
38. "Secondary Electron Effects in Photon Stimulated Desorption", D.E. Ramaker, T.E. Madey, R.L. Kurtz, and H. Sambe, Phys. Rev. B38, 2099 (1988).

39. "Image Charge, Coherent Scattering, and Symmetry Effects in Electron Stimulated Desorption: O⁻ from O₂ Condensed on Metals", D.E. Ramaker and H. Sambe, published in Desorption Induced by Electronic Transition, DIET III, ed by R. Stulen and M. Knotek, Springer Series in Surface Sci., (Springer, Berlin Heidelberg, 1988), p. 85.
40. "The Magnitude of Secondary Electron Contributions in Photon Stimulated Desorption", D.E. Ramaker, T.E. Madey, R.L. Kurtz, and H. Sambe, published in Desorption Induced by Electronic Transition, DIET III, ed by R. Stulen and M. Knotek, Springer Series in Surface Sci., (Springer, Berlin Heidelberg, 1988), p. 182.
41. "Interpretation of the Ethylenic, Carbodic and Graphitic Auger Lineshapes of Chemisorbed Carbon Species", F.L. Hutson and D.E. Ramaker, J. Vac. Soc. Technol. A6, 1105 (1988).
42. "Electron Stimulated Desorption and Coherent Scattering", H. Sambe and D.E. Ramaker, J. Vac. Sci. Technol. A6, 836 (1988).
43. "Review of Photoelectron and Auger Data for the High Temperature Superconductors", D.E. Ramaker, In Thin Film Processing and Characterization of High Temperature Superconductors, J.M. Harper, J.H. Colton, L.C. Feldman eds, AVS Series No. 3, (AIP, New York, 1988) p. 284.
44. "Electron Spectroscopic Data for the High Temperature Superconductors - What can We Learn from It?", D.E. Ramaker, Chemistry of High-Temperature Superconductors, edited by D.L. Nelson and T.F. George, ACS Symposium Series 377 (ACS, Washington, DC, 1988). p. 84.
45. "Utilization of a Hubbard U Model to Understand the Valence Band Photoelectron Data for the High Temperature Superconductors", D. E. Ramaker, Phys. Rev. B38, 11816 (1988).
46. "Understanding Core Level Decay Processes in the High-Temperature Superconductors", D.E. Ramaker, N.H. Turner, and F.L. Hutson, Phys. Rev. B38, 11368 (1988).

h. Technical Reports Issued

1. "Final State Correlation Effects in Auger Lineshapes, Application to Silicon Dioxide", D.E. Ramaker.
2. "Symmetry of the Au(110) Surface Reconstruction Studied by Spin-polarized Low-Energy Electron Diffraction", B. Reihl and B.I. Dunlap.
3. "Symmetry Properties of Spin-polarized LEED", B.I. Dunlap.
4. "Auger Lineshapes of Solid Surfaces - Atomic, Bandlike, or Something Else?", B.I. Dunlap, F.L. Hutson, and D.E. Ramaker.
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32. "Image Charge Effects in Electron Stimulated Desorption: O⁻ from O₂ condensed on Ar Films Grown on Pt", H. Sambe, D.E. Ramaker, L. Parenteau and L. Sanche.

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39. "Interpretation of the Ethylenic, Carbodic and Graphitic Auger Lineshapes of Chemisorbed Carbon Species", F.L. Hutson and D.E. Ramaker.
40. "Electron Stimulated Desorption and Coherent Scattering", H. Sambe and D.E. Ramaker.
41. Interpretation of the Carbon Auger Line Shapes from Adsorbed and Fragmented Ethylene on Ni(100)", F.L. Hutson and D.E. Ramaker.
42. "Forbidden Electron Attachment in O₂", H. Sambe and D.E. Ramaker, submitted to Phys. Rev. B.
43. "Review of Photoelectron and Auger Data for the High Temperature Superconductors", D.E. Ramaker.
44. "Utilization of a Hubbard U Model to Understand the Valence Band Photoelectron Data for the High Temperature Superconductors", D. E. Ramaker.
45. "Understanding Core Level Decay Processes in the High-Temperature Superconductors", D.E. Ramaker, N.H. Turner, and F.L. Hutson.
46. "Electron Spectroscopic Data for the High Temperature Superconductors - What can We Learn from It?", D.E. Ramaker.

47. "Utilization of a Highly Correlated Cluster Model for Interpretation of Electronic Spectroscopic Data for the High Temperature Superconductors", D.E. Ramaker.
48. "Chemical Effects in the Carbon KVV Auger Line Shapes", D.E. Ramaker.

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