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FINAL REPORT

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QUANTITATIVE INTERPRETATION OF AUGER LINESHAPES
AND ELECTRON/PHOTON STIMULATED DESORPTION

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- a. **Principal Investigator: David E. Ramaker**
- b. **Cognizant ONR Scientific Officer: David Nelson/Mark Ross**
- 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. We have most recently examined XPS, XAS, and AES data for the transition metal halides with applications to the high temperature superconductors, and CEELS, AES, and NEXAFS data for chemisorbed carbon species on metals. Electron/photon stimulated desorption (ESD/PSD) was also of interest. Here, an interpretation of spectroscopic data allowed for the first quantitative determination of a dissociative attachment cross-section on a surface and new knowledge about the trajectory of the desorbing atom.

- e. **Significant Results**

Table 1 summarizes our significant accomplishments in electron spectroscopy (AES, NEXAFS, and XPS), and in ESD/PSD. In each case, the table indicates the system studied, the significance of the work, and the numerical sequence (as indicated below) of the papers (P) and technical reports (TR) published.

TABLE 1 - Review of Recent Accomplishments
(October 1988 - February 1991)

SYSTEM	SIGNIFICANCE	PRODUCTIVITY (P and TR)*
<u>Interpretation of electron spectra</u>		
1. TMX_n (X=halides, oxides), HTSC's	Obtained an understanding of anion electronegativity effects in PES and AES spectra with applications to HTSC's.	P-2 TR-4
2. C_2/Ni	First evidence that C_2 is formed on Ni, which then tips up to serve as a nucleation site for graphite formation at higher Temp.	P-5,6,7,8 TR-1,9,10
3. Hydrocarbons and other carbon	Reviews of previous work in AES of carbonaceous materials.	P-11,12 TR-3,7
<u>ESD and PSD</u>		
4. $O_2/Ar/Pt$	First quantitative determination of a dissociative attachment cross-section on a surface	P-1,9 TR-2,5
5. Diatomics/Pt	First evidence that X^- desorption may proceed via an indirect bounce trajectory.	P-10 TR-6
6. Diatomics, O_2, N_2	Role of symmetry and forbidden transitions in dissociative attachment of small molecules.	P-3,4 TR-8

*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: 10/1/88 - 2/28/91
Understanding the nature of
dissociation/desorption of small molecules and
negative ion desorption.
2. Mr. Fred Hutson - Research Associate, part time
Period worked: 10/1/88 - 12/31/90
Applications of electron spectroscopic data.
3. Mr. Hengxiang Yang - Graduate Student, summer
support
Period worked: 3 summer months of 89 and 90.
Experimental study of thin films.
4. Ms. Xiaowei Jin - Graduate Student, summer support
Period worked: 3 summer months of 90.
Theoretical studies on NEXAFS data.

g. Publications emanating from contract.

1. H. Sambe, D.E. Ramaker, M. Deschenes and L. Sanche, "Absolute Cross Section for Dissociative Electron Attachment in O₂ Condensed on Kr Film", *Phys. Rev. Letters*. **64**, 523 (1990).
2. D.E. Ramaker, "Understanding Electronegativity Effects in Photoelectron Spectra: Application to the High T_c Superconductors", *J. Electron Spectroscopy and Related Phenomena* **51/52**, 987 (1990).
3. H. Sambe and D.E. Ramaker, "Forbidden Electron Attachment in O₂", *Phys. Rev.* **A40**, 3651 (1989).
4. "Dissociative Electron Attachment in NO", H. Sambe and D.E. Ramaker, *Chemical Physics* **94**, 2548 (1991).
5. "Evidence for Vertical C₂ on Ni as a Precursor for Graphite Nucleation", *Applic. Surf. Sci.* **48**, 242 (1991).
6. "Interpretation of the Carbon Auger Line Shapes from Adsorbed and Fragmented Ethylene on Ni(100)", F.L. Hutson and D.E. Ramaker, *Surf. Sci.* **248**, 148 (1991).
7. "Spectroscopic Evidence for Carbon-Carbon Bonding in Carbodic Layers on Metals", F.L. Hutson, D.E. Ramaker, and B.E. Koel, *Surf. Sci.* **248**, 327 (1991).
8. "CEELS as a Probe of the Carbide to Graphite Transformation on Ni", D.E. Ramaker, *New Diamond Science and Technology* (Proc. 2nd Intn. Conf. on New Diamond Science and Technology), eds. R. Messier and J.T. Glass, MRS Intn. Conf. Proc. Series (Materials Research Soc., Pittsburg, PA, 1991).
9. "Lower Limits on the Absolute Dissociative Electron Attachment Cross Section from O₂ Condensed on Rare-Gas Films", H. Sambe, D.E. Ramaker, M. Deschenes, and L. Sance, submitted to Desorption Induced by Electronic Transitions, DIET IV, ed by G. Betz and P. Varga, Springer Series in Surface Sci., (Springer, Berlin Heidelberg, 1990).
10. "Electron-Stimulated O⁻ Desorption from O₂ Condensed on Rare-Gas Films: Evidence for an Indirect "Bounce" Trajectory", H. Sambe and D.E. Ramaker, submitted to Desorption Induced by Electronic Transitions, DIET IV, ed. by G. Betz and P. Varga, Springer Series in Surface Sci., (Springer, Berlin Heidelberg, 1990).
11. "The Past, Present, and Future of Auger Line Shape Analysis", D.E. Ramaker, submitted to "Critical Reviews in Solid State Physics".
12. "Extracting Chemical Information from Auger Line shapes", D.E. Ramaker, *Scanning Microscopy Supplement* **4**, 207 (1990).

h. Technical Reports Issued

1. F.L. Hutson, D.E. Ramaker, and B.E. Koel, "Spectroscopic Evidence for Carbon-Carbon Bonding in Carbide Layers on Metals", ONR Technical Report No. 49.
2. H. Sambe, D.E. Ramaker, M. Deschenes and L. Sanche, "Lower Bound Estimates of the Dissociative Electron Attachment Cross Section for O₂ Condensed on a Kr Film", ONR Technical Report No. 50.
3. D.E. Ramaker, "Extracting Chemical Information from Auger Lineshapes", ONR Technical Report No. 51.
4. D.E. Ramaker, "Understanding Electronegativity Effects in Photoelectron Spectra: Application to the High T_c Superconductors", ONR Technical Report No. 52.
5. H. Sambe, D.E. Ramaker, M. Deschenes, and L. Sanche, "Lower Limits on the Absolute Dissociative Electron Attachment Cross Section from O₂ Condensed on Rare-Gas Films", ONR Technical Report No. 53.
6. H. Sambe and D.E. Ramaker, "Electron-Stimulated O⁻ Desorption from O₂ Condensed on Rare-Gas Films: Evidence for an Indirect "Bounce" Trajectory", ONR Technical Report No. 54.
7. "The Past, Present, and Future of Auger Line Shape Analysis", D.E. Ramaker, ONR Technical Report No. 55.
8. "Dissociative Electron Attachment in NO", H. Sambe and D.E. Ramaker, ONR Technical Report No. 56.
9. "Evidence for Vertical C₂ on Ni as a Precursor for Graphite Nucleation", D.E. Ramaker, ONR Technical Report 57.
10. "CEELS as a Probe of the Carbide to Graphite Transformation on Ni", D.E. Ramaker, ONR Technical Report 58.

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