Quantitative Interpretation of Auger Line shapes and Electron/Photon Stimulated Desorption

D.E. Ramaker

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Auger Spectroscopy, Electron Stimulated Desorption, Photon Stimulated Desorption

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 line shapes. 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.
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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>
<thead>
<tr>
<th>SYSTEM</th>
<th>SIGNIFICANCE</th>
<th>PRODUCTIVITY (TR, P)</th>
</tr>
</thead>
<tbody>
<tr>
<td>NO&lt;sub&gt;3&lt;/sub&gt;<em>, SO&lt;sub&gt;4&lt;/sub&gt;</em>, SiO&lt;sub&gt;2&lt;/sub&gt;</td>
<td>Proposed intermediate localization model. First det'm. of theo. shake/Auger lineshapes.</td>
<td>P- 1,2,6 TR- 1,4,7,14</td>
</tr>
<tr>
<td>O&lt;sub&gt;2&lt;/sub&gt; gas</td>
<td>First ab-initio determination of experimental Auger widths</td>
<td>P- 3,23 TR- 6,30</td>
</tr>
<tr>
<td>NO&lt;sub&gt;3&lt;/sub&gt;-</td>
<td>Effect of Mulliken vs. local populations on Auger intensity.</td>
<td>P- 4 TR- 5</td>
</tr>
<tr>
<td>NO&lt;sub&gt;2&lt;/sub&gt;-, O&lt;sub&gt;2&lt;/sub&gt;, C&lt;sub&gt;2&lt;/sub&gt;H&lt;sub&gt;3&lt;/sub&gt;, Cu, Be,</td>
<td>Proposed final state rule for Auger lineshapes.</td>
<td>P- 5,8,12 TR- 8</td>
</tr>
<tr>
<td>C&lt;sub&gt;6&lt;/sub&gt;Li, C&lt;sub&gt;6&lt;/sub&gt;Cs</td>
<td>Proposed orthogonalized final state rule to account for enhanced intercalant peak</td>
<td>P- 7,9</td>
</tr>
<tr>
<td>N&lt;sub&gt;2&lt;/sub&gt;, CO, O&lt;sub&gt;2&lt;/sub&gt;, NO</td>
<td>Systematic and consistent interpretation of spectra for diatomic molecules</td>
<td>P- 13,25,28,29 TR- 11,21,26,27,28</td>
</tr>
<tr>
<td>Graphite</td>
<td>Established first case of localization in extended covalent system; first obs. of shakedown satellite.</td>
<td>P- 14,20,24,27 TR- 13,19,22,24</td>
</tr>
<tr>
<td>Atoms with atomic # = 8-54</td>
<td>Det'm. of semi-empirical KVV and L&lt;sub&gt;2&lt;/sub&gt;VV atomic Auger matrix elements.</td>
<td>P- 16</td>
</tr>
<tr>
<td>TM carbides, nitrides, oxides, SiC</td>
<td>Related Auger lineshapes to ionic bonding effects</td>
<td>P- 19 TR- 17</td>
</tr>
<tr>
<td>Si</td>
<td>First quantitative interpretation of CCV Auger lineshapes;</td>
<td>P- 21 TR- 15</td>
</tr>
<tr>
<td>Benzene, Cyclohexane, Polyethylene</td>
<td>Consistent interpretation and comparison of DU's in molecules and solids</td>
<td>P- 26,34,41 TR- 25,33,39,48</td>
</tr>
<tr>
<td>Diamond</td>
<td>Established evidence for antiferromagnetic ordering on surface</td>
<td>P- 30 TR- 29</td>
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<tr>
<td>13.</td>
<td>Polyethylene, diamond</td>
<td>Established the role of diamond excitation and shakeoff in AES processes.</td>
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<td>P= 31</td>
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<tr>
<td></td>
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<td>TR- 30</td>
</tr>
<tr>
<td>14.</td>
<td>Benzene, Transition metals</td>
<td>Interpretation of Auger line shapes for systems with less than 1/2 filled VB.</td>
</tr>
<tr>
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<td>P- 32</td>
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<tr>
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<td>TR -31</td>
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<tr>
<td>15.</td>
<td>Y-BA-Cu-O, La-Sr-Cu-O</td>
<td>Interpretation of AES and XPS data indicates the Cu-O bond covalency correlates with Tc, and that no Cu^{3+} is present.</td>
</tr>
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<td>P- 37,43,44,45,46</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TR- 37,43,44,45,46,47</td>
</tr>
<tr>
<td>16.</td>
<td>C_{2}H_{6}/Ni, C_{2}H_{4}/Ni, CH/Ni</td>
<td>First quantitative interpretation of Auger line shapes for chemisorbed systems.</td>
</tr>
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<td>TR- 41</td>
</tr>
</tbody>
</table>

*P and TR indicate sequence numbers of publications and ONR technical reports as listed below.*
TABLE 2  Summary of significant accomplishments in ESD/PSD.

<table>
<thead>
<tr>
<th>SYSTEM</th>
<th>SIGNIFICANCE</th>
<th>PRODUCTIVITY (TR, P)*</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. CO,N₂,H₂O</td>
<td>Established role of 2h1e type states in PSD of chemisorbed systems.</td>
<td>P- 10,11,15 TR- 9,10,12</td>
</tr>
<tr>
<td>2. OH/Ti, Cr,</td>
<td>Established the Auger induced desorption mechanism for non-maximal valency</td>
<td>P- 19 TR- 18</td>
</tr>
<tr>
<td>Cu, O/Cr</td>
<td>systems.</td>
<td></td>
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<tr>
<td>3. H₂O,OH/TiO₂</td>
<td>Resonant dissociative attachment mechanism found to be active for OH⁺ and O⁻.</td>
<td>P- 22 TR- 23</td>
</tr>
<tr>
<td>O/W, O/Mo</td>
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<tr>
<td>4. NH₃/Ru</td>
<td>Role of secondary electrons in desorption yields.</td>
<td>P- 18,38,40 TR- 16,36</td>
</tr>
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<td>mixed N₂O₂</td>
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<tr>
<td>5. O₂/Ar/Pt</td>
<td>Elucidated the role of image charge effects in PSD.</td>
<td>P- 33,39 TR- 32</td>
</tr>
<tr>
<td>6. O₂/Ar/Pt</td>
<td>Established the role of coherent scattering effects in the enhancement of</td>
<td>P- 35,42 TR- 34,40</td>
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<tr>
<td></td>
<td>ESD cross-section.</td>
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<tr>
<td>7. O₂/Pt,W</td>
<td>Elucidated the role of symmetry and its breakdown at surfaces in ESD</td>
<td>P-36 TR- 35,38,42</td>
</tr>
</tbody>
</table>

*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.


h. **Technical Reports Issued**


41. Interpretation of the Carbon Auger Line Shapes from Adsorbed and Fragmented Ethylene on Ni(100)", F.L. Hutson and D.E. Ramaker.


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