

probe the surface coverages. We use this equation to analyze the data of Gronwald and Henzler⁴ who have measured LEED profiles with a high resolution diffractometer for Si deposited on Si(111). Their data agree well with the above expression and values of the surface coverages can be extracted.

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Summary Abstract: Pseudodipole selection rules for extended fine structure in APS: Calculations and applications

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In extended appearance potential fine structure (EAPFS), one uses a beam of electrons to obtain EXAFS-like absorption structure. Details of the experiment and its several applications have been published.¹⁻³ A major question in the analysis is the angular momentum of the two final state electrons, especially the higher energy one bearing the EXAFS-like information, since knowledge of the phase shifts determines the precision to which one can resolve nearest neighbor spacings. In this paper we summarize model calculations to suggest that EAPFS has a pseudodipole excitation rule (i.e., that it can be analyzed with the same phase shift as would be used for EXAFS) and to show that previous experiments are consistent with this view. Detailed reports will appear elsewhere.⁴

Our initial calculations using hydrogenlike core electrons and OPW extended states convinced us that OPW is not valid for this problem (let alone the simplified version used previously⁵), since matrix elements which were expected to be rather slowly changing with incident electron energy E_i showed pronounced structure. We thus selected a model where the neighborhood of the target ionic core is treated realistically. We used the model developed by Bryant⁶ to calculate the bound and continuum wave functions of an ion imbedded in jellium. To compare with Refs. 1 and 2, we used an Al⁺³ ion in jellium with $r_s = 2.1$ and a Ti⁺⁴ ion in jellium with $r_s = 1.9$ and looked at the K and L_3 edges, respectively.

To calculate matrix elements we made a partial wave expansion of the wave functions. After some manipulation of $3j$ and $6j$ symbols, the matrix element can be expressed as a sum over the angular momenta of the incident electron and the two final state continuum electrons. We evaluated the con-

tribution to the total matrix element from each of these channels. We found that, for the Al- K edge, slightly over half of the total matrix element comes from one channel, that in which the incident electron has angular momentum $l_i = 2$, and both of the final state electrons have angular momentum 1. In the case of the Ti- L_3 edge, we found that the channel having $l_i = 3$ and both final electrons with $l = 2$ accounted for 1/2-1/3 of the total. In both cases these results weaken approximately 500 eV above threshold, the upper limit of typical EAPFS experiments.¹ The Al matrix element is nearly independent of the distribution of energy between the outgoing electrons. Similar results hold for titanium except when a final electron is near the $3d$ resonance, which, at least in this model, is just above the Fermi level. We also found that most of the interaction can be accounted for by the dipole part of the Coulomb interaction (the $r\langle/r\rangle^{-2}$ part of its partial wave expansion). Note that in both the aluminum and titanium cases the largest channels represent the case where the core electron gains one quantum of angular momentum and the incident electron loses one quantum, consistent with the dipole interaction.

We have also calculated matrix elements for simple model potentials, usually of the Thomas-Fermi type, varying both their strength and range. We found three trends. If the core electron has a nodeless wave function, (viz., $1s$ or $2p$, but not $2s$, $3s$ or $3p$) and if there is also another bound state of the same angular momentum (e.g., a $2s$ state if we are looking at a $1s$ core electron) then: (i) The transition is dominated by the dipole part of the Coulomb interaction. (ii) If the core electron has angular momentum l_c , then the largest channel is one in which the incident electron has angular momentum

$l_c + 2$, and both final electrons have angular momentum $l_c + 1$, consistent with (i). (iii) The matrix element is not significantly dependent on the distribution of energy between the two final state electrons, in agreement with previous claims.³ These trends hold best for the K edge, and fairly well for the L_3 edge. It is substantially less successful for the $M_{4,5}$ edges, where the dominant channel may account for only a fifth of the final signal. The requirement that the core wave function be nodeless is essential. For example, in L_1 excitation, the monopole and quadrupole parts of the Coulomb interaction dominate. Perhaps the requirement of a second bound state of the same l_c should be replaced by the requirement of a resonant or bound state of angular momentum $l_c + 1$, since both are often present. Finally, as the incident electron's energy increases condition (ii) fails, while condition (i) remains.

Condition (iii) corroborates previous work and allows differentiation of the EAPFS signal with respect to E_i to obtain EXAFS-like information from the electron with E_i minus the core and Fermi energies. Condition (ii) shows that this EXAFS-like electron has the same angular momentum as an electron in a true EXAFS experiment. Thus condition (ii) leads to a "pseudodipole selection rule." Note that for the Al- K edge, the second largest channel adds over 10% to this $l = 1$ dominance.

We have tested the conjecture in the context of our model by placing a spherical potential shell about the central atom and calculating the resulting EAPFS signal.⁶ Differentiating with respect to E_i , we find that the distance of the shell from

the origin calculated by standard EXAFS techniques is within $\pm 0.04 \text{ \AA}$ for Ti- L_3 and $\pm 0.01 \text{ \AA}$ for Al- K .

In reanalyzing the data of Refs. 1 and 2, we find the Lee-Beni procedure compensates partially for formerly using monopole excitation rules. Using $l = 1$ central atom phase shifts for the oxygen K edge, we calculate an O-Al distance of 2.02 \AA , consistent with the previous work.⁸ In the Ti experiment we use $l = 2$ phase shifts and find the Ti-Ti spacing to be 2.88 \AA as compared to the known crystal spacing of 2.89 \AA . Our success encourages us to believe that EAPFS can be a valid tool in surface measurements. Further work remains to understand the numerical trends we discovered.

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Summary Abstract: Multilayer reconstruction of the (2×2) GaAs(111) surface

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Earlier, we have reported on the structure of the GaAs(111) surface, which undergoes a (2×2) reconstruction.¹ In that report, we considered only the rearrangement of atoms in the topmost double layer. In a (2×2) structure, there are four Ga atoms and four As atoms in a unit cell of the double layer. We found that three Ga atoms in the unit cell were depressed to an almost coplanar position with the As atoms below. The resulting perpendicular separation between Ga and As planes of atoms was $0.07 \pm 0.02 \text{ \AA}$. The fourth Ga atom was popped up to $1.31 \pm 0.05 \text{ \AA}$ above the plane of As atoms.

By comparing results of calculated IV curves from dynamical theory with measured data of the $(\frac{1}{2}, 0)$ and $(0, \frac{1}{2})$ beams, we found that sizable lateral shifts ($0.1 \pm 0.03 \text{ \AA}$ and $0.28 \pm 0.03 \text{ \AA}$, respectively) must occur for Ga and As atoms in the first double layer. Also, the complete lack of symmetry

in the measured data for these two beams is a good indication of the presence of large shifts which break the symmetry of the Ga plane of atoms. In this reconstruction model, while the vertical and lateral displacements are large, the Ga-As bond length variation is generally $\leq 2\%$. With this model, we obtained good agreement in all five measured integral order beams, and fair agreement in three of five half-integral order beams.

We have now included in our model reconstruction of the second double layer. First, we find that the As atoms in the first double layer do not lie in the same plane. One As atom per unit cell is depressed by $0.07 \pm 0.03 \text{ \AA}$ (see Fig. 1 and also, d_3 of Fig. 2). The Ga atoms directly below these As atoms are in turn depressed by $0.04 \pm 0.02 \text{ \AA}$. This leads to a second double layer having the (2×2) structure (see Fig. 2).