

## ERRATA

ADSORPTION SITES AND BOND LENGTHS OF IODINE ON Cu{111} AND Cu{100} FROM SURFACE EXTENDED X-RAY-ABSORPTION FINE STRUCTURE. P. H. Citrin, P. Eisenberger,<sup>(a)</sup> and R. C. Hewitt [Phys. Rev. Lett. **45**, 1948 (1980)].

Ed Stern has pointed out to us that the omission of a cross term in the  $L_{2,3}$ -edge extended x-ray-absorption fine-structure (EXAFS) amplitude function modifies the numerical values listed in our Table I. The conclusions reached in our work are unaltered. The existence of this cross term, which couples the  $p-d$  and  $p-s$  transition probabilities, is well known<sup>1-3</sup> and was ignored by us because its contribution to the absolute magnitudes for the occupied threefold and fourfold adsorption sites in the systems studied amounted to only  $\sim 10\%$ . However, because this contribution is of opposite sign for the  $\tilde{\epsilon}_{\parallel}$  and  $\tilde{\epsilon}_{\perp}$  data and is of larger relative size for the onefold site, its effect on the ratio of absolute amplitudes for all the sites is not negligible and should therefore be included. If we take the amplitude of the  $p-s$  transition to be about 0.2 of that of the  $p-d$  transition (this is true for all atoms<sup>2</sup>), the effective coordination number  $N_s$  for the adsorbate atom is modified from  $\sum_i (\frac{1}{3} + |\tilde{\epsilon} \cdot \tilde{r}_i|^2)$  to  $\sum_i (1.4/3 + 0.6|\tilde{\epsilon} \cdot \tilde{r}_i|^2)$ , where the same notation applies.<sup>4</sup> The corrected calculated values for  $N_s$  are given in Table I along with our experimental results. As emphasized in our Letter it is the use of *both* absolute and relative surface extended x-ray-absorption fine-structure amplitudes which establishes the adsorption site, and in this regard the threefold and fourfold hollow-site assignments remain unchanged. The relatively weak polarization dependence for these two systems<sup>5</sup> clearly dictates the need for obtaining particularly reliable absolute amplitudes. If the polarization dependence of surface extended x-ray-absorption fine-structure

TABLE I. Calculated vs experimental  $N_s$  values for I on Cu.

	Atop	Bridge	Hollow	Expt.
Cu{111}				
$\tilde{\epsilon}_{\parallel}$	0.47	1.07	1.67	$1.6 \pm 0.2$
$\tilde{\epsilon}_{\perp}$	1.00	1.76	2.53	$3.0 \pm 0.6$
$\tilde{\epsilon}_{\perp}/\tilde{\epsilon}_{\parallel}$	2.13	1.65	1.52	$1.9 \pm 0.4$
Cu{100}				
$\tilde{\epsilon}_{\parallel}$	0.47	1.06	2.42	$1.9 \pm 0.2$
$\tilde{\epsilon}_{\perp}$	1.00	1.75	3.09	$2.8 \pm 0.6$
$\tilde{\epsilon}_{\perp}/\tilde{\epsilon}_{\parallel}$	2.13	1.66	1.28	$1.5 \pm 0.3$

amplitudes is to be used as an independent means for establishing adsorption sites, the measurement of  $L_1$  and  $K$  edges is more desirable ( $N_s$  is then simply proportional to  $\sum_i |\tilde{\epsilon} \cdot \tilde{r}_i|^2$ ). This has been done for  $\text{Br}_2$  on Grafoil<sup>6</sup> and for S on Ni{100}.<sup>7</sup>

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<sup>1</sup>S. M. Heald and E. A. Stern, Phys. Rev. B **16**, 5549 (1977).

<sup>2</sup>B. K. Teo and P. A. Lee, J. Am. Chem. Soc. **101**, 2813 (1979).

<sup>3</sup>P. A. Lee, P. H. Citrin, P. Eisenberger, and B. M. Kincaid, Rev. Mod. Phys. **53**, 769 (1981).

<sup>4</sup>For angularly averaged  $L_{2,3}$ -edge EXAFS amplitudes the cross term drops out and the expression  $\sum_i (\frac{1}{3} + |\tilde{\epsilon} \cdot \tilde{r}_i|^2)$  remains applicable.

<sup>5</sup>The systems studied, i.e., close-packed {111} and {100} surfaces of an fcc metal, actually represent least favorable cases. The polarization dependence of adsorbate  $L_{2,3}$ -edge EXAFS amplitudes is enhanced for substrates having either more open structures (e.g., Si{111}, W{111}), or lower symmetry (e.g., Cu{110}).

<sup>6</sup>S. M. Heald and E. A. Stern, Phys. Rev. B **17**, 4069 (1978).

<sup>7</sup>S. Brennan, J. Stöhr, and R. Jaeger, to be published.