Abstract: Determining surface relaxation from LEED via a transform method*

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A method for determining the degree of relaxation of a clean metal surface from realistic LEED data is presented, using the complex Fourier transform of the beam intensity as a function of electron momentum (the Patterson function). As shown by Landman and Adams,[1] the calculated Patterson function $P_c(z)$ corresponding to an analysis of kinematic (not dynamic) LEED data is given by the convolution integral

$$P_c(z) = \int_{-\infty}^{\infty} W(z')P_d(z - z')dz', \tag{1}$$

where $W(z)$ is the complex Fourier transform of the envelope of the LEED data in momentum space (specifically including the cutoff at finite momentum). $P_d(z)$ is given by

$$P_d(z) = \sum_i g_i[\delta(z - z_i) + \delta(z + z_i)], \tag{2}$$

where the set $\{z_i\}$ is a map of all the distances between layers in the crystal surface region and the coefficients $\{g_i\}$ decrease in amplitude for increasing z_i. Combining Eqs. (1) and (2) gives

$$P_c(z) = \sum_i g_i[W(z - z_i) + W(z + z_i)]. \tag{3}$$

In our method a quantity called the residual R is determined by

$$R^2 = \int_0^{\infty} [P_c(z) - P_0(z)]^2 dz, \tag{4}$$

where $P_0(z)$ is the Patterson function of the actual LEED data. For an assumed set of positions $\{z_i\}$, the coefficients $\{g_i\}$ are determined in the least-square sense to minimize the residual. By varying the positions of the delta functions as well as the value of the inner potential, and by looking for the smallest residual as well as the most physical set of coefficients $\{g_i\}$, the structure can be determined.

To illustrate the method, we show in Fig. 1(a) the kinematic I-V curve for the (11) beam of a material with a bulk spacing of $d = 2.23$ Å, a surface layer relaxed outward by $t = 9\%$, and an inner potential $V_0 = 16$ eV. The constant line is the window function. For the case of a single layer relaxing, the set of positions $\{z_i\}$ can be completely determined by one parameter t to be

$$\{z_i\} = 0, nd, (n + t)d, \qquad n = 1,2,3 \ldots . \tag{5}$$

By varying the choices of V_0 and t, the residual can be calculated to give the surface shown in Fig. 1(b). In Fig. 1(c) we show the topographic plot of this surface. The residual values have been normalized by dividing each value by

$$R_0^2 = \int_0^{\infty} P_0^2(z)dz. \tag{6}$$

The minimum at $V_0 = 17$ eV and $t = 8\%$ is very pronounced. The reasons why this minimum does not occur at exactly the correct solution for this kinematic data are fully discussed.

Using this method, the bulk of the work presented is the

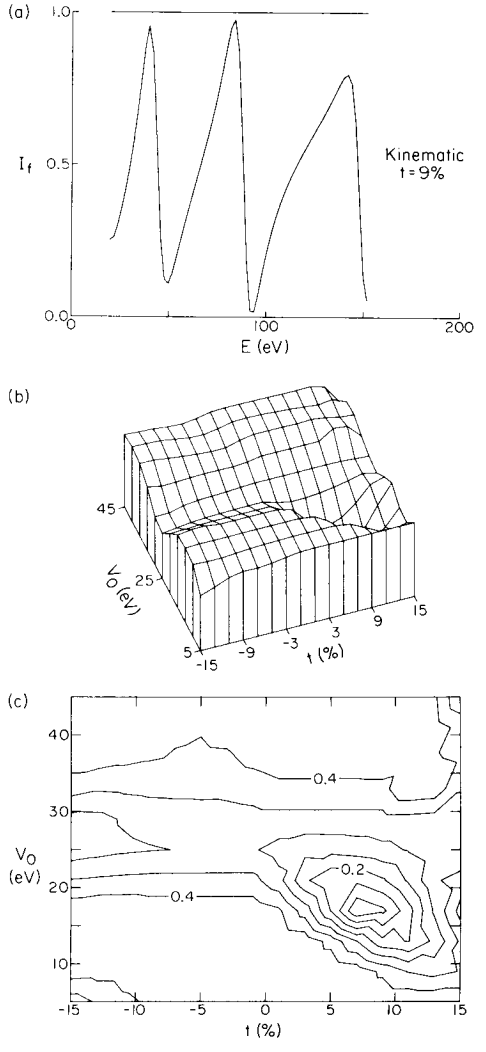

FIG. 1. (a) Kinematic interference function and constant window function appropriate for $W(110)$ using parameters in Ref. 2 and assuming $V_0 = 16$ eV and a surface relaxation outward of $t = 9\%$. (b) Plot of the residual R as a function of choice of inner potential V_0 and percent relaxation t. (c) Topographic contour plot of the surface in (b). All contours are separated by $\Delta R = 0.05$.

analysis of fully dynamic data (calculated) for four beams from the $W(110)$ surface for assumed relaxation of $t = 9\%$, -9%, and 0% as calculated by Van Hove and Tong.[2] We present analysis of data with different energy ranges as well as with different choices for the window function. We conclude that at its best the method can completely determine the surface relaxation, and at its worst it can narrow down considerably the choices of structure which may have to be analyzed with multiple scattering programs. This is the first evidence that a transform method can determine the degree of relaxation of a highly dynamic scattering material.

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