Truncation, potential, and temperature effects in the transform-deconvolution method

David L. Adams, Uzi Landman, and John C. Hamilton*

Xerox Corp., Webster Research Center, Webster, New York 14580

(Received 3 September 1974; in final form 10 October 1974)

Fourier transforms of LEED intensities contain convolution products of functions of the interatomic vectors with data truncation, lattice vibration, and potential windows. The composite and individual effects of the windows in the deconvolution of transforms of LEED intensities are studied using calculated and experimentally measured intensities. In the analysis of LEED intensities from Al(100), lattice motion is found to be of major importance along with data truncation and potential characteristics.

I. INTRODUCTION

A large number of properties of solids exhibit a marked dependence upon the atomic arrangement in the topmost layers. Structural parameters of the surface on the atomic scale and the correlation between the geometrical and electronic structure are of fundamental importance in the understanding of surface phenomena. The use of low energy electron diffraction (LEED) for surface-structure determination has been the subject of intensive efforts in the last ten years.[1]

Recently, we have described for the first time a *practical direct method* for surface structure analysis via LEED.[2,3] As we have shown, Fourier transformations of LEED intensities contain convolution products of functions of the interatomic vectors with functions (windows) of the scattering potential, temperature factors and data-truncation effects. Thus, to extract the geometrical information from the transform a deconvolution of the nonstructural components must be performed in order to achieve accurate and unambiguous structural assignments.

In this paper we briefly illustrate, with reference to experimental data from Al(100),[4] the individual and composite effects of data-truncation, scattering potential characteristics, and temperature dependence on the deconvolution results and the interrelationships between them.

II. TRANSFORM WINDOWS AND DECONVOLUTIONS

The Fourier transform of LEED intensities defines a *three-dimensional* vector space.[2,3] The first step in our procedure consists of the determination of interlayer spacings from *one-dimensional projections* of the transform, the results of which are utilized in the determination of interlayer registries via *two-dimensional transform sections* as we have previously demonstrated.[2]

The one-dimensional projection is defined as

$$P(Z)=\int_{-\infty}^{\infty} dS I_{00}(S)\omega_B(S;S_1,S_2)\exp[2\pi i S z], \quad [1]$$

where I_{00} is the intensity of the specular beam and $\omega_B(S;S_1,S_2)$ is a "box car" truncation function (unit magnitude for values of the normal momentum transfer $S_1<S<S_2$ and zero otherwise. $P(z)$ contains the projections of interatomic vectors on the surface normal.[3] The one-dimensional projection (Eq. 1) of a kinematical expression for the intensity of electrons diffracted from a uniform clean substrate with layer spacing d is given by[3]

$$P(z)=F_{BTP}(z)*(1-\alpha^2)^{-1}\sum_{\nu=-\infty}^{\infty}\alpha^{|\nu|}\delta(z+\nu d), \quad [2]$$

where '*' denotes a convolution operation; $\alpha=\exp(-\mu d/\cos\theta)$, μ is the attenuation coefficient, and θ the angle of incidence. The function $F_{BTP}(z)$ is the transform of the truncated scattering potential renormalized with respect to atomic motion, i.e.,

$$F_{BTP}(z)=\int_{-\infty}^{\infty} dS\omega_B(S;S_1,S_2)\omega_T(S)\omega_P(S)\exp[2\pi i S z],$$
$$=F_{BT}(z)*F_{BP}(z); \quad [3a]$$

$$F_{BT}(z)=\int_{-\infty}^{\infty} dS\omega_{BT}(S;S_1,S_2)\exp[2\pi i S z]; \quad [3b]$$

$$F_{BP}(z)=\int_{-\infty}^{\infty} dS\omega_{BP}(S;S_1,S_2)\exp[2\pi i S z]; \quad [3c]$$

$$\omega_{BT}=\omega_B(S;S_1,S_2)\omega_T(S);$$
$$\omega_{BP}=\omega_B(S;S_1,S_2)\omega_P(S); \quad [3d]$$

where the idempotency of ω_B is used. In the above, $\omega_T(S)=\exp[-\alpha(S)S^2]$ is the Debye–Waller[5] factor. Elastic scattering from an ion core is described by the

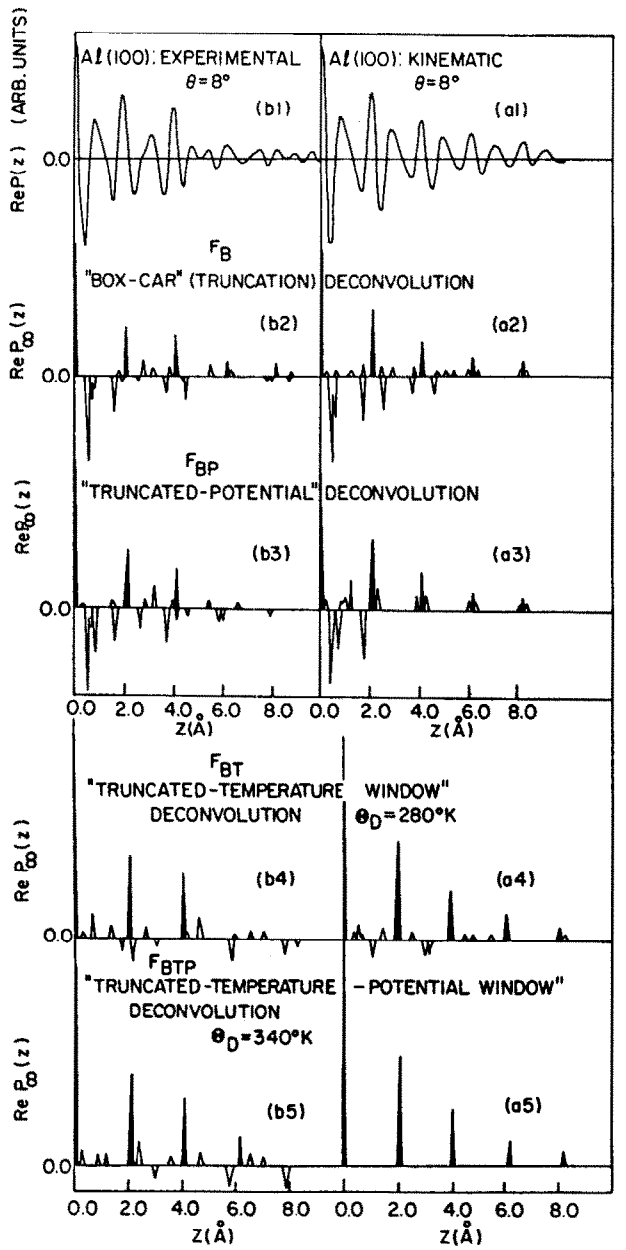

FIG. 1. Transforms $P(z)$ and deconvolutions $[P_\infty(z)]$. (a1). Real part of the $P(z)$ transform of a kinematically calculated[3] (00) beam intensity from Al(100) for incidence angle $\theta=8°$. In the calculation of the intensity 14 phase-shifts derived from Snow's potential were used with an interlayer spacing $d=2.05$ Å; $V_0=14$ eV, attenuation coefficient $\mu=0.32$ Å^{-1}, $\Theta_D=340°$ K and $T=295°$ K. (a2–a5). Deconvolutions of the transform of the kinematically calculated intensity. The deconvolutions in (a2)–(a5) were performed using the window functions defined in Eqs. (4), (3b), (3c), and (3a), respectively. A modified Southwell method was used.[8] (b1). Real part of the $P(z)$ transform of a measured (00) beam intensity profile from Al(100), for angle of incidence $\phi=0°$ and $\theta=8°$ at room temperature. (b2–b5). Deconvolution of the transform of the experimental intensity. The meaning of the various window components are as indicated in caption (a2)–(a5). The base width of the peaks is ±0.05 Å. Structural peaks forming a consistent weighted vector set have been filled.

atomic scattering factor expanded in a series of partial waves,[6–7] with $\omega_p(S)$ its squared magnitude.

From Eq. 2, it is evident that the extraction of geometrical information from the LEED transform requires a deconvolution of the complex window function $F_{BTP}(z)$ [Eq. 3(a)] from the transform. To facilitate our discussion of the effects of the components of the window, we have introduced the functions F_{BT} and F_{BP} [Eqs. 3(b) and 3(c), respectively], which represent the truncated temperature and potential windows, respectively. In addition, we define the window function F_B which represents the effect of data-truncation

$$F_B=\int_{-\infty}^{\infty} dS\omega_B(S;S_1,S_2)\exp[2\pi iSz]. \qquad [4]$$

In the following analysis we have used kinematical specularly diffracted intensities[3] from Al(100) for angle of incidence $\theta=8°$ calculated by using 14 phase-shifts with a Debye temperature $\Theta_D=340°$K, $T=295°$K and an interlayer spacing $d=2.05$ Å, and specularly diffracted intensities from Al(100) measured[4] at room temperature for the same angle of incidence, which exhibits marked multiple scattering features. The real parts of the one-dimensional transform projections of these intensities are shown in Figs. 1(a1) and 1(b1) for the calculated and experimental measured intensities, respectively. In both the kinematical and experimental cases, the transforms exhibit marked peak broadening and pronounced extra features which are of nonstructural origin. These effects are the result of the convolution of functions of the interatomic vectors with the truncated potential and temperature windows. The appearance of pronounced nonstructural features in the transform clearly precludes direct structure determination on the basis of the transform alone, demonstrating the necessity of an appropriate deconvolution. It is instructive to note the strong similarity between the transforms of the kinematically calculated and the measured intensities which exhibit pronounced multiple-scattering features. This similarity demonstrates the effective averaging introduced upon Fourier transformation of LEED intensities.[2,3]

We turn now to an examination of the effects of the data-truncation, potential, and temperature components of the window [Eqs. (3), (4)] on the deconvolution. We proceed by performing deconvolutions[8] of the above $P(z)$ transforms of the intensities with respect to the individual contributions to the window $F_{BTP}(z)$ [Eqs. (3) and (4)]. First a deconvolution of data truncation alone, represented by the F_B window [Eq. (4)] is performed. Figures 1(a2) and 1(b2) contain the computer deconvolutions of the complex function F_B from the complex transforms of the kinematical and experimental intensities, respectively. We observe that deconvolution of data-truncation alone is not sufficient to account for all the nonstructural components in the transforms. Improved results are obtained by the deconvolution of the truncated potential window, F_{BP} [Eq. (3c)], shown in Figs. 1(a3) and 1(b3) for the kinematical and experimental cases, respectively. However, the deconvolution results still contain nonstructural features which interfere with the accuracy of the analysis. Next, we study the results of deconvoluting the truncated temperature effect from the

original transforms. Since in analyzing experimental data the effective Debye temperature is unknown, a variation is performed to achieve an optimized deconvolution. (The convergence criterion employed is that a *convolution* of the *deconvolution result* with the corresponding *window*, *recovers* the *original transform* to a few percent.) The results of deconvoluting the F_{BT} window [Eq. (3b)] shown in Figs. 1(a4) and 1(ab4) for the kinematical and experimental cases, respectively, are surprisingly good, though an additional improvement is achieved by the deconvolution of the composite truncated potential-temperature window [Eq. (3a)], shown in Figs. 1(a5) and 1(b5) for the kinematical and experimental cases, respectively.

While a complete study of temperature effects is obviously beyond the scope of this paper, it will be discussed in a forthcoming publication where the analysis is extended to intensities measured at different temperatures.[4] We emphasize here the correlated effects of lattice dynamics and scattering potential in the analysis of LEED intensities.[6,7,10] This results in different values of the Debye temperature needed to achieve an optimized deconvolution, depending on the window function used.

Examination of the various deconvolutions of the kinematical transform [Figs. 1(a2)–1(a5)] reveals a variable degree of "noise" depending upon the window function used in the deconvolution ("noise" of negative value is included in these figures although no structural significance is associated with it in our analysis). Similar noise occurs in the deconvolutions of the transforms of the experimental data [Figs. 1(b2)–1(b5)].[4] Consequently, at this time, it is difficult to determine the source of the noise in the experimental deconvolutions. Since, as demonstrated in the kinematical case, an incomplete description of the window function results in noise in the deconvolution, we estimate that a significant part of the noise in the deconvolution of the experimental transforms derives from an incomplete description of the temperature and potential components of the window function and does not necessarily represent multiple-scattering effects.[8]

The result of the deconvolution of the composite window from the transform of the experimental intensity is shown in Fig. 1(b5) (other angles of incidence yield similar results).[4] In these results prominent peaks occur only at $2.05N$ Å ($N=0$, 1, 2, etc.) and form the only consistent periodic vector set. The unique value of the interlayer spacing determined from different intensity profiles, despite its strong variation with angle of incidence, demonstrates the consistency and applicability of the method. The determined value of 2.05 Å is in agreement with the bulk interlayer spacing of 2.025 Å to within our estimated accuracy of ± 0.05 Å.

The above results demonstrate the importance of data-truncation, vibronic and scattering potential effects in the analysis of LEED intensities. Specifically, in the surface structure analysis of Al(100), lattice motion is found to be of major importance along with data truncation and scattering potential characteristics.

ACKNOWLEDGMENTS

The authors are indebted to Dr. J. E. Demuth and Dr. P. M. Marcus for their assistance in deriving the phase-shifts used in this calculation. We are grateful to Ms. C. Troy for her invaluable assistance in the preparation of the manuscript.

*Present address: Bard Hall, Cornell University, Ithaca, NY 14850.

[1]Phys. Today **27**, 17 (1974).
[2]U. Landman and D. L. Adams, J. Vac. Sci. Technol. **11**, 195 (1974).
[3]D. L. Adams and U. Landman, Phys. Rev. Lett. **33**, 585 (1974).
[4]D. L. Adams and U. Landman (to be published).
[5]A. Guinier, *X-Ray Diffraction* (W. H. Freeman, San Francisco, 1963).
[6]D. W. Jepsen, P. M. Marcus, and F. Jona, Phys. Rev. B **5**, 3933 (1972).
[7]C. B. Duke, N. O. Lipari, and U. Landman, Phys. Rev. B **8**, 2454 (1973).
[8]A modified relaxation method due to Southwell (Ref. 9) has been used in performing the deconvolution; for details, see U. Landman and D. L. Adams (to be published).
[9]R. V. Southwell, *Relaxation Methods in Theoretical Physics* (Oxford U. P., New York, 1946).
[10]G. E. Laramore, Phys. Rev. B **6**, 1097 (1972).