

SURFACE SCIENCE LETTERS

HARD CORRUGATED WALL POTENTIAL: NUMERICAL CALCULATION OF DIFFRACTED PEAK INTENSITIES FOR ANY TYPE OF CORRUGATION

G. ARMAND, J. LAPUJOLADE and J.R. MANSON *

*Service de Physique Atomique, Section d'Etudes de Interactions Gaz–Solides, Centre d'Etudes
Nucléaires de Saclay, BP 2, F-91190 Gif-sur-Yvette, France*

Received 16 May 1978; manuscript received in final form 10 November 1978

In the present state of the art it seems that the so-called Hard Corrugated Wall is a potential which gives one of the best representations of the neutral atom–solid surface diffraction phenomena. In fact this potential has recently been coupled with an attractive well to give some very impressive agreement with experimental data [1,2]. In this paper we develop a formalism for the repulsive hard corrugated wall which is valid for all corrugations, even in the case of discontinuities in the shape function. Taking Oz as the direction normal to the surface, this potential is defined by

$$V(x, y) = 0 \quad \text{if} \quad z > \varphi(x, y) = \varphi(\mathbf{R}),$$

$$V(x, y) = \infty \quad \text{if} \quad z < \varphi(x, y) = \varphi(\mathbf{R}).$$

With this particular type of potential the Lippmann–Schwinger equation can be solved and one gets for the incoming plus scattered waves [3]:

$$\begin{aligned} \psi = \exp[i(\mathbf{K}_0 \cdot \mathbf{R} - k_{0z}z)] + \sum_{\mathbf{G}} \frac{\exp[i(\mathbf{K}_0 + \mathbf{G}) \cdot \mathbf{R}]}{k_{Gz}} \\ \times \int_{\text{unit cell}} F(\mathbf{R}') \exp(-i\mathbf{G} \cdot \mathbf{R}') \exp[ik_{Gz}|z - \varphi(\mathbf{R}')|] d^2\mathbf{R}', \end{aligned} \quad (1)$$

where

$$k_{Gz}^2 = k_0^2 - (\mathbf{K}_0 + \mathbf{G})^2,$$

in which, as usual, \mathbf{k}_0 is the incident particle wavevector of component \mathbf{K}_0 parallel, and k_{0z} perpendicular to the surface, \mathbf{G} is a surface reciprocal lattice vector, and

* Permanent address: Department of Physics and Astronomy, Clemson University, Clemson, South Carolina 29631, USA.

(R, z) is the position vector. $F(R)$ is the unknown source function which is to be determined by applying the boundary condition

$$\psi(R, z = \varphi(R)) = 0, \quad (2)$$

i.e., by solving the following integral equation:

$$0 = \exp[-ik_{Gz}\varphi(R)] + \sum_G \frac{\exp(iG \cdot R)}{k_{Gz}} \times \int_{\text{unit cell}} F(R') \exp(-iG \cdot R') \exp[ik_{Gz}|\varphi(R) - \varphi(R')|] d^2R'. \quad (3)$$

For z greater than the maximum value of φ , ψ consists of an incoming plus a sum of outgoing diffracted waves of amplitude

$$A_G = (k_{Gz})^{-1} \int_{\text{unit cell}} F(R') \exp(-iG \cdot R') \exp[-ik_{Gz}\varphi(R')] d^2R'. \quad (4)$$

So knowing the source function F the reflection coefficients are easily calculated using

$$R_G = \frac{\cos \theta_G}{\cos \theta_0} |A_G|^2,$$

where θ_G is the scattering angle measured from the normal. The set of R_G values will satisfy the unitarity condition

$$\sum_{G(k_{Gz}^2 > 0)} R_G = 1. \quad (5)$$

Several other methods of applying the boundary conditions giving simpler equations for determining the source function have been presented. A comparison with these other methods and a discussion of the problems involved with them is given elsewhere [4]. Recently, Garcia and Cabrera [5] have presented a numerical method which allows one to solve the integral equation (3). They restrict their calculation, without loss of generality, to the two-dimensional case: the corrugation function φ , and consequently the source function F are not dependent on y , a description which gives a good representation of stepped surfaces, for instance. Their method, called RR' , consists in replacing the integral in eq. (3) with a finite sum by dividing the one-dimensional unit cell of length a into $2N$ intervals of equal length. The resulting equation is regarded as a system of $2N$ linear algebraic equations for the $2N$ unknown values $F(X_n)$. In other words, the ψ function is forced to be zero at the set of $2N$ points $X = X_n, Z = \varphi(X_n)$. The system is inverted to obtain the $F(X_n)$ values and then the reflection coefficients are calculated by numerical

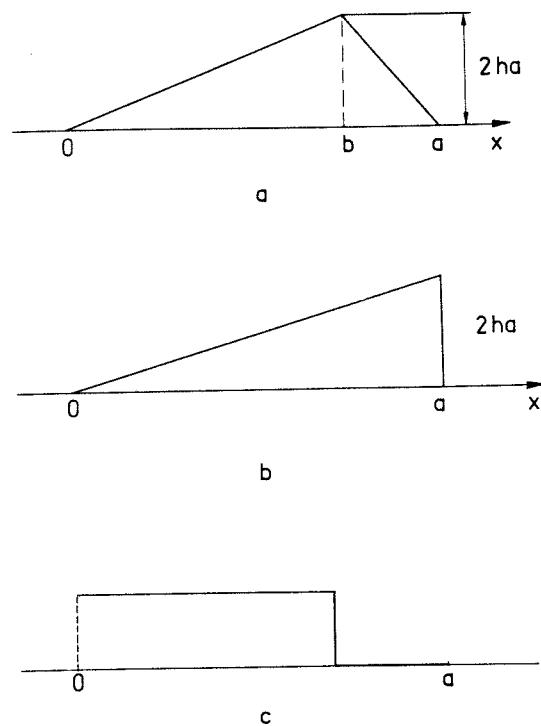


Fig. 1. (a) The triangular corrugation profile; (b) the saw-tooth profile; (c) the dental profile.

integration of eq. (4). The number N should be sufficiently large so that the calculated R_G values satisfy the unitarity relationship (5).

This method, which has been successfully applied to the interpretation of diffracted peak intensities from a vicinal surface [6,7] where the corrugation is of a triangular type (fig. 1a), is not suitable when the profile presents a "vertical" part (a discontinuity in the $\varphi(x)$ function) such as the saw-tooth corrugation (fig. 1b). In this latter case the numerical integration does not take into account the vertical line of the discontinuity and consequently the ψ function does not necessarily vanish on this part of the profile. We propose here a numerical method, called $RR'Z$, which allows the problem to be solved for any kind of corrugation, even in the case of discontinuities.

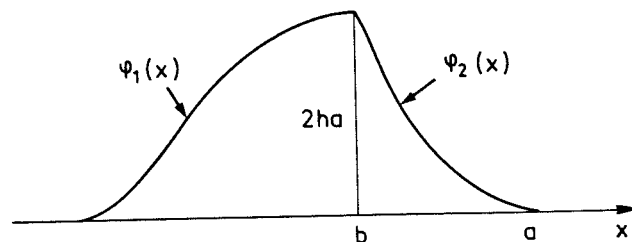


Fig. 2. A general corrugation profile of height $2ha$, described by the two functions $\varphi_1(x)$ and $\varphi_2(x)$.

Let us consider the one-dimensional profile of a unit cell of length a (fig. 2) defined by

$$z = \varphi_1(x), \quad 0 \leq x \leq b; \quad z = \varphi_2(x), \quad b \leq x \leq a,$$

where, for simplicity, φ_1 and φ_2 are taken to be monotonic functions. Eq. (1) reduces to:

$$\begin{aligned} \psi = \exp[i(K_0 \cdot R - k_{0z}z)] + \sum_{G_x} \frac{\exp[i(K_0 \cdot R + G_x x)]}{k_{Gz}} \\ \times \left\{ \int_0^b F_1(X) \exp(-iG_x X) \exp[ik_{Gz}|z - \varphi_1(X)|] dX \right. \\ \left. + \int_b^a F_2(X) \exp(-iG_x X) \exp[ik_{Gz}|z - \varphi_2(X)|] dX \right\}, \end{aligned} \quad (6)$$

where

$$k_{Gz}^2 = k_0^2 - (K_{0x} + G_x)^2 - (K_{0y})^2.$$

We change the variable of integration from X to Z . Putting

$$F(\varphi^{-1}(Z)) \frac{d(\varphi^{-1}(Z))}{dZ} = F'(Z),$$

we get for the boundary condition and beam amplitudes:

$$\begin{aligned} 0 = \exp(-ik_{0z}z) + \sum_{G_x} \frac{\exp(iG_x x)}{k_{Gz}} \\ \times \left\{ \int_0^{2ha} F'_1(Z) \exp[-iG_x \varphi_1^{-1}(Z)] \exp[ik_{Gz}|z - Z|] dZ \right. \\ \left. - \int_0^{2ha} F'_2(Z) \exp(-iG_x \varphi_2^{-1}(Z)) \exp[ik_{Gz}|z - Z|] dZ \right\}, \end{aligned} \quad (7)$$

$$\begin{aligned} A_G = \frac{1}{k_{Gz}} \int_0^{2ha} \{F'_1(Z) \exp[-iG_x \varphi_1^{-1}(Z)] - F'_2(Z) \exp[-iG_x \varphi_2^{-1}(Z)]\} \\ \times \exp(-ik_{Gz}Z) dZ. \end{aligned} \quad (8)$$

Now we divide the integration interval ($0 \leq Z \leq 2ha$) into N subintervals and put

2) $Z_n = n(2ha/N)$. Carrying out the numerical integration, eq. (7) can be written as

$$0 = \exp(-ik_{0z}z) + \frac{2ha}{N}$$

$$1) \quad \times \left\{ \sum_{n=0}^{N-1} F_1'(Z_n) \sum_{G_x} \frac{\exp\{iG_x[x - \varphi_1^{-1}(Z_n)]\}}{k_{Gz}} \exp(ik_{Gz}|z - Z_n|) \right. \\ \left. - \sum_{n=1}^N F_2'(Z_n) \sum_{G_x} \frac{\exp\{iG_x[x - \varphi_2^{-1}(Z_n)]\}}{k_{Gz}} \exp(ik_{Gz}|z - Z_n|) \right\}. \quad (9)$$

For a given point on the profile, that is to say for a pair $z, x = \varphi^{-1}(z)$, this equation contains N unknown values of each function $F_1'(Z)$ and $F_2'(Z)$ or a total of $2N$ unknown quantities. To convert eq. (9) into a system of linear algebraic equations one choose N points on each profile section, $X_{n'} = \varphi_1^{-1}(Z_{n'})$ and $X_{n'} = \varphi_2^{-1}(Z_{n'})$, with for instance $Z_{n'} = (n' + \epsilon) 2ha/N$, $0 \leq \epsilon < 1$. Note that, with ϵ different from zero, the set of points $X_{n'}$ where $\psi = 0$, is different from the set X_n where the F function is determined. Evaluating eq. (9) at the set of points $X_{n'}, Z_{n'}$ gives a set of $2N$ linear equations in the $2N$ unknown quantities F_1' and F_2' . The system can be inverted and the diffraction amplitudes are obtained from (8) by numerical integration.

With this procedure we have forced the ψ function to be zero on only $2N$ points of the profile, and not, as it should be, on the continuous set of profile points. In order for the boundary conditions to be well approximated, the number N will be certainly large. Furthermore, we will obtain a good evaluation of the integrals in eqs. (1) and (8) by the numerical procedure only if the integral does not vary strongly over the interval $Z_{n+1} - Z_n = 2ha/N$. This condition is difficult to formulate as the F function is unknown, but it certainly implies again that N should be equal to a large number and additionally imposes a condition on $|G_{\max}| = (2\pi/a)P$ the maximum value of G in the sum of eq. (9). (In principle this sum extends from $-\infty$ to $+\infty$.) In this way the sum becomes

$$\frac{2ha}{N} \sum_{-P}^{+P} \frac{1}{k_{Gz}} \exp\{iG_x[\varphi_{1,2}^{-1}(Z_{n'}) - \varphi_{1,2}^{-1}(Z_n)]\} \exp\left(ik_{Gz}|n' + \epsilon - n| \frac{2ha}{N}\right). \quad (10)$$

For the particular case where $n = n'$ and both $\varphi(Z_n)$ and $\varphi(Z_{n'})$ lie on the same portion of the profile, it reduces to

$$\frac{2ha}{N} \sum_{-P}^{+P} \frac{1}{k_{Gz}} \exp\left(ik_{Gz}\epsilon \frac{2ha}{N}\right), \quad (11)$$

a sum which remains convergent as N goes to infinity even in the case $\epsilon = 0$ if P is of the order of N .

Table 1

Comparison of the RR' method and the $RR'Z$ method with a triangular corrugation profile for a system exhibiting seven diffracted beams; the incident beam is perpendicular to the surface

Beam	$RR', \epsilon = 0.5$	$RR', \epsilon = 0$	$RR'Z, \epsilon = 0$
$\bar{3}0$	0.236×10^{-2}	0.236×10^{-2}	0.224×10^{-2}
$\bar{2}0$	0.434×10^{-2}	0.434×10^{-2}	0.430×10^{-2}
$\bar{1}0$	0.52340	0.52368	0.52203
00	0.18088	0.18069	0.18218
10	0.14749	0.14739	0.14859
20	0.10796	0.10804	0.107812
30	0.3336×10^{-1}	0.3347×10^{-1}	0.3269×10^{-1}
ΣR_G	0.99981	1.00000	0.99987

$$h = 0.05, a = 3 \times 10^{-8} \text{ cm}, |k_0| = 7.06 \times 10^8 \text{ cm}^{-1}, |k_0|a = 21.18, b/a = 0.75, K_0 = 0.$$

Thus, it appears that in the numerical procedure one has to choose two values, P and N , the P value being certainly equal to or near the N value. The numerical result should be a convergent process: the calculated peak intensities should reach their asymptotic values and the unitarity sum should approach unity as N increases. In practice one increases N until the desired unitarity is obtained.

Table 1 gives result obtained with a triangular shaped profile (fig. 1a). Between the two results $\epsilon = 0.5$ and $\epsilon = 0$ with the RR' method there is only a difference of 3×10^{-4} on the most intense peak ($\bar{1}0$) which is of the order of the unitarity defect. The $\epsilon = 0$ procedure seems to be the best one for this profile. Calculation with the new saw-tooth corrugation leads to the same conclusion. This means that in either case the sums over G are sufficiently precise taking $P = N$ in (10) and consequently in (11). But the difference probably comes from the fact that the source function F is not determined on the same set of profile points. Particularly, if $\epsilon = 0$, the vertices of the profile are points where the wave function is forced to zero, but if $\epsilon \neq 0$ this is no longer the case. Between the RR' and $RR'Z$ methods, the difference is a little greater (0.5% on the 00 peak) but this can certainly be reduced by increasing the number of points $2N$ which would have the effect of improving the unitarity of the $RR'Z$ procedure. Nevertheless, the two methods are seen to be equivalent for this profile.

Table 2 gives the results for the saw-tooth profile ($b/a = 1$). As the relative height increases, the unitarity given by the RR' method is progressively destroyed, as could be expected, if the ψ function does not completely vanish on the vertical part of the corrugation. With the new method exposed here ($RR'Z$), the unitarity slowly decreases as h increases but remains within 1% of 1. In fact, for the highest profile taking $2N = 150$ in place of 100, the unitarity becomes better. This illustrates the convergence of the process and confirms the validity of the method used.

Note that for $h = 0.15$ the classical rainbow coincides approximately with the $\bar{2}0$ peak.

Table 2
Comparison of the RR' method and the $RR'Z$ method for the saw-tooth profile

Beam	$b/a = 1, 2N = 100, \epsilon = 0$				$b/a = 1, 2N = 150, \epsilon = 0$			
	$h = 0.05$		$h = 0.15$		$h = 0.2$		$h = 0.2$	
	RR'	$RR'Z$	RR'	$RR'Z$	RR'	$RR'Z$	RR'	$RR'Z$
30	0.351×10^{-2}	0.252×10^{-2}	0.1044×10^{-1}	0.627×10^{-2}	0.7929×10^{-1}	0.7227×10^{-1}	0.7311×10^{-1}	0.7311×10^{-1}
20	0.2071×10^{-1}	0.1712×10^{-1}	0.77333	0.69503	0.62169	0.64730	0.64833	0.64833
10	0.55957	0.53464	0.2932×10^{-1}	0.6011×10^{-1}	0.7627×10^{-1}	0.10343	0.10352	0.10352
00	0.24784	0.26350	0.3135×10^{-1}	0.6639×10^{-1}	0.3084×10^{-1}	0.8616×10^{-1}	0.8708×10^{-1}	0.8708×10^{-1}
10	0.7667×10^{-1}	0.8527×10^{-1}	0.5606×10^{-1}	0.895×10^{-1}	0.149×10^{-2}	0.2884×10^{-1}	0.2962×10^{-1}	0.2962×10^{-1}
20	0.5577×10^{-1}	0.6144×10^{-1}	0.1082×10^{-1}	0.1672×10^{-1}	0.1946×10^{-1}	0.3165×10^{-1}	0.3296×10^{-1}	0.3296×10^{-1}
30	0.3008×10^{-1}	0.3195×10^{-1}	0.3156×10^{-1}	0.6048×10^{-1}	0.2665×10^{-1}	0.2377×10^{-1}	0.2236×10^{-1}	0.2236×10^{-1}
ΣR_G	0.99417	0.99647	0.94290	0.99453	0.85573	0.99344	0.99700	0.99700

$a = 3 \times 10^{-8}$ cm, $|k_0| = 7.06 \times 10^8$ cm $^{-1}$, $|k_0|a = 21.18$, $K_0 = 0$.

The two methods of solution, integration over Ox and Oz , can be combined in order to calculate diffraction peak intensities from corrugation profiles having both horizontal and vertical part like the "dental" corrugation depicted in fig. 1c.

Although one does not normally expect surface profiles with discontinuous $\varphi(x)$ in atom-surface scattering this approach may be a useful method for certain types of stepped surfaces. In addition, such surfaces are often found in the field of acoustic wave scattering, which is relevant to the same formalism.

References

- [1] C.E. Harvie and J.H. Weare, *Phys. Rev. Letters* 40 (1978) 187.
- [2] N. Garcia, F.O. Goodman, V. Celli and N.R. Hill, to be published.
- [3] R.I. Masel, R.P. Merrill and W.H. Miller, *Phys. Rev. B* 12 (1975) 5545.
- [4] G. Armand and J.R. Manson, *Phys. Rev. B*, to be published.
- [5] N. Garcia and N. Cabrera, in: *Proc. 7th Intern. Vacuum Congr. and 3rd Intern. Conf. on Solid Surfaces*, Vol. I (Vienna, 1977) p. 379.
- [6] N. Garcia and J. Lapujoulade, to be published.
- [7] G. Armand and J.R. Manson, *Phys. Rev. B*, to be published.