Normalized distorted-wave Born approximation for soft potentials in atom-surface scattering

N. Garcia*
IBM Zurich Research Laboratory, 8803 Rüschlikon-Zurich, Switzerland
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In recent papers Armand and Manson have dealt with atom-surface scattering from a soft exponential corrugated potential. In this work we present a normalized distorted-wave Born approximation whose results compare well with exact calculations by Armand. This approximation may reproduce the intensities of the main beams for He scattering from dense metallic surfaces where the corrugations are not too large.

In two recent papers, Armand and Manson[1,2] have used the so-called CCGM (Cabrera, Celli, Goodman, Manson) theory[3] and have solved without approximation the problem of atom-surface scattering from a soft exponential corrugated potential

$$V(\vec{R},z)=Ce^{-\chi[z-D(\vec{R})]}, \tag{1}$$

where the position vector is $\vec{r}=(\vec{R},z)$, $\vec{R}$ and z being the parallel and perpendicular coordinates to the surface, C is an energy constant irrelevant for the intensities, $D(\vec{R})$ is the corrugation function, and χ gives information on the softness of the potential: for $\chi\to\infty$, the hard corrugated-surface (HCS) model with corrugation $D(\vec{R})$ is obtained.

The CCGM theory[3] starts by solving the Hamiltonian

$$H_0(z)=-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}+V_0(z) \tag{2}$$

with m mass of the particle; then perturbation theory is applied to the eigenfunctions $\phi_p(z)e^{i\vec{K}\cdot\vec{R}}$. Here $(\vec{K},p)$ is a wave vector with parallel and perpendicular components $\vec{K}$ and p, respectively [for the incident particle $\vec{k}_i=(\vec{K},k_{\vec{0}z})$]. The total scattered wave function is

$$|\psi_i^+\rangle=\sum_{\vec{G}}\psi_{\vec{G}}(z)e^{i(\vec{K}+\vec{G})\cdot\vec{R}}, \tag{3}$$

$\vec{G}$ being the two-dimensional reciprocal vectors, and

$$\psi_{\vec{G}}(z)=\int_0^\infty b_{\vec{G}}(p)\phi_p(z)dp, \tag{4}$$

an expansion in terms of the $\phi_p(z)$. The outline of the theory can be followed in Refs. 1–3. Armand and Manson[1] and Armand[2] (we concentrate on Ref. 2) took

$$V_0(z)=Ce^{-\chi z} \tag{5}$$

for which solutions are the modified Bessel functions, $K_{ip}(z)$. For the case of potential (1), the distorted-wave Born approximation (DWBA) gives the scattering amplitude of the beam $\vec{G}$ as

$$A_{\vec{G}}=-\frac{\pi}{4}\frac{F_{\vec{G}}}{P_{\vec{G}}} \tag{6}$$

[see Ref. 2, Eq. (28)], where

$$F_{\vec{G}}=(V_{\vec{G},\vec{0}}-\delta_{\vec{G},\vec{0}})f(P_{\vec{G}},P_{\vec{0}}), \tag{7}$$

$$P^2_{\vec{G}}=\frac{4}{\chi^2}k^2_{\vec{G}z}, \tag{8}$$

$$V_{\vec{G},\vec{0}}=\frac{1}{S_0}\int_{S_0}e^{-i\vec{G}\cdot\vec{R}}e^{\chi D(\vec{R})}d\vec{R}, \tag{9}$$

S_0 being the surface of the unit cell, and the matrix elements of $e^{-\chi z}$ are[4]

$$f(P_{\vec{G}},P_{\vec{0}})=[P_{\vec{G}}\sinh(\pi P_{\vec{G}})P_{\vec{0}}\sinh(\pi P_{\vec{0}})]^{1/2}\frac{(P_G^2-P_0^2)}{\cosh(\pi P_{\vec{G}})-\cosh(\pi P_{\vec{0}})}(1-\delta_{\vec{G},\vec{0}})+\frac{2}{\pi}P_G^2\delta_{\vec{G},\vec{0}}. \tag{10}$$

The expressions for a corrugated Morse potential for $V_{\vec{G},\vec{0}}$ are the same, but the matrix elements are different as shown in Ref. 3. Finally, the diffraction intensities $I_{\vec{G}}$ are given by

$$I_{\vec{G}}=\frac{k_{\vec{G}z}}{k_{\vec{0}z}}|i\delta_{\vec{G},\vec{0}}-2A_{\vec{G}}|^2. \tag{11}$$

It is well known that the specular beam is not

well described by the DWBA and that unitarity is not fulfilled. For example, looking at the specular intensity in (11) for $A_{\vec{0}}$ real, this being the case at hand [see Eqs. (9) and (10)], we observe that it is always larger than one.

Thus, to obtain results from the DWBA, a way has to be chosen to normalize the intensity. Usually this is done[3] by redefining the specular $I^R_{\vec{0}}$ as

$$I^R_{\vec{0}} = 1 - \sum_{\vec{G} \neq \vec{0}} I_{\vec{G}} \ , \tag{12}$$

where $\vec{G}$ runs for any channel such that $k^2_{\vec{G}z} \geq 0$. Here, we propose a normalized solution $I^N_{\vec{G}}$ reading

$$I^N_{\vec{G}} = \frac{I_{\vec{G}}}{\sum_{\vec{G}} I_{\vec{G}}} \ . \tag{13}$$

We call this result normalized distorted-wave Born approximation (NDWBA), and its validity has to be checked numerically against exact calculations. We have done this for the examples given by Armand[2] for a square unit cell of size $a = 2.55$ Å, and the corrugation

$$D(\vec{R}) = ha\left[\cos\left[\frac{2\pi}{a}x\right] + \cos\left[\frac{2\pi}{a}y\right]\right] \tag{14}$$

with $h = 0.02$, an azimuthal angle $\phi = 45°$, and $|\vec{k}_i| = 8.6$ Å^{-1}. Tables I and II show the Armand results[2] in comparison to those obtained with NDWBA for two different incident angles, $\theta_i = 31°$ and $60.5°$. The value U in the first line indicates the unitarity obtained with DWBA (i.e., the specular peak in NDWBA is approximately $1/U$). The number in parentheses gives the percentage error for the specular beam as compared with the exact results[2]; when not indicated, the deviation is smaller than 1%. This approximation works better than (12). From the calculations we notice: (i) as expected, the approximation is better the smaller U is (i.e., $U \to 1$), (ii) for a given corrugation, the approximation is better the smaller χ is (i.e., the potential is softer), (iii) the approximation is better when the angle of incident θ_i increases, or when the value of $k_{\vec{0}z}$ becomes smaller—but we should stress that these cases are more interesting because then the softness parameter χ plays an important role with respect to the corrugation strength h,[5,6] (iv) although all the beams are not described with the same accuracy, the more intense beams are well described, and these are the interesting ones from the experimental point of view, (v) also, the limits of validity of the NDWBA are within the range of the dense metallic surfaces as, for example, a recent analysis of Rieder's experimental data[5,6] for He/Ni(110) has shown, (vi) it is clear that when χ increases, the approximation fails but this also happens with the exact calculations. In these cases, the approach that works better is to expand around the HCS as a zero-order solution. This gives the correct limit for $\chi \to \infty$, and is good for χ large for any corrugation in which the HCS can be solved.[6]

In conclusion, we have proposed a simple computational method to calculate atom-surface scattering intensities from soft corrugated potentials which is based on a normalized distorted-wave Born approximation. We have shown that it works well by comparing with the results of exact calculations for a soft exponential corrugated potential performed by Armand.[2] The method can be generalized to any potential by solving numerically the Hamiltonian $H_0(z)$, and calculating the

TABLE I. Comparison for the intensity in different beams between exact solutions (Ref. 2) and NDWBA in this paper. $k_i = 8.6$ Å^{-1}, $h = 0.02$, $\theta_1 = 31°$, $(-n)$ denotes 10^{-n}.

U	1.103		1.370 (5%)		1.489 (7%)		1.541 (8%)	
χ (Å^{-1})	1		3		5		6	
	Exact	NDWBA	Exact	NDWBA	Exact	NDWBA	Exact	NDWBA
$I_{0,0}$	0.9037	0.9066	0.6958	0.7320	0.6294	0.6770	0.6145	0.6623
$I_{1,1} \times 100$	0.16(−6)	<1.(−5)	0.038 16	0.0010	0.1878	0.014	0.2536	0.0330
$I_{1,0} \times 10$	0.37(−2)	0.36(−2)	0.3671	0.3369	0.6188	0.5600	0.6785	0.6163
$I_{1,\bar{1}} \times 10$	0.41(−3)	<1.(−5)	0.0492	0.0041	0.0883	0.0128	0.0980	0.0187
$I_{0,\bar{1}}$	0.0432	0.0462	0.0967	0.0996	0.0987	0.1030	0.0987	0.1030
$I_{\bar{1},\bar{1}} \times 10$	0.0276	0.003	0.1630	0.0005	0.1859	0.015	0.1897	0.0230

TABLE II. The same as in Table I for $\theta_i = 60.5°$; $(-n)$ denotes 10^{-n}.

U	1.000		1.044		1.096		1.115	
χ (Å^{-1})	1		3		5		6	
	Exact	NDWBA	Exact	NDWBA	Exact	NDWBA	Exact	NDWBA
$I_{0,0}$	0.9998	0.9998	0.9595	0.9589	0.9169	0.9145	0.9051	0.9008
$I_{0,\bar{1}} \times 10$	0.58(−3)	<0.6(−3)	0.1904	0.2048	0.3820	0.4250	0.4340	0.4873
$I_{\bar{1},\bar{1}} \times 100$	0.63(−5)	<1.(−5)	0.1103	0.0200	0.3570	0.0370	0.4428	0.0780
$I_{1,\bar{1}} \times 10^3$	0.31(−4)	<1.(−5)	0.0889	0.0500	0.3649	0.290	0.4964	0.4700

matrix elements with the remainder of the potential (this work is now in progress). We claim that this simple and "cheap" approximation is enough to study the atom-surface scattering from compact metallic surfaces where the softness is more important. In case of harder potentials, we suggest that the approach of a distorted-wave Born approximation starting with the HCS as zero-order solution may give a good description of the elastic intensities.

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*Permanent address: Departamento Fisica Fundamental, Universidad Autonoma de Madrid, Canto Blanco, Madrid 34, Spain.

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