# Neutral-atom scattering from random isolated adsorbate atoms on clean metal surfaces: Oxygen and carbon monoxide on nickel (001)

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The intensity I of the specular beam of a helium nozzle beam scattered from a Ni(001) surface has been measured as a function of adsorbate coverage  $\Theta$  for both oxygen and CO exposures at 350 K for different angles of incidence. A linear relationship is found between ln  $(I/I_0)$  ( $I_0$ , the intensity of the specular beam from the clean surface) and  $\Theta$  up to  $\Theta = 0.15$  monolayer of O on Ni and  $\Theta = 0.1$  monolayer of CO on Ni. A model is proposed in which the scattering is governed by the repulsive part of the gas-surface potential, the latter being described by a hard-wall corrugation. A constant attractive well depth and a temperature-dependent vibration amplitude of the atoms are also incorporated into the model. The adsorbate atoms are treated as a shot noise on a flat metal surface. By means of suitable averaging, a formula is found that explains the linear dependence indicated. From the best fit of the model to the experimental data, a set of parameters describing the corrugation of a single adsorbate is derived. Cross sections for the helium-adatom scattering are 65 and 26 Å<sup>2</sup> for CO and O, respectively. The corresponding corrugations have been fitted with Gaussians of height 0.62 Å (for CO) and 0.32 Å (for O).

## I. INTRODUCTION

Neutral-atom scattering (NAS) has been developed in recent years as a sensitive probe of electronic charge distribution in periodic surface structures.<sup>1-6</sup> For example, Rieder and Engel<sup>6</sup> recently used NAS in order to analyze the crystallography of an ordered layer of hydrogen on nickel (011) and were able to recognize different surface structures as a function of hydrogen coverage. It has also been proved,<sup>7</sup> following earlier theoretical suggestions,<sup>8</sup> that NAS can give important information concerning surface excitations and, in particular, surface phonons. However, NAS has seldom been used to explore adsorption processes at low coverages when the particles of the adsorbate can be considered to be mostly at random sites on the surface. Only recently, Mason et al.<sup>9</sup> have shown, from a comparison of the coherent and incoherent elastic scattering signals of helium atoms impinging on a copper (001) surface, that information can be gained about the mechanisms involved in those first stages of adsorption. In an earlier publication<sup>10</sup> we described a first attempt to use NAS as a real probe of the electronic charge distribution around isolated adsorbate atoms

on a metal surface at very low coverages ( $\Theta \sim 0.03$ ). In the present paper this preliminary work is extended (i) by studying the experimental variation of the scattered intensities as a function of coverage and (ii) by developing a theoretical model in which the disorder of the adsorbed layer is properly taken into account when treated as a random gas and as a lattice gas (defined later, Sec. IV). We have measured, as a function of gas coverage, the dependence of the specular beam intensity of a helium beam on the incident angle  $\theta_i$  when either oxygen or carbon monoxide is adsorbed on a well-characterized Ni(001) surface. Our model is shown to be in very good agreement with the experimental data, and geometrical parameters associated with the electronic charge distribution around the adsorbate atoms are derived from an optimized fitting of the experimental results.

# **II. EXPERIMENTAL**

The experiments were carried out in an ionpumped ultrahigh-vacuum chamber with a base

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pressure of  $2 \times 10^{-10}$  Torr. With the beam on, the pressure rose to  $2 \times 10^{-9}$  Torr, but peaks other than helium did not significantly increase. The helium beam was generated from a nozzle source of the specific design of Campargue.<sup>11</sup> The wavelength in our experiments was  $\lambda = 0.57$  Å (wave vector k = 11.0 Å<sup>-1</sup>). Detection was performed by means of a quadrupole that could be rotated in both polar and azimuthal angles. The angular resolution of the detector was approximately 0.9°. A complete description of the equipment can be found elsewhere.<sup>12</sup>

The Ni(001) sample was in the form of a disk and was cleaned in the standard way by argon-ion bombardment, followed by annealing and oxygen treatments at elevated temperatures. After cleaning, no traces of the usual contaminants, such as carbon, sulfur, oxygen, etc., were detected by Auger spectroscopy. In the course of our experiments, we found that the helium specular intensity from the metal surface was, in fact, a much more sensitive probe of surface cleanliness than Auger spectroscopy. Routinely, we therefore used the specular intensity as a monitor of impurity adsorption or segregation. This was particularly important in connection with hydrogen contamination that could not, obviously, be detected by Auger measurements. Hydrogen is by far the most abundant component of the residual atmosphere in the vacuum chamber and adsorbs readily on the nickel surface. We performed flash desorption runs of hydrogen-contaminated surfaces and found that the desorption peak has its maximum at  $\sim 360$  K. In the following, we carried out our experiments at a surface temperature of at least 350 K and, therefore, hydrogen contamination was thought to be negligible.

As is well known, the helium specular intensity is very sensitive to surface order. In order to obtain a maximum specular peak, the nickel sample had to be annealed at high temperature (~1300 K). As a figure or merit for the cleanest surface, we quote a value of 0.55 for the ratio of the intensity of the specular beam to that of the incident beam for an incident angle of  $\theta_i = 70^\circ$  and a surface temperature of T = 350 K.

As will become apparent in subsequent sections, an accurate measurement of oxygen and carbon monoxide exposure is mandatory. We did these measurements by integrating over exposure times recorder traces of gauge overpressure (with respect to the background pressure) and correcting for the ionization probability of the corresponding gas. Exposures were converted into coverages by using available data on sticking probabilities as described below.

# **III. RESULTS**

For both carbon monoxide and oxygen we have measured, as a function of the total reactive gas exposure S, the intensity of the helium specular peak I for different values of the incident polar angle  $\theta_i$ . The azimuthal angle has always been kept constant with the projection of the incident direction on the specimen plane lying along [110]. These values of the specular intensities have been normalized to the corresponding specular intensity from the clean surface (at the given angle)  $I_0$ , by defining a relative intensity J:

$$J = I/I_0 . (1)$$

It is worth pointing out that a quantity such as J is free of certain errors that can arise in the measurements of either I or  $I_0$  separately, for example, those errors connected with glancing incidence angles when the cross section of the beam becomes larger than the diameter of the specimen. It is clear that, in this case, both I and  $I_0$  measurements would certainly give anomalously low values, but they would not result in incorrect values of J.

In order to convert exposures S into coverages  $\Theta$  the values of the sticking probability s must be taken into account. For carbon monoxide, we have taken s = 1 in the whole range of our experiments.<sup>13</sup> For oxygen we have used a dependence of the form  $s(\Theta)=1-k\Theta$ . If the exposure is normalized to the surface density of atoms, we obtain immediately

$$\Theta = \frac{1}{k} (1 - e^{-kS}) . \tag{2}$$

From a systematic Auger study of oxygen-nickel interactions, Holloway and Hudson<sup>14</sup> suggest a value of k = 4. We have tried to optimize the value of k by comparison with our own scattering data. We have made different plots of  $\ln J$  vs  $\Theta$  assuming different values of the constant k in Eq. (2). An example is shown in Fig. 2 for k = 4.5. All the plots have a linear region for any k in the range 3 < k < 5 but for that corresponding to k = 4.5 the linear region extends to higher  $\Theta$ . As in our theoretical model, to be discussed later, a linear dependence of  $\ln J$  vs  $\Theta$  is obtained we take as the best value of k the one that preserves the linearity for a longer range. In the following, all the data for oxygen are plotted under the assumption that k = 4.5 in Eq. (2). This value compares reasonably well with that obtained by Holloway and Hudson.

Our experimental values for both carbon monoxide and oxygen are plotted in a  $\ln J$ -vs- $\Theta$  representation in Figs. 1 and 2, respectively. It is clear that for both gases, and for each angle of incidence  $\theta_i$ , the



FIG. 1. Experimental values of  $\ln J$  as a function of the coverage  $\Theta$  of CO for different values of the incident angle  $\theta_i$ . Note that J is equal to the specular intensity normalized to the value from the clean surface at the given angle. Solid line: Best fitting of Eq. (8).

curves have a linear region. A least-squares fitting of the corresponding slopes, p, is plotted versus the angle of incidence  $\theta_i$  in Figs. 3 and 4. Notice the very different qualitative behavior of the p plot for both gases.

#### **IV. THEORETICAL MODEL**

## A. Random Gas

We consider, first, the case of a random gas, i.e., a collection of gas adatoms (coverage  $\Theta$ ) on a flat surface. No lattice structure is included and an adatom can, consequently, be placed at any position on the surface plane. No correlation between the positions of different adatoms is considered.

Our model assumes that helium scattering from the adsorbate-covered surface can be treated in the hard-wall approximation.<sup>1</sup> The metal surface is assumed to have no corrugation of its own, and the adsorbate corrugation is represented by a function

$$Z(\vec{R}) = \sum_{j} Z_0(\vec{R} - \vec{R}_j)$$
, (3)

where  $\vec{R}$  is a position vector parallel to the surface,  $\vec{R}_j$  refers to the position of adatom j ( $\vec{R}_j$  is not a lattice vector in this case), and  $Z_0$  is the corrugation function of a single adatom. The central assumption of the random-gas model is that Eq. (3) can be considered as shot noise in the statistical sense.<sup>15</sup>

The helium scattering amplitude A is computed now in the Kirchhoff approximation.<sup>16</sup> Let us call  $\vec{Q}$  and  $q_z$  the momentum transfer parallel and perpendicular to the surface, respectively. The scattered coherent amplitude is

$$A(\vec{Q},q_z) = \frac{F}{S} \int_{S} \exp(i\vec{Q}\cdot\vec{R}) \\ \times \exp[iq_z Z(\vec{R})] d\vec{R} , \qquad (4)$$

where F is a numerical factor (equal to unity for the



FIG. 2. Experimental values of  $\ln J$  as a function of the coverage  $\Theta$  of O (atomic) for different values of the incident angle  $\theta_i$ . Solid line: Best fitting of Eq. (8).



FIG. 3. Slope, p, of the linear part of the plot of Fig. 1 as a function of the corresponding incident angle  $\theta_i$ . The solid line is a fitting of the experimental values of p with the help of Eq. (15) and the parameters of Table I for CO.



FIG. 4. Slope, p, of the linear part of the plot of Fig. 2 as a function of the corresponding incident angle  $\theta_i$ . The solid line is a fitting of the experimental values of p with the help of Eq. (15) and the parameters of Table I for O.

specular beam) involving the angle, S is the area associated with the transfer width,<sup>17</sup> and the integral is extended precisely over this area S.

If we restrict attention to the specular intensity and, for convenience, drop from the notation the symbol  $\vec{Q}$  by writing  $A(q_z) = A(\vec{0}, q_z)$ , we have

$$A(q_z) = \frac{A_0(q_z)}{S} \int_S \exp[iq_z Z(\vec{R})] d\vec{R} , \qquad (5)$$

where  $A_0(q_z)$  designates the specular amplitude from the clean surface.

As we have a random distribution of adatoms, we must average A over the different possible distributions. A well-known property of random-noise averages<sup>15</sup> allows us to write the average value of the exponential in Eq. (5) in terms of the surface density  $\lambda$ of scattering centers. Following Ref. 15 we write  $\lambda = \Theta/b_0^2$ , where  $b_0$  designates the nearest-neighbor distance in the metal surface. We obtain

$$\frac{A(q_z)}{A_0(q_z)} = \langle \exp[iq_z Z(\vec{R})] \rangle = \exp\left[\frac{\Theta}{b_0^2} \int_{\sigma b_0^2} \{\exp[iq_z Z_0(\vec{R})] - 1\} d\vec{R}\right].$$
(6)

It is clear that for a random gas  $\langle \exp[iq_z Z(\vec{R})] \rangle$  does not depend on  $\vec{R}$ , as expected. We are interested in the intensity *I*, which can be written in terms of the intensity from the clean surface  $I_0(q_z)$ ,

$$I(q_z) = I_0(q_z) \exp\left[\frac{2\Theta}{b_0^2} \int_{\sigma b_0^2} \{\cos[q_z Z_0(\vec{R})] - 1\} d\vec{R}\right].$$
(7)

In Eqs. (6) and (7) we introduced the quantity  $\sigma$  as the effective cross section of an adatom for the scattering process. If we recall our definition of J given by Eq. (1), we can rewrite Eq. (7) as

$$\ln J = -2\sigma \Theta[1 - H(q_z)] ,$$

$$H(q_z) = \frac{1}{\sigma b_0^2} \int_{\sigma b_0^2} \cos[q_z Z_0(\vec{R})] d\vec{R} ,$$
(8)

where the integral is extended [as in Eq. (7)] to the area of the adatom, represented by  $\sigma b_0^2$ .

Equation (8) is the basis of our interpretation of the experimental data. Note that the  $q_z$  dependence

of H leads to a dependence of I on the angle of incidence  $\theta_i$  as  $q_z$  is given by

$$q_z = 2 \left[ k^2 \cos^2 \theta_i + \frac{2m}{\hbar^2} D \right]^{1/2}, \qquad (9)$$

where k is the incident momentum, m the mass of the helium atom,  $\hbar$  the Planck constant divided by  $2\pi$ , and D the attractive potential well depth.<sup>18</sup>

## B. Lattice gas

The random-gas model of the preceding section fails to be realistic, particularly at short distances

between adatoms, due to the fact that adatoms are actually constrained to sit on a set of lattice points. We argue in this section that, assuming low coverages  $\Theta \ll 1$ , the consideration of a lattice gas does not result in substantial modifications of Eq. (8).

A lattice gas is still given by a corrugation function like that in Eq. (3) provided that the surface density of scattering centers  $\lambda$  of shot-noise theory is now made position dependent. With the notation of Ref. 15 we can now write

$$\lambda(\vec{\mathbf{R}}) = \Theta \sum_{j} \delta(\vec{\mathbf{R}} - \vec{\mathbf{R}}_{j}^{0}) , \qquad (10)$$

where  $\vec{R}_j^0$  designates a set of lattice points [for example, the set of fourfold sites corresponding to the ordered structure of oxygen on nickel (001)]. A straightforward substitution for  $\lambda$  from Eq. (10) into the corresponding averaging formula leads to

$$\langle \exp[iq_z Z(\vec{R})] \rangle = \exp(-\Theta\{1 - \exp[iq_z Z_0(\vec{\rho})]\}),$$
  
(11)

where  $\vec{\rho}$  designates a coordinate parallel to the surface restricted to the unit cell of the lattice. Comparison of Eqs. (11) and (6) shows that the average  $\langle \exp[iq_z Z(\vec{R})] \rangle$  is a constant for the random gas but does depend on the position of the point in the unit cell for the lattice gas. Substitution of Eq. (11) into Eq. (5) leads finally to

$$A(q_z) = \frac{A_0(q_z)}{b_0^2} \times \int_{\sigma b_0^2} \exp(-\Theta\{1 - \exp[iq_z Z_0(\vec{\mathbf{R}})]\}) d\vec{\mathbf{R}} .$$
(12)

We argue now that the values of the amplitude in both random-gas and lattice-gas models [Eqs. (12) and (6)] are the same to the first order in  $\Theta$ . It is easily shown, by expanding both equations to the first order in  $\Theta$ , that in either case the linear term is

$$\frac{A(q_z)}{A_0(q_z)} \simeq 1 - \sigma \Theta + \frac{\Theta}{b_0^2} \int_{\sigma b_0^2} \exp[iq_z Z_0(\vec{R})] d\vec{R} .$$
(13)

It is also worth pointing out that Eq. (13) is exactly equal to the equation that we used for analysis of our data in a previous publication<sup>10</sup>; that equation was derived on the basis of very simple arguments. This equation is thought to be sufficiently accurate for very low  $\Theta$  but is expected to fail at the higher coverages considered in the present paper (in Ref. 10 only values of  $\Theta < 0.03$  were considered).

It is much easier to compare the experimental re-

sults with Eq. (6) than Eq. (12). Therefore, we have tried to estimate the range for which both of them can be interchanged within experimental error. This has been found numerically (for a variety of trial models) to be possible for coverages  $\Theta < 0.3$ . As all our analysis is carried out for values of  $\Theta$  definitely lower than this upper bound, Eq. (6) has been systematically used for the analysis of our data.

## C. Temperature effects

The above-mentioned model has been derived in terms of a stationary corrugation and must be slightly modified to account for temperature effects. Although a full analysis of Debye-Waller effects in atom scattering from surfaces is still lacking,<sup>19</sup> a simple correction has been incorporated in our model. We assume that the intensity from the adsorbate-covered surface has a different Debye-Waller factor than the clean one due to the fact that the mean-square amplitude (MSA) of vibration of surface atoms is different when an adsorbate is present. Denoting by W and  $W_0$  the corresponding Debye-Waller factors for the adsorbate-covered and clean surface, respectively, we have a temperature-corrected intensity given by

$$I(q_z) = I_0(q_z) \exp[-2(W_0 - W)]$$
$$\times \exp\{-2\sigma\Theta[1 - H(q_z)]\}$$

A simple assumption of linearity in  $\Theta$  for the average MSA of the adsorbate-covered surface<sup>10</sup> leads finally to a temperature-corrected law of dependence between r and  $\Theta$ :

$$\ln J = -\Theta\{q_z^2 \Delta u^2 + 2\sigma[1 - H(q_z)]\}, \qquad (14)$$

where  $\Delta u^2$  is the difference between the MSA of an adsorbate and a substrate atom. Equation (14) is the final expression that will be compared with the experimental results.

#### V. DISCUSSION

A comparison of Eq. (14) with the experimental curves for both carbon monoxide and oxygen (Figs. 1 and 2) reveals remarkable agreement. We can see that linearity between  $\ln J$  and  $\Theta$  is preserved until rather high values of  $\Theta$  are reached ( $\Theta \sim 0.1$  for CO and  $\Theta \sim 0.15$  for oxygen). At higher coverages two effects are expected to contribute to a departure from that linear relationship: island formation and lattice-gas effects. The latter have been computed, as indicated above, to occur at values of  $\Theta$  higher than those corresponding to a departure from linearity in Figs. 1 and 2 and, therefore, island formation seems a good candidate to account for the deviation from linearity in the data. It is worth noting that the onset of observation of diffraction peaks in oxygen [corresponding to a superlattice spot  $(\frac{1}{2},0)$  of the  $p(2\times 2)$  structure] has been reported at a comparable coverage.<sup>20</sup>

On the basis of our model, the experimental values of the slope p in Figs. 3 and 4 should be identified with the quantity in curly brackets in Eq. (14), which we shall call the theoretical slope,  $p^{\text{theor}}$ :

$$p^{\text{theor}} = q_z \Delta u^2 + 2\sigma [1 - H(q_z)]. \qquad (15)$$

Equation (15) has been adjusted to the experimental data by taking the difference between the MSA of adsorbate and substrate,  $\Delta u^2$ , and the scattering cross section  $\sigma$  as adjustable parameters. The adatom corrugation  $Z_0(\vec{R})$  appearing in the function  $H(q_z)$  has been taken in the shape of a Gaussian:

$$Z_0(\vec{R}) = a \exp(-R^2/2b^2)$$
 (16)

with adjustable height a and width b. The potential well depth D of Eq. (9) has been taken as D = 7.5 meV from the data of Rieder<sup>21</sup> in the system oxygen on Ni(011).

The values of the parameters giving the best fit to the experimental data are given in Table I. The corresponding graphs of Eq. (15) are given as solid lines in Figs. 3 and 4. We can see that the agreement with experiment is good.<sup>22</sup> We discuss in the following the significance of the values obtained for the different parameters.

One general question, that may be asked first, is to what extent the set of parameters of Table I can be considered as unique. In particular, one can wonder whether changing the corrugation to a different shape (for example, a paraboloid) can give rise to very different geometrical parameters. The answer to that question, obtained after many computations using Eqs. (15) and (8), is that the parameters a and  $\sigma$  are remarkably independent of the shape of the impurities within less than 20%. In other words, trying to fit the data of Fig. 4 with a paraboloid of height a and radius  $d (d = b_0 \sqrt{\sigma/\pi})$ would result in a best value of a that did not differ from the one in Table I by more than 20%. Of

TABLE I. Numerical values of the corrugation parameters and of the Debye-Waller correction corresponding to the best fitting of Eq. (15) to the experimental data of Figs. 3 and 4.

	a (Å)	σ	<b>b</b> (Å)	$\Delta u^2$ (Å <sup>2</sup> )
со	0.615	10.55	6.15	0.012
0	0.32	4.2	3.3	0.006

course, the latter fitting would be, in any case, worse, resulting in a larger value of the sum of the squared deviations from the experimental points. A general discussion of the role of the different parameters in the value of  $H(q_z)$  can be found in Ref. 10, where different impurity shapes are also compared.

Our value of a = 0.32 Å for oxygen in a disordered layer on Ni(001) is in good agreement with a recent determination by Rieder<sup>23</sup> for an ordered  $p(2\times2)$  layer of oxygen on that particular nickel face. Our results confirm the widely extended belief that the first stages of oxygen interaction with Ni(001) are dominated by the adsorption of oxygen atoms in second-neighbor fourfold sites at a distance of  $2b_0$  along [110].

Concerning the actual values of a, we must bear in mind that NAS probes the electronic surface structure at a certain distance above the plane of the surface-atom cores, in fact, at the so-called turning point of the helium-atom-surface interaction potential. It is expected, and has actually been calculated for some systems,<sup>24</sup> that the corrugation at the turning point is smoother than that at the level of the atom cores. Quantitative comparisons of corrugations obtained from NAS (ordered or disordered layers) and surface-atom core positions await the development of realistic calculations along the lines of those of Ref. 24, for a number of adsorbatesubstrate systems. Nevertheless, the fact that the value we have obtained for a in CO is roughly twice that obtained in O does seem reasonable in view of the well-known fact that CO adsorbs on Ni(001) in an upright position.

Our results for the cross section  $\sigma$  (note that they correspond to absolute values  $\sigma b_0^2$  of 65 and 26 Å<sup>2</sup> for CO and O) support the long-standing belief that NAS is extremely sensitive to minor concentrations of impurities or defects on the surface. The value of  $\sigma_{\rm CO} = 10$  is in excellent agreement with the data of Mason et al.<sup>9</sup> in CO on Cu(001), in which they quote a decrease of 20% in the specular peak for a CO coverage of 1% (this is equivalent to  $\sigma = 10$  because the intensity decreases with coverage as  $2\sigma\Theta$ , the factor 2 arising from the conversion of amplitudes to intensities). It is also worth pointing out that our result of  $\sigma_0 = 4.2$  is such that there is just no overlap between two neighboring oxygen atoms at a distance  $2b_0$  along [110]. This justifies our assumption of taking the oxygen adatom corrugation as arising from isolated oxygen atoms even if the adatoms themselves are arranged in pairs. Our cross sections are, however, smaller by about a factor of 3 of those recently estimated<sup>25</sup> by Comsa and coworkers in CO on Ni(111). The reasons for it are not clear, but it seems that long-range attractive potentials do not play a key role in our experiment.

We finally want to discuss the value we obtain for the Debye-Waller parameter. Our value of  $\Delta u^2 = 6 \times 10^{-3} \text{ Å}^2$  can be compared with that estimated by Lapujoulade *et al.*<sup>26</sup> on the basis of their measurements on ordered layers of oxygen on Cu(001). They obtain upper and lower bounds for  $\Delta u^2$  of 9 and  $3 \times 10^{-3} \text{ Å}^2$ . In the absence of direct measurements for oxygen on nickel, the agreement between our fitted parameter and the above data seems reasonable.

#### **VI. CONCLUSIONS**

We have shown in this paper that the scattering of neutral helium beams from surfaces can give information about the electronic charge distribution around disordered adsorbate atoms at the turning point of the incoming particle. We have been able to obtain a set of parameters that characterize quantitatively the geometry of the corrugation by which that electronic distribution is represented.

Apart from the intrinsic interest of these results in what concerns the study of the initial stages of gas-surface interactions [for example, we have shown here that the vertical distance from the oxygen atom to the surface is the same in the initial disordered state and in the ordered  $p(2\times2)$  structure], we want to point out that the present work suggests that surface defects (such as surface vacancies) can be studied also with the help of this technique. This possibility would be most welcome, in

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view of the present scarcity of surface-defect probes. The utilization of atom scattering in these fields would be favored by the large cross section of any surface irregularity to the atom beam, this cross section having been measured, unambiguously, for the first time in the present work. We must stress, however, that any attempt to correlate measurements of the electronic corrugation, as those reported here, to actual displacements of atom cores at the surface require realistic calculations of the interaction potential between a helium atom and the clean or adsorbate-covered surface. We hope that the present results will foster these types of calculations.

Note added in Proof. After submission of this paper a model for the treatment of atom scattering from random surface impurities has appeared in the literature [A. Levi *et al.*, Surf. Sci. <u>121</u>, 504 (1982)]. Although their approach is different the results of their calculations agree with ours.

## ACKNOWLEDGMENTS

The authors are indebted to Professor N. Cabrera for continuous guidance and advice. The help of Carmen Ocal with the numerical adjustments and rewarding discussions with Dr. A. M. Baró, Dr. R. Miranda, and Professor G. Comsa are gratefully acknowledged. Thanks are due the Instituto de Estudios Nucleares and Comisión Asesora (Contract No. 4150/79) for financial help.

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