

Simulation for Helium Atom Scattering From Stepped Surfaces

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Abstract — A computer program has been developed to simulate the helium atom scattering from stepped surface for both up hill and down hill scattering with diffraction kinematics chosen to be both in-and out-of-phase relative to the terraces. Codes from the program perform calculation in 3D geometries with normal incidence spectra of helium atoms having beam energy in the range from 15 meV to 60 meV and the smoothing of the step edge atom. Program codes apply the overall phase associated with each point over the surface for three different ranges of potentials, which are prepared by using the modified sudden approximation method of scattering calculation and realistic helium-surface interaction potential. The computations have been executed in the case of a Cu (001) surface. It is observed that the scattering is sensitive to the details in the helium-step interaction potentials.

Keywords: Scattering, simulation, helium, atom, Surface, sudden approximation.

1.0 Introduction

The availability of high-resolution diffractometers for helium atom scattering in the late nineties has provided the opportunity to study a wide range of surface structures and understanding the involving mechanism in the surface growth. The metal-on-metal epitaxy is technologically important and in recent years helium scattering has been widely used to characterize the growth of thin metal film [14-16]. It is necessary to have a clear and perfect understanding of the scattering from growing surfaces to characterize the growth system. Atomic steps represent probably the most common defect species on crystalline surfaces; they are certainly always present, even on surfaces that have been prepared using the latest state of the art technique [1]. In order to characterize the growth of thin metal films by helium scattering, it is necessary to understand the helium scattering from isolated steps on metal surfaces both qualitatively and quantitatively. These study provided quantitative information on vertical surface morphology, that is, step heights and average step densities [2]. The experiment of Lahee *et al.* [3] was the first of its kind to provide information on the size and shape of an isolated step from the diffusely scattered helium intensities. Different theoretical analyses [3-7] of experimentally observed diffraction intensities gave qualitative information on size, shape and distribution of steps [3]. Quantitative information on the structure of the step edge from experimental data requires the detailed knowledge of the helium-step interaction potential. The realistic helium-step interaction potential model proposed by Sultana [8] facilitated the quantitative investigation of helium scattering from an isolated step on low index Cu (001) surface. The scattering calculations have been performed using the sudden approximation [9]. In this paper, we study the elastic atom scattering intensities for isolated atomic steps on low index Cu (001) surface by employing the helium-surface interaction potential and modified sudden approximation. Simulations of helium scattering from an isolated Cu (001) step have been performed for a range of incident beam energy from 15 meV to 60 meV. The simulated diffraction patterns have been analyzed and observed that the scattering is sensitive to the details in the helium-step interaction potentials.

2.0 Computational Method

Helium atom scattering has been treated by a quantum mechanical model known as Modified Sudden Approximation [5,9,10]. The atom - solid surface interaction is characterized by an interaction potential for an isolated step of Cu (001). The applied interaction potential describes the properties of ideally periodic or disordered surfaces, respectively.

The modified Sudden Approximation has been introduced into atom-surface scattering theory by Gerber and coworkers [9,11]. The original sudden approximation was modified by Hinch [5] where the incident and final values of the phase factors $i \eta$ and $f \eta$ were distinguished. The initial phase factor η_i is defined solely by $V(R, Z)$ and the final state

perpendicular wave vector K_{mn}^z . The scattered amplitude $A_{00, mn}$ from the 00^{th} to the mn^{th} channel in the modified sudden approximation [5] is written as $A_{00, mn} = \frac{1}{F} \int_{u.c} \int e^{-G_{mn,R}} e^{i(\eta_i(R) + \eta_f(R))} d^2 R$, where the phase factor η_i is evaluated in the

WKB approximation and takes the following form: $\eta_i = \int_{z_i(R)}^{\infty} [k_i^z(R, z) - k_{00}^z] dz - k_{00}^z z_i(R)$, -----(1), where k_{00}^z is the

magnitude of incident perpendicular wave vector and $k_i^z(R, z)$ is defined at each point in the space by $[k_i^z(R, z)]^2 = (k_{00}^z)^2 - \frac{2mV(R, z)}{\hbar^2}$. $z_i(R)$ is the classical turning point, that is, the height over the surface at a point \mathbf{R} at

which k_i^z is equal to zero. Similarly, $\eta_f = \int_{z_f(R)}^{\infty} [k_f^z(R, z) - k_{mn}^z] dz - k_{mn}^z z_f(R)$, -----(2) and

$[k_f^z(R, z)]^2 = (k_{mn}^z)^2 - \frac{2mV(R, z)}{\hbar^2}$ and $z_f(R)$, the classical turning point for the outgoing channel is defined such that

$\frac{\hbar k_{mn}^z}{2m} = V(R, z = z_f(R))$. The final scattered intensity, $I_{00, mn}$ are then expressed in terms of the amplitudes:

$$I_{00, mn} = |A_{00, mn}|^2.$$

3.0 Computational strategies

3.1 Geometry and Approximation for Phase Calculations

Scattering phase shifts for each unique potentials are necessary for the calculation of detailed diffraction pattern. Fortran programs have been written to calculate the helium diffraction pattern from helium-step interaction potential for any incident wave vector (i.e., beam energy) and incident angles. The geometry and the type of approximation used to define a phase associated with each point over the surface can be explained in the following way. To calculate the phase: $\varphi = \eta_i(x) + \eta_f(x) - \Delta k_{\parallel} x$, we have to do the integration (1) and (2). From these two equations it is seen that

turning point (i.e., either z_i or z_f) $z = ZTP$, the integrand is equal to $-KZ$, where KZ = perpendicular component of wave vector $KVEC$ (either K_{00}^z or K_{mn}^z). This is due to the fact at turning point, $K_i^z(x, ZTP)$ and $K_f^z(x, ZTP)$ are zero. At

point after the turning point, that is, at $NZTP$ (see fig-1) the integrand $= \left[(KZ)^2 - \frac{2mV(x, z)}{\hbar^2} \right]^{\frac{1}{2}} - KZ$

$= [(KZ)^2 - POT(z(NZ), x) \times CON]^{\frac{1}{2}} - KZ$, where $CON = \frac{2m}{\hbar^2} = 1.9150328$ is calculated such that the potential is in meV. At the

end point of $ZARRAY$, that is, of Range 1 (at point NZ) the integrand is $= [(KZ)^2 - POT(z(NZ), x) \times CON]^{\frac{1}{2}} - KZ$.

Now let us consider the function F to be $F = \left[(KZ)^2 - \frac{2mV(x, z)}{\hbar^2} \right]^{\frac{1}{2}} - KZ$ and let us plot F as a function of Z Schematically().

The area $A = \frac{1}{2} [-KZ + F(NZTP)] \times [z(NZTP) - ZTP]$. So using the simple trapezoidal rule the total integral is

$$= A + \left[\frac{F(NZTP)}{2} + F(NZTP+1) + \dots + F(NZ-1) + \frac{F(NZ)}{2} \right] \times DZ = A + \left[\frac{F(NZTP)}{2} + \frac{F(NZ)}{2} \right] \times DZ + [F(NZTP+1) + \dots + F(NZ-1)] \times DZ$$

$$= \left\{ \frac{1}{2} [-KZ + F(NZTP)] \times \frac{[ZARRAY(NZTP) - ZTP]}{DZ} + [F(NZTP) + F(NZ)] \times \frac{1}{2} + [F(NZTP+1) + \dots + F(NZ-1)] \right\} \times DZ$$

The integral for the limit from $z(NZTP)$ to $z(NZ)$ has been evaluated using the extended trapezoidal rule [12]. The phase η for the 1st range of potential is $\eta_1 = Integral - KZ \times ZTP$. For the 2nd range of potential the phase η is $\eta_2 = Integral = \{ [F(1) + F(NZ)]/2 + [F(2) + F(3) + \dots + F(NZ-1)] \} \times DZ$. And for the 3rd range of the potential the phase η is $\eta_3 = Integral = \{ [F(1) + F(NZ)]/2 + [F(2) + F(3) + \dots + F(NZ-1)] \} \times DZ$. The phase $\eta = \eta_1 + \eta_2 + \eta_3 \dots (3)$ is for the whole range of the potential which could be either for the incident wave or for the scattered wave.

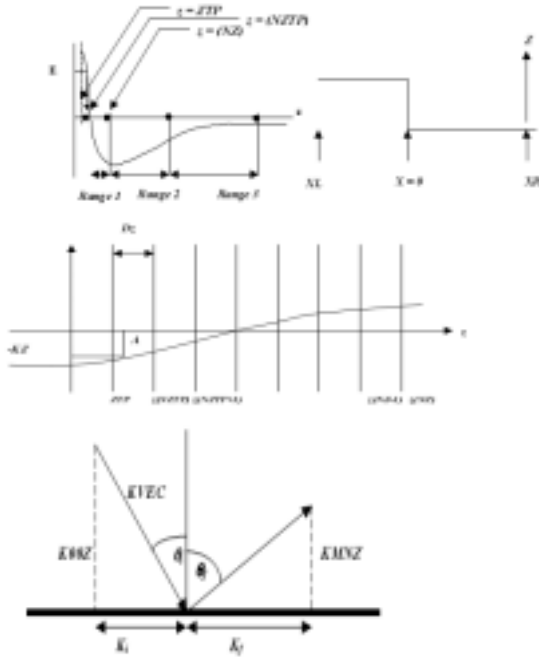


Fig.1: The left diagram shows the interaction potential for a particular value of x (any point on the step shown in the right diagram) for different values of z (distance of the He atom from the surface) in three parts. Range 1, Range 2 and Range 3 indicating the turning point ZTP .

Fig. 2(a): Schematic diagram of variation of the integrand F as a function of z .

Fig.2(b): Schematic diagram of scattering kinematics showing the incident wavevector $KVEC$, the Z -component of $KVEC$ and the Z -component of the scattered wavevector, that is, $KOOZ$ and $KMNZ$ and the incident and scattered angles θ_i and θ_f respectively.

3.2 Adjustment of KZ values

The KZ values are divided into $NINT$ number of points such that the KZ values are equally spaced. Now for any KZ value (i.e., for a particular k_i) we get a $KOOZ$ and a $KMNZ$ which corresponds to an incident wavevector k_i and scattered wavevector k_f we are able to determine the total phase η (eqn.3) at each x -value on a surface. So for each x , we can calculate η values for a set of KZ (K_i or K_f) values and store it. From the scattering kinematics in Fig. 2(b) it is clear that $K_i = k VEC \sin \theta_i$ and $K_f = k VEC \sin \theta_f$, where θ_i and θ_f are the incident and the scattered angle respectively. Let us suppose we want to calculate phase η at a particular x for a particular value of K_i and K_f . We can obtain it easily by interpolating the value of η from the above set of η values that has been calculated for different KZ values at each x . We should choose the value of $NINT$ in such a way that the interpolated value of η is a correct one. Once the phase $\eta(x)$ is obtained we can evaluate $\phi(x)$ over the surface to calculate the scattered amplitude $A_{00,mm}$.

3.3 Potential Parameters

In the fitting the potential energy data, as calculated by realistic potential model proposed by Sultana[8] emphasis has been put on the smoothing parameter λ . The potential parameters used for the calculation of He-Cu(001) interaction potential are as follow: the strength of repulsive pair potential, $A=8.0 meV$, steepness of repulsive pair potential, $b=2.34 \text{ \AA}^{-1}$, dispersion constant, $C_6= 5085 meV$ and dispersion constant, $C_8 = 7500 meV$. The smoothing parameter γ has been chosen to be 1.5 which ensures that the surface corrugation is less than 0.15 \AA^{-1} peak to peak for the energy range between $0 meV$ to $60 meV$ [8]. This implies that the surface corrugation of a clean, unconstructed (001) closed packed surface of Cu is very low as suggested by the experimental data [13].

3.4 Surface Parameters

We use the surface parameters of Sultana [8] for the calculation of the He-Cu(001) potential. The surface parameters for Cu(001) are lattice constant of FCC bulk unit cell $a_1=3.63 \text{ \AA}$; surface lattice constant, $a = 2.55 \text{ \AA}$, inter layer distance $=1.803 \text{ \AA}^{-1}$, atom densities in the metal $4/a_1^3 = 0.0845 \text{ \AA}^{-3}$ and $b = 2.34 \text{ \AA}^{-1}$. The minimum potential well is obtained in present calculation is $-6.138 meV$ which is very close to experimental one $-6.35 meV$ for Cu (110) surface [8,13]. The calculated contour plot of potential for down oriented step edge of Cu(001) and for up oriented step edge of Cu(001) are shown in Fig.4 and Fig.6, respectively.

3.5 Structure of the FORTRAN Codes

The STEPSCAT.FOR code is written in FORTRAN-77 in double precision to input data in complex *16 accuracy. A possibility for batch processing is included in the program that permits fast and comfortable treatment of expected simulation. The code is organized as files. Each file performs numerical calculation to create database after accomplishing the run. Separate database for each process are easier for control and suitable for new simulation. All the parameters have the same meaning and same values have unique name in all the parts of the STEPSCAT codes. The above programs can be run as batch files. The output of AMPDK.FOR can be plotted using any plotting routine. The structures of the FORTRAN codes are schematically shown in Fig. 3.

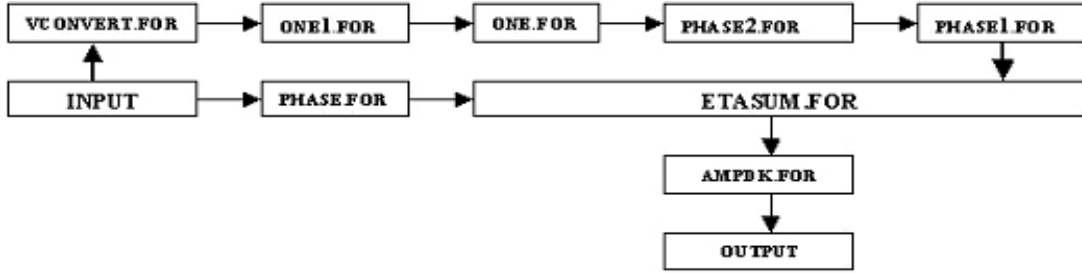


Fig.3: The structure of the Fortran codes. The output contains the scattered intensity for each value of parallel momentum transfer.

4.0 Results and Discussion

This section looks at the results obtained from the FORTRAN-77 codes. The scattering calculations have been performed using modified sudden approximation. It can be seen that in all of the graphs that the specular intensity is the highest calculated intensity. All of the other intensities have been calculated relative to this one. Let us first look at the simulated diffraction patterns in Fig. 5, for helium scattering from a down oriented Cu (001) step at normal incidence. The normalized scattered intensity has been plotted as a function of parallel momentum exchange (denoted as DKP in Fig. 5). All the scattering calculations have been performed for normal incidence. We have not varied the angle of incidence but beam energies have been varied. The specular peak is at in-phase-condition for the incident wave vector $k_i = 712 \text{ \AA}^{-1}$ and out-of-phase condition for $k_i = 9.7 \text{ \AA}^{-1}$. The largest proportion of scattered intensity, other than that associated with specular intensity, is found from positive parallel momentum exchange. The interference between the beams scattered from the upper level and lower level terraces gives rise to the specular peak at $\Delta k_{||} = 0$. The phase shift between the beams scattered from the upper terrace and the lower terrace depends on the step height, the angle of incidence and the helium wavelength (that is, beam energy). Changing the incident beam energy can thus give rise to strong intensity variations of the specular peak. Constructive interference between the scattered beams from the upper and the lower level terraces occurs for the in-phase-condition chosen. Similarly, destructive interference occurs for the out-of-phase condition. In out-of-phase condition the specular peak is splitted and the intensity at $\Delta k_{||} = 0$ is very small compared to the two peaks at either side of $\Delta k_{||} = 0$ having equal magnitudes. In the positive parallel momentum exchange region intensity is greater which can be explained by the classical deflection of the atom from the sloped portion of the step. The broad intensity oscillations are due to the interference between the scattering from different sections of the sloped portion of the step, or the interference between beams directly scattered from the flat surface. Consequently, these oscillations are directly related to the dimension of the step edge. The period of large angle oscillations represents the length of the step edge extension, approximately 5 \AA , observed in the potential related. In the negative parallel momentum exchange region, the magnitude of the scattered intensity decreases very quickly. The smaller period of oscillations in the negative parallel momentum exchange region represents the total width of the step; here 26.775 \AA for Cu (001) step. This is the surface over which the integration was performed. We have studied the angular distribution of scattering intensity from single Cu (001) up-step using our Fortran codes. The wavevector $k_i = 5.227 \text{ \AA}^{-1}$ and $k_i = 10.455 \text{ \AA}^{-1}$ correspond to the beam energies 14.18 meV and 57.71 meV respectively. The largest proportion of scattered intensity is found in the negative parallel momentum exchange region only corresponding to up-hill scattering from the step edge. The positive parallel momentum exchange region is classically

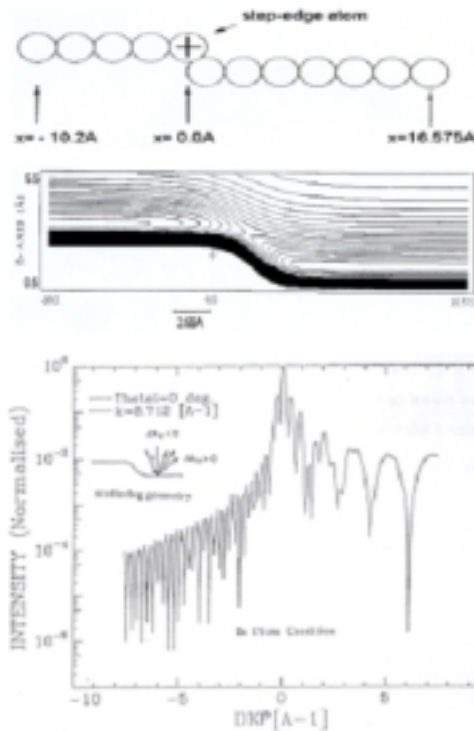


Fig. 5: Normalize intensities for a down steps of Cu (001) with the potential of Fig. 4 at incident wavevectors $k_i = 8.712 \text{ \AA}^{-1}$ and $k_i = 9.7 \text{ \AA}^{-1}$. The largest proportion of scattered intensity, other than that associate with the specular intensity, is found in the positive parallel momentum exchange only.

Fig. 4: A cross-section of a Cu (001) down step is shown in the upper diagram. Contour plot of potential calculated using modified pair-wise potential [8] to represent at a down oriented step-edge of Cu (001).The Z-axis is perpendicular to, and the X-axis parallel to, the surface. The step width = 26.775 \AA ; step height = 1.803 \AA , the calculated well depth = -6.4 meV and the smoothing parameter = 1.5 . In this case the step edge atom has been smoothed like the rest of the atoms on the surface. The contour spacing is 0.164 meV . A very small hill is observed at the step-edge (figure taken from ref. [8])

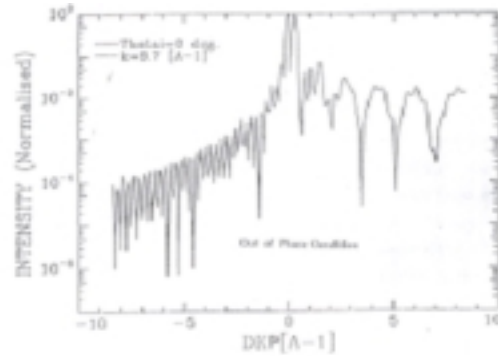


Fig. 6: A cross- section of a Cu (001) down step is shown in the upper diagram. The lower diagram shows a contour plot of a potential to represent the total helium interaction at Cu (001) step-edge (an up step).The Z-axis is perpendicular to, and the X-axis is parallel to, the surface. The step height = 1.803 \AA , and the calculated potential minimum is -6.4 meV . The contour between -6 and -1 meV are drawn in steps of 0.5 meV and between 10 and 80 meV in step of 10 meV . The smoothing parameter used in the potential Calculation was $= 1.5$ (figure taken from ref. [8])

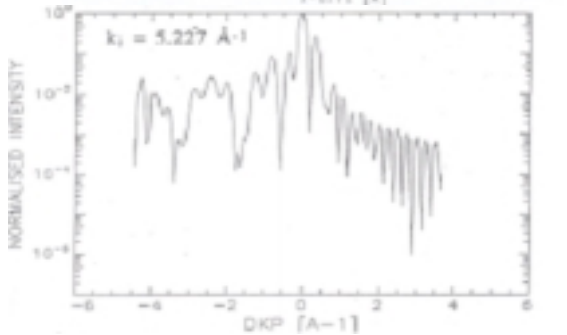


Fig. 7: The curves show the calculated intensities from model step edge of Cu (001) using the potential of Fig. 6 for low ($k_i = 5.227 \text{ \AA}^{-1}$) and high ($k_i = 10.455 \text{ \AA}^{-1}$) beam energies. In both the cases, the largest proportion of scattered intensity, other than that associated with the specular intensity, is found in the negative parallel momentum exchange region. The specular beam is at the in-phase condition for the chosen wave vectors at normal incidence.

forbidden for scattering for an up step. We found that peak shape and peak position depend on the details of the potential as seen by the helium atoms. So, at high beam energy, the step appear more abrupt to the helium atoms than at low beam energy.

5.0 Conclusion

The step edges are known to play a dominant role in surface growth. This paper illustrates the different aspects of the helium scattering from isolated metal steps. Our simulated results show that the helium atom scattering from an isolated step on Cu (001) metal surface is independent on incident beam energy and the scattering depends on the details of the interaction potential. The findings and the calculational procedure adopted in this paper can be used analyzing the experimental data for helium scattering from growing metal surfaces. It is easy to simulate helium scattering from any stepped surface (say vicinal surfaces or other growth systems) if the scattering from isolated steps are known. Our Fortran codes are able to facilitate us to quantitative step structure analyses provided more experimental data are available.

6.0 References

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