Detection of Tamm Surface-State Resonances in VLEED, LEEM and TCS

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We have identified, for the first time, surface-state resonances in above–vacuum surface spectroscopies which are due to the gradual rise in average interstitial potential of atomic layers on approach to the surface.

1. Introduction

Tamm surface states and resonances have their electron density centred mainly on the crystal side of the top layer of atoms in contrast to Shockley surface states and resonances which have their electron density centred mainly on the vacuum side of the top atomic layer. In a scattering picture, surface states or resonances occur when a standing wave is formed by scattering between surface and bulk potentials. Shockley surface resonances have been detected in VLEED and occur typically within ~5 eV of the vacuum emergence of non-specular electrons. VLEED, LEEM and TCS data for Cu(111) has unexplained peaks, for instance, at ~20 eV at normal incidence. This is typical of such data for other metal surfaces as well. The aim of this work is to determine possible origins of unexplained peaks in VLEED, LEEM and TCS data beginning with the ~20 eV peak on Cu(111) at normal incidence.

2. Method

The correct form of the surface potential for Cu(111) (in the muffin-tin approximation) is shown schematically in Fig. 1. We use our layer-by-layer KKR surface energy-band structure method to calculate the energy of the surface resonances [1]. We also use the layer-by-layer KKR scattering method to calculate the reflectivity of the specular backscattered 00 beam from Cu(111) at normal incidence [2]. In all calculations the bulk scattering potential was obtained from the band structure in Ref. [3]. A number of surface scattering potentials were used. Shown in this work are results for a step potential in the surface region.

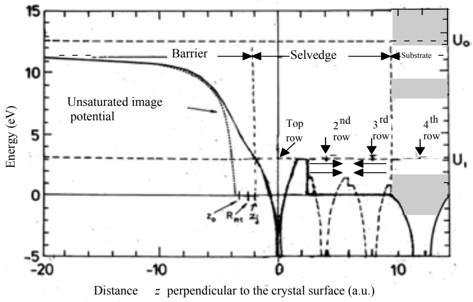


Fig.1. Horizontal arrows in the atomic selvedge region indicate scattered electrons which can produce Tamm surface states and resonances. Unshaded regions in the substrate represent surface-projected bulk-band gaps.

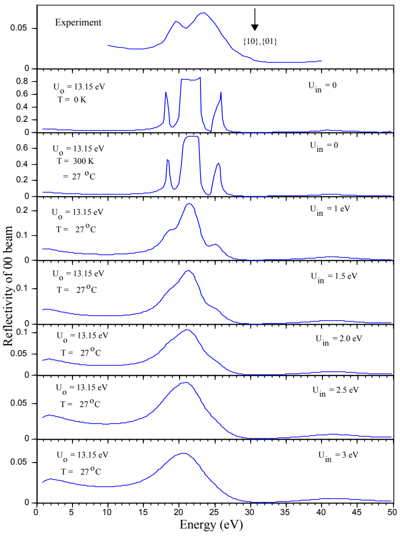


Fig. 2 Top frame is experimental LEEM data [4]; U_o is inner potential of 13.15 eV and step height; U_{in} is bulk isotropic inelastic scattering potential. In all cases a non-reflecting step surface potential is placed at the jellium discontinuity z_j = -1.97 a.u.

3. Results

In Fig. 2 we show calculated reflectivities which do not allow for the inclusion of surface resonances. For $U_{in} < \sim 2.3$ eV the bulk crystal Bragg peak and two satellite peaks are present. For $U_{in} > \sim 2.3$ eV only the central Bragg peak remains. Neither of these cases corresponds to the experimental results of two peaks at ~20 and 23.5 eV. A surface resonance

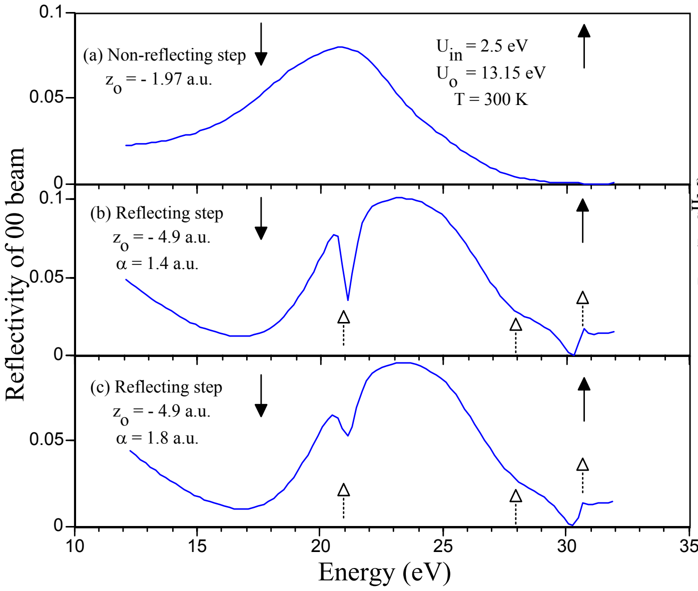


Fig. 3. For the reflecting step calculations, surface inelastic scattering is included by a potential of Gaussian form on the vacuum side of the origin of coordinates, with a height equal to $-U_{in}$ and halfwidth given by α.[2] Open arrows represent surface resonance features.

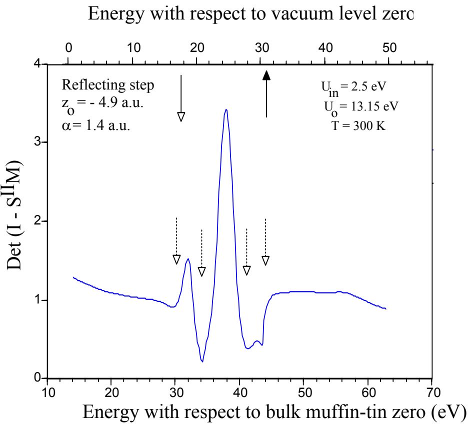
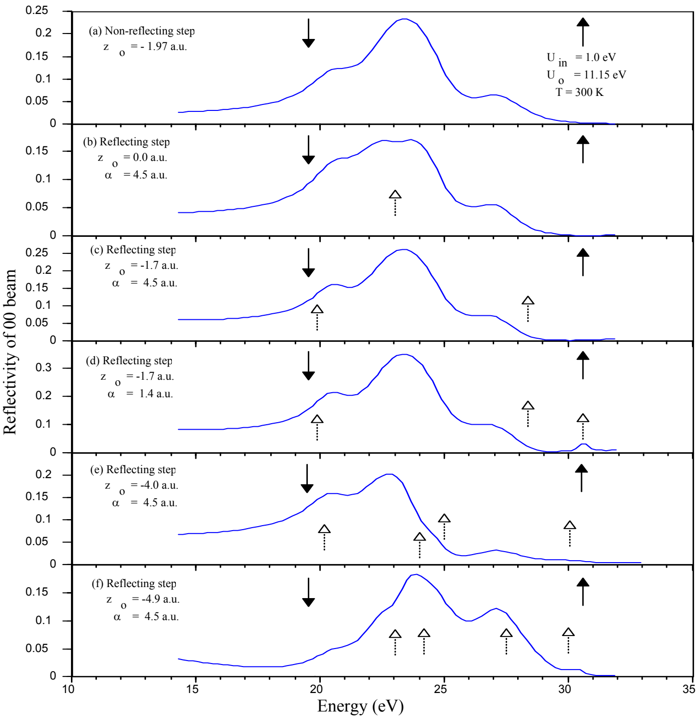


Fig. 4. Open downward arrows indicate the energies of the surface resonances. Solid arrows indicate crystal and vacuum emergence of the six {01}, {10} beam sets.



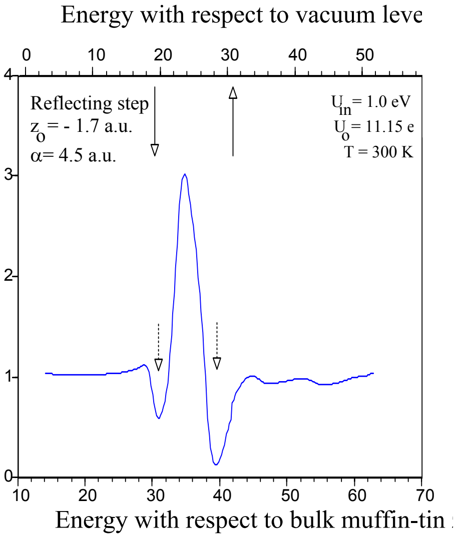


Fig. 6. Open downward arrows indicate the energies of the surface resonances. Solid arrows indicate crystal and vacuum emergence of the six {01}, {10} beam sets.

Fig. 5. For the reflecting step calculations, surface inelastic scattering is of the same form as described in Fig. 3. Open arrows represent surface resonance features.

feature can appear in LEED/LEEM beam reflectivities as a peak, a dip, or a peak and dip combination. In Fig. 3 a reflecting step potential, which allows for the inclusion of surface states, is included in the calculation. The step is located at z_o = - 4.9 a.u. from the top layer of atoms and two values of the surface inelastic scattering potential are included. The surface resonance feature near 21 eV splits the Bragg peak giving rise to the experimentally obtained two peak structure at the correct energies. Using our surface band structure calculation, the energy of the surface resonances for $k_{||} = 0$, formed by the same surface potential as used in Fig. 3(b), is found from the minima shown in the plot in Fig. 4. Typical results for the case of bulk isotropic scattering potential of $U_{in} < \sim 2.3$ eV are shown in Fig. 5. In Fig. 5(c) for U_{in} = 1.0 eV, a surface resonance feature occurs at ~20 eV which enhances the bulk peak already present in the reflectivity for step positions z_o = - 1.7 a.u. and - 4.0 a.u. However the higher energy peak is also present for this bulk potential which does not appear in the experimental data. Using our surface band structure calculation, the energy of the surface resonances for $k_{||} = 0$, formed by the same surface potential as used in Fig. 5(c), is found from the minima shown in the plot in Fig. 6.

4. Conclusion

For the bulk scattering potential used here [3], isotropic electron absorption corresponding to ~2.5 eV gives best agreement with experiment. The ~20 eV peak seen in the experimental result is due to a surface resonance centred at 20.95 eV as shown in Fig. 4. This resonance is strong because it has a relatively long lifetime. It is responsible for splitting the single Bragg peak into two peaks. The centre of this resonance occurs only 3.4 eV above the bulk muffin-tin zero and 9.75 eV below the vacuum level for for Cu(111) with an inner potential of 13.15 eV. In this case the electron wavefunction and density are mostly centred on the crystal side of the top layer of atoms which corresponds to a Tamm-type surface resonance. This is the first time a Tamm-type surface resonance has been found to influence VLEED/LEEM reflectivities. It is suggested that the step potential model we have used here simulates the gradual rise of the constant interstitial potential between muffin-tin wells of atomic layers on approach to the vacuum interface as illustrated in Fig. 1. Surface resonances arising from this effect are not usually included in VLEED/LEEM calculations. Further calculations are being performed to include detailed models of the surface potential which give rise to the Tamm surface states and resonances and also the Shockley and Rydberg states and resonances.

It is suggested that failure to model the surface potential realistically in this atomic selvedge region is a major cause of the discrepancies between theory and experiment in the ~30 year history of VLEED.

Acknowledgments

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