The interpretation of angular distributions in resonance electron scattering: multiple scattering and selection rules

1989 J. Phys.: Condens. Matter 1 SB225

(http://iopscience.iop.org/0953-8984/1/SB/052)

J. Phys.: Condens. Matter **1** (1989) SB225–SB226. Printed in the UK

The interpretation of angular distributions in resonance electron scattering: multiple scattering and selection rules

P J Roust[†] and R E Palmer[‡]

[†] Lawrence Berkeley Laboratory, 1 Cyclotron Road, Berkeley, California 94720, USA
[‡] Cavendish Laboratory, Madingley Road, Cambridge CB3 0HE, UK

Received 28 March 1989

Abstract. The angular distributions observed in resonance electron scattering from adsorbed molecules constitute a new probe of molecular orientation on the surface. We describe how selection rules can be invoked to simplify the interpretation of these distributions.

Within the last two years, the first observations of the angular distributions obtained in resonance electron scattering from adsorbed molecules have been reported, for both physisorbed [1] and chemisorbed [2] molecules. These distributions are of particular interest because they depend upon the orientation of the molecule on the surface, and thus represent a new probe of molecular orientation. The distributions are obtained by measuring the angular dependence of the intensity of a molecular vibrational loss mode as observed in angle-resolved electron energy-loss spectroscopy (EELS), under conditions where the molecular excitation occurs via transient negative-ion resonance formation, i.e. an electron is temporarily trapped in an anti-bonding molecular orbital. Such resonance formation leads to substantially enhanced vibrational excitation cross sections. If the electron wave field impinging on the molecule is expanded in terms of partial waves, then in general the partial wave of lowest angular momentum consistent with the symmetry of the host molecular orbital is the one captured into and re-emitted from the molecular resonance, so distinctive angular scattering profiles will be observed. For the hypothetical case of an isolated, oriented molecule the observed emission profile will just be the emitted partial wave, referenced to the orientation of the molecular axis [3]. However, for molecules on a surface, multiple elastic electron scattering between electron emission from the resonance and detection by the EELS analyser means that the angular profile can be dramatically altered by interference effects [1, 4]. Thus the straightforward relation between the observed angular distributions and the molecular orientation is destroyed and detailed calculations of the multiple scattering using 'LEED-style' computer programs are needed in order to make an orientation determination [4]. Thus we are motivated to ask whether there are cases in which detailed calculations can be avoided.

Our prime purpose here is to demonstrate briefly that in certain cases of resonance electron scattering selection rules will apply that will simplify the interpretation of the measured angular distributions. Consider a specific example. A homonuclear diatomic molecule stands upright on a surface, and an electron is emitted in a partial wave of p_y symmetry. In the absence of multiple scattering there would therefore be a node in the emitted intensity in the direction normal to the surface. Now suppose that the centre of symmetry of the molecule lies in a mirror plane of the surface. Subject to this condition, the node in intensity in the normal direction will be preserved. Why? Because emission on one side of the mirror plane has the opposite phase to emission on the other side, and for every multiple-scattering path beginning on one side of the mirror plane there is a symmetrical path beginning on the other side. These pairs of scattering paths interfere destructively producing a zero in the emitted intensity along the surface normal. Generalising, a node normal to the surface will be observed given such mirror plane symmetry and a partial wave with odd parity with respect to reflection in the mirror plane. We believe such selection rules enhance the power of resonance electron scattering as a probe of molecule orientation on surfaces. Details of this work will be found in [5].

References

[1] Palmer R E, Rous P J, Wilkes J L and Willis R F 1988 *Phys. Rev. Lett.* **60** 329
[2] Jones T S and Richardson N V 1988 *Phys. Rev. Lett.* **61** 1752
[3] Davenport J W, Ho W and Schrieffer J R 1978 *Phys. Rev.* B **17** 3115
[4] Rous P J and Palmer R E 1989 *Phys. Rev.* **11** 7552
[5] Rous P J and Palmer R E 1989 *Phys. Rev.* B submitted