ATOM LOCATION USING RECOIL ION SPECTROSCOPY

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INTRODUCTION

Low energy ion scattering(LEIS) using inert gas and alkali ions is widely used in studies of the surface atomic layer. The extreme surface sensitivity of this technique ensures that it yields both compositional and structural information on clean and adsorbate covered surfaces. A number of investigations have been carried out on initial adsorbate site location using inert gas ion LEIS. The conclusions usually invoke blocking or shadowing of substrate atoms to explain changes in reflected ion yield though attention is rarely paid to possible problems arising from variations in the charge exchange process.

It is possible to substantiate the structures determined by LEIS by using a slight variation of the technique which yield substantially different information. This variation involves the use of of the highly sensitive negatively charged recoils for adsorbates which have a strong chance of being found in the negatively charged state (e.g. oxygen). In general the detection of recoil ions is difficult in the positive spectrum as they may correspond to energies at which there is a strong scattered ion signal, or they may lie on the tail of a scattered ion signal. These problems can be avoided by monitoring the negatively charged particles.

The advantages associated with the use of negatively charged recoils are:

(a) Being negatively charged they do not need to be extracted from an intense background of positively charged scattered ions if inert gas primary projectiles are used as the probability of creating negatively charged inert gas ions is exceedingly small.

(b) The angular distribution of ejected adsorbate atoms carries with it direct information about the site from which ejection occurred. This is a much more direct measurement of the adsorption site than that obtained by inference from changes in scattered ion yield.

Low Energy Negative recoil Spectroscopy (LENRS) has been applied to a study of oxygen on Ni(110) to gauge the sensitivity to coverage and site location. The adsorption procedure followed was aimed at reproducing conditions reported in similar LEIS and LEED studies of oxygen on Ni(110) to yield a (2x1) LEED pattern. After target cleaning and annealing of damage the sample was exposed to 0.4 Langmuirs of oxygen at a sample temperature of 450K. The measurements were performed with a beam dose which was experimentally found to produce minimal changes to the surface structure by sputtering or surface damage. After each measurement the target was cleaned with sputter bombardment at 700K.

RESULTS AND DISCUSSION

An energy spectrum of the negatively charged particles emitted from the surface comprises a relatively narrow low energy peak which results from a single binary event creating a direct recoil particle. There is often observed one or two higher energy peaks in the negative particle energy spectrum which have been identified as originating from deflected recoil processes. The term 'deflected recoil' is collectively given to the processes which involve scattering of an atom after the initial recoil event, and to the recoil event where the projectile has previously been scattered by another atom. There is no general rule to distinguish these two processes, and they must therefore be differentiated by reference to computer simulations.

An effective demonstration of the usefulness of recoil ions is revealed in fig. 1. The recoiling O^- is shown for a recoil angle of 60^o while the angle of incidence is increased from 0^o (measured to the surface) up to 60^o when a 2 keV Ne^+ projectile is used. The magnitude of the direct recoil signal exhibits marked differences between the case when the experiment is performed along the <001> surface chain and the <110> surface chain. These differences can be used to distinguish between different adsorption sites. It is possible to call on previous extensive studies of this surface or the currently accepted reconstruction model to eliminate some the suggested adsorption sites. However it is instructive to apply LENRS to this surface without assuming any a priori knowledge of the surface structure to illustrate the potential application of this technique to as yet unstudied surfaces. The results in fig 1 preclude the possibility that the oxygen is sitting in a centrefold site. If this were so the recoil signals would be comparable along the two surface alignments. The short bridge site (between atoms in the <110> surface direction) is also ruled out as that would yield a higher signal along the <001> surface direction. The only oxygen position consistent with these results is a long bridge site (between atoms in the <001> surface direction). Under the experimental conditions used in this study the projectile is prevented from striking the oxygen along the <001> direction because it lies in the shadow cones formed by the neighbouring Ni atoms. Using the Moliere function with an appropriate screening length correction to predict the shadow cone dimensions it is possible to determine that the oxygen must be more than 0.42 Å above the Ni surface in order that a comparable yield to the <110> direction is seen along the <001> direction under these experimental conditions. The results in fig. 1 indicate that the oxygen is closer than 0.42 Å to the surface.

To more accurately locate the oxygen atom a detailed survey of the recoiling ions is necessary. This can be acquired by monitoring the negative ion yield as a function of the azimuthal angle (fig 2). The negative ion yield is low when incident along the <100> surface chain, but as the target is rotated away from this direction the ion yield increases indicating that the oxygen is emerging from the shadow cone formed by the neighbouring Ni surface atom. Detailed analysis reveals that the height of the oxygen above the surface is 0.2 ± 0.1 Å. This height results in a Ni-O bond length of 1.77 Å which is in close agreement with recently reported theoretical value of 1.75Å.

While there exists a wealth of structural information in the angular distribution of the directly recoiling atoms there is a greater potential for information to be extracted from the deflected recoils. As these events involve both a recoiling event and a scattering event they may be used to determine the relative positions of the Ni and O atoms. This aspect requires more attention and comparison to computer simulation.

CONCLUSIONS

The use of negatively charged recoil ions greatly extends the capabilities of low energy scattering techniques; in particular to the electronegative elements. This method has been successfully applied to a study of O on Ni(110) and located the adsorbate in the long bridge site just above the surface. Additional work is in progress to assess the suitability of the deflected recoils to more detailed structural information.

Fig. 1

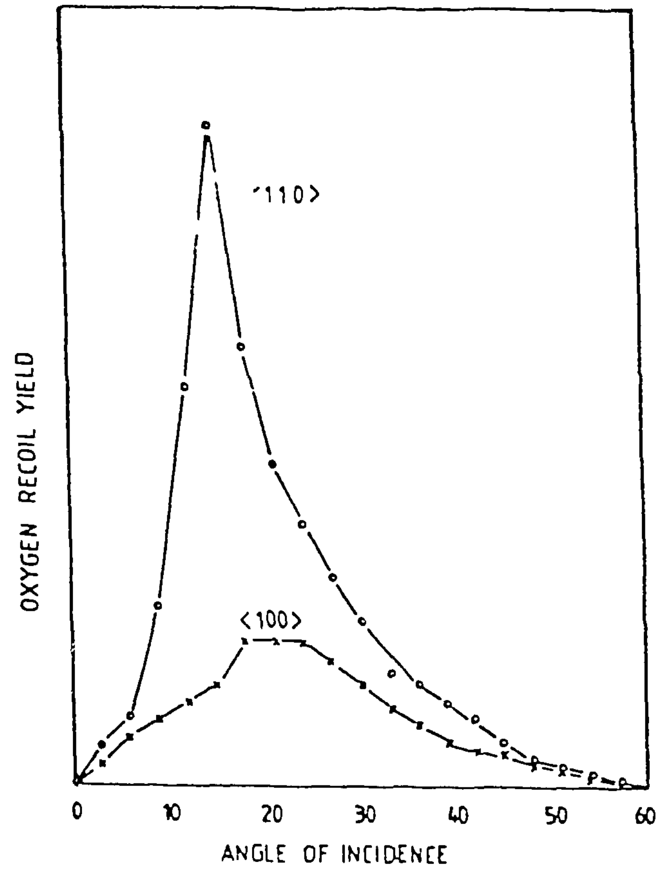
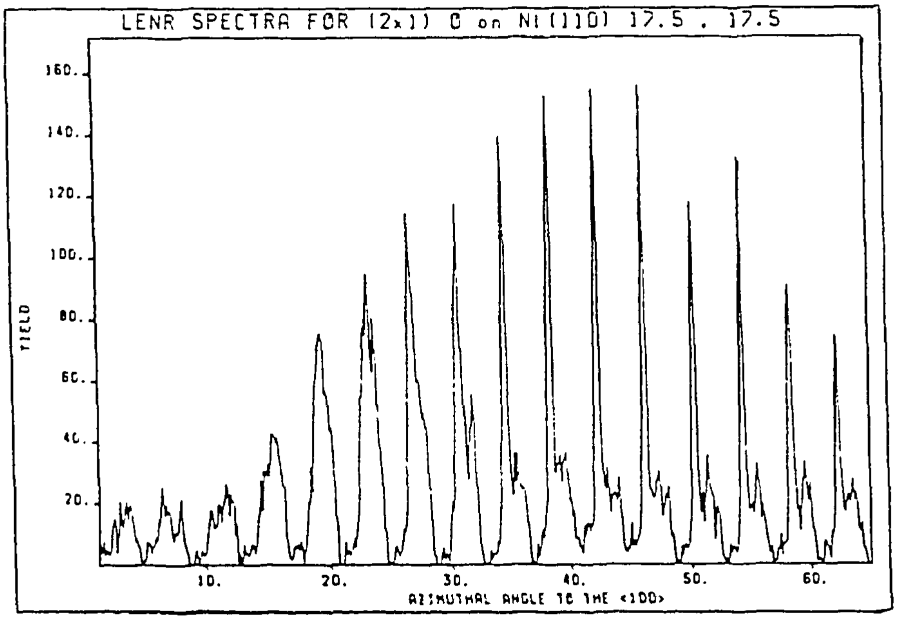

OXYGEN RECOIL YIELD
<110>
<100>
0
10
20
30
40
50
60
ANGLE OF INCIDENCE

Fig. 2


LENR SPECTRA FOR (2x1) O on Ni(110) 17.5 . 17.5
YIELD
160.
140.
120.
100.
80.
60.
40.
20.
10.
20.
30.
40.
50.
60.
AZIMUTHAL ANGLE TO THE <100>