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MEASUREMENT OF THE DISPERSION CURVES OF SURFACE VIBRATIONS ON Ni (100) AND Ni (100) C (2 x 2) O BY ELECTRON ENERGY LOSS SPECTROSCOPY

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Résumé- Les courbes de dispersion de plusieurs vibrations de surface ont été mesurées sur toute la zone de Brillouin à deux dimensions dans la direction (110) sur Ni(100) et Ni(100) C(2x2) O. Le phonon de Rayleigh a été observé dans les deux cas. Sur Ni(100) C(2x2) O nous avons de plus observé une résonance et deux vibrations de l'oxygène, perpendiculairement et parallèlement à la surface. La discussion des résultats dans le cadre d'un modèle simple de la dynamique du réseau donne des renseignements sur la relaxation de la surface et la distance Ni-O.

Abstract- The dispersion curves of several surface vibrations have been measured throughout the two-dimensional Brillouin zone in the direction (110) on Ni(100) and Ni(100) C(2x2)O. The Rayleigh phonon has been observed on both systems. Besides a resonance and two O-vibrations associated with motions perpendicular and parallel to the surface have been observed on Ni(100) C(2x2)O. Those results are discussed within the framework of a simple model of the lattice dynamics, which yields information upon surface relaxation and the Ni-O distance.

By contrast to most of electron energy loss spectroscopy (EELS) measurements carried out so far at vanishing wave-number q of the detected vibration, we report here the EELS observation of vibrational losses at large q on Ni (100) and Ni (100) C (2 x 2) O throughout the two -dimensional Brillouin zone (B. Z). The measurement of the dispersion curve $\omega(q)$ (ω is the vibrational frequency) provides information about force constants and interatomic distances at the surface.

I - EXPERIMENTAL

The Ni single crystal was prepared and cleaned according to standard procedures /1/. The exposure to oxygen was done so that it produced sharp, half integer spots characteristic of the C (2 x 2) structure in the electron diffraction pattern /2/.

In the EELS measurement an incoming electron of energy E_i and wave-number k_i impinges on the surface, emits or absorbs a phonon (ω, q) and emerges with E_s and k_s . In our working conditions, k_i , k_s and the normal direction to the (100) surface lie in the scattering plane. Two conservation laws hold which read, taking into account that $\hbar\omega \ll E_i$:

$$E_i - E_s \pm \hbar\omega = 0 \quad (1)$$

$$k_i (\sin\theta_i - \sin\theta_s) = q \quad (2)$$

where θ_i and θ_s are the angles of the incoming and outgoing beams respectively measured from the normal direction. The + or - sign in eq. 1 refers to annihilation or creation of a phonon, which corresponds in turn in the EELS spectrum to a gain or a loss. In all experiments θ_s was always set to $\sim 70^\circ$ and θ_i varied by steps with E_i kept constant so that q was scanned over the whole B.Z. in the direction (110) from $\Gamma(q=0)$ to the zone edge point X ($q=1.26 \text{ \AA}^{-1}$) and the loss spectrum was recorded for each θ_i value.

II - THE CLEAN SURFACE : Ni (100)

The measurements were made at 300 K and at $E_i = 180$ and 322 eV. The spectrum recorded at X shows (fig. 1c) an elastic contribution, the loss peak on its right side and the gain peak lying at the same distance on the left side. As q decreases, ω goes to zero and both loss and gain features grow at the expense of the loss-less peak which disappears (fig. 1b) till finally loss and gain merge into a single peak (see fig. 1a).

The frequency ω has been plotted versus q in fig. 2. By using symmetry considerations and comparing the experimental curve with calculated phonon dispersion data /3/ one identifies the measured branch in fig. 2 to the Rayleigh mode /1/.

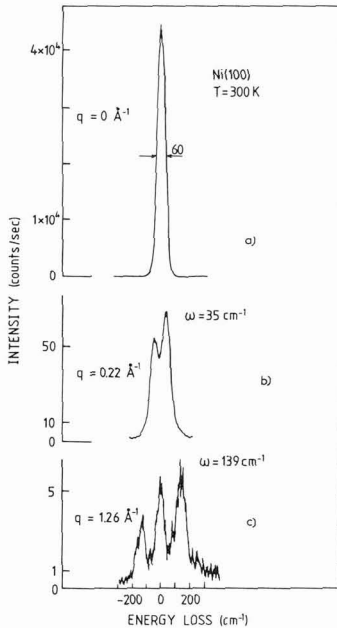


Fig. 1 - EELS spectra taken at $E_i = 180$ eV on Ni (100).

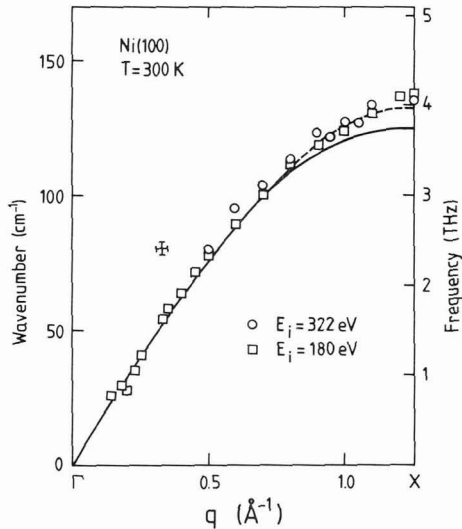


Fig. 2 - Measured frequency ω of the Rayleigh phonon (open circles and squares) versus q on Ni (100). The data are fitted by the solid and dashed lines as explained in the text.

Each Ni-atom is then assumed to interact only with its nearest neighbours via central forces described by the force constant K_b which is assessed independently from bulk phonon dispersion data. With K_b at hand Rahman and Mills /1/ have calculated the solid curve. The disagreement occurring at the zone edge is lifted by increasing the force constant K_s between Ni-atoms in the first and second layers by 25% with respect to K_b , which yields the dashed line in fig. 2. Such a stiffening of K_s is consistent with a contraction of the first Ni-plane which has moreover been reported independently by Frenken, Smeenk, Van der Veen from ion blocking measurements.

III - THE O-COVERED SURFACE : Ni (100) C (2 x 2) O

All spectra have been taken at 150K and at several impact energies E_i because of the large q - and E_i dependence of the losses /2/illustrated in fig. 3. The four observed vibrational modes (their dispersion is represented in fig. 4) comprise two modes of oxygen ($O_{//}$ and O_{\perp} in fig. 3, 4) and two resonances (R and R_{\perp} in fig. 3, 4). It has been shown /2/ using selection rules that the oxygen atom moves at Γ parallel to the surface for the $O_{//}$ and R modes and perpendicular to it for the O_{\perp} -one. At last R_{\perp} has been identified to the Rayleigh phonon /2/.

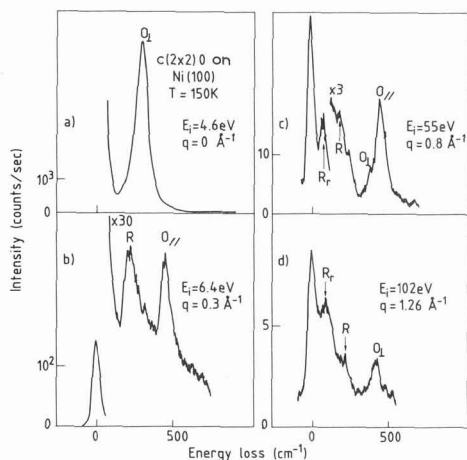


Fig. 3 - EELS spectra taken on Ni (100) C (2 x 2) O at several E_i - and q -values.

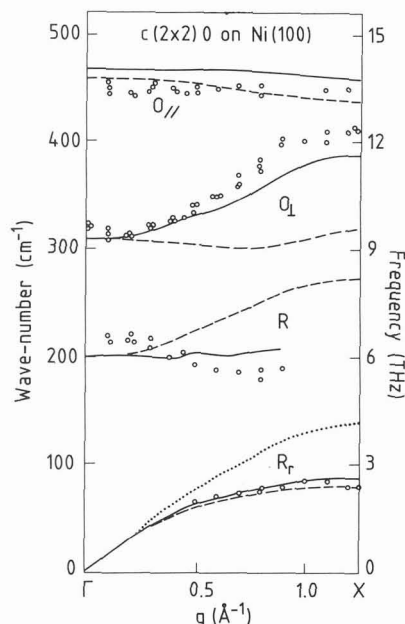


Fig. 4 -Dispersion data (open circles) of surface vibrations on Ni (100) C (2 x 2) O. Solid and dashed lines are theoretical dispersion curves, calculated as explained in the text. The dotted line represents the Rayleigh branch on Ni (100).

Rahman, Black and Mills have extended the model used in the preceding section to fit the data. Two extra force-constants K_{NiO} and K_{OO} have been introduced to account for the central interaction of each oxygen with its Ni- and O- nearest neighbours respectively. The distance d between the O-layer and the first Ni plane must also be inserted into the calculation and has been assigned to a value of 0.88 Å provided by SEXAFS measurements /4/. The best fit determines K_{NiO} and K_{OO} and gives the solid lines in fig. 4. Then K_s is matched to reproduce the Rayleigh curve and is found smaller than K_p , which is indicative of an outwards expansion of the first Ni layer, consistent with already quoted measurements by Frenken et al. The agreement of the solid curves with the data is good apart from the overall dispersion of O_{\perp} which is smaller than the measured one. Upton and Goddard /5/ have claimed that $d = 0.26$ Å and Rahman, Black and Mills have tried to fit the dispersion data with that assumption. It is then required to introduce bond bending forces to fit the O_{\perp} and $O_{//}$ branches at Γ . The result of the calculation is indicated by the dashed lines in fig. 4 and the large discrepancy allows to discard the d -value of Upton and Goddard.

IV - CONCLUSION

The measurement of surface phonon dispersion on Ni (100) and Ni (100) C (2 x 2) O reveals a relaxation of the Ni surface directed inwards on Ni (100) and outwards on Ni (100) C (2 x 2) O and supports the SEXAFS determination of the distance separating the O-layer from the surface.

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