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SPIN POLARIZATION EFFECT IN THE THEORY OF MAGNETIC SCATTERING FROM ANTIFERROMAGNETIC NiO (111) SURFACES BY POLARIZED LOW ENERGY ELECTRON DIFFRACTION*

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Dynamical calculations are performed to determine the differential cross section of low energy electrons scattered from antiferromagnetic NiO (111) surfaces. We find that the spin-dependence of this quantity with respect to the incident electron polarization depends strongly on: (1) the magnetization of the topmost layer, (2) the exchange potential model used, and (3) the incident beam angle.

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Very successful neutron diffraction methods[1] have made it possible to obtain correct bulk descriptions of the detailed magnetic arrangements in solids. Such success, however, cannot be achieved for magnetic surfaces because of a lack of surface sensitivity inherent in this technique. Low energy electron diffraction (LEED)[2] is, however, a useful tool for surface geometry determinations, which possesses both high surface sensitivity and experimental simplicity. Due to the rapid advances in polarized electron beam technology,[3] it has become feasible and attractive to study surface magnetization via spin-polarized low energy electron diffraction (PLEED). The basic physics underlying the PLEED process follows.

Low energy electrons can be scattered not only by the Coulombic potentials of the surface atoms but also by the exchange potential associated with the magnetic structure. The differentially scattered currents $I^{\uparrow}$ (spin up) and $I^{\downarrow}$ (spin down) will, in general, be different for incident electron beams having a spin polarization parallel ($\uparrow$) or antiparallel ($\downarrow$) to a given crystal direction. The difference, $I^{\uparrow}-I^{\downarrow}$, or the polarization P,[4] $P=\frac{I^{\uparrow}-I^{\downarrow}}{I^{\uparrow}+I^{\downarrow}}$, provides the most direct means for studying the role of exchange in electron scattering. In the case of PLEED, the electrons penetrate the surface only a few lattice spacings and therefore should be extremely sensitive to the spin structure of a magnetic surface. The aim of this paper is to demonstrate what kind of detailed information can be obtained from a theoretical investigation of magnetic electron scattering by an antiferromagnetic NiO (111) surface and thus present guidelines for future PLEED experiments.

NiO has the NaCl structure.[5] Assuming a bulk termination of the (111) surface, the layer stacking sequence perpendicular to the surface consists of alternate hexagonal layers of oxygen and nickel, with both the oxygen and nickel sublattices having the fcc structure. Figure 1 shows the nickel sublattice only. Neutron diffraction studies[6] have shown that the NiO crystal is antiferromagnetically ordered below the Néel temperature (523K). The 3d electrons localized on the Ni^{+2} ion with two unpaired spins contribute a magnetic moment of $2\mu_B$ (μ_B is the Bohr magneton) since the orbital magnetic moments are essentially quenched in solids. All the magnetic moments lie in the (111) plane and are directed along $[0\bar{1}1]$ and $[01\bar{1}]$ directions in alternate sheets, as shown in Fig. 1. The difference in the scattering cross sections for up and down spins is caused mainly by the opposite signs of the magnetic exchange for the two spin orientations. A free electron gas model for the exchange potential

between the incident electron and the Ni^{+2} electron density is[7] (atomic units with $e = \hbar = 1$ will be used throughout)

$$\tilde{V}^{\alpha}_{ex}(\vec{r};\vec{\mu_1},\vec{\mu_2}) = V^{\alpha}_{ex}(\vec{r}) + U^{\alpha}_{ex}(\vec{r};\vec{\mu_1},\vec{\mu_2}) \qquad (1)$$

where $U^{\alpha}_{ex}(\vec{r};\vec{\mu_1},\vec{\mu_2}) = -\left[\frac{1}{3}(\rho_s/\rho)V^{\alpha}_{ex}(\vec{r})\right]\vec{\mu_1}\cdot\vec{\mu_2}$

$\rho = \rho_\uparrow + \rho_\downarrow$ = charge density

$\rho_s = \rho_\uparrow - \rho_\downarrow$ = spin density

Here $\vec{\mu_1}$ and $\vec{\mu_2}$ are the unit vectors which specify the spin directions of the incident electrons and the Ni^{+2} magnetic moments, respectively. V^{α}_{ex} is the usual Slater exchange potential for a nonmagnetic nickel ion. If $\vec{\mu_1} \perp \vec{\mu_2}$, $\vec{\mu_1}\cdot\vec{\mu_2} = 0$, then $\tilde{V}^{\alpha,\uparrow}_{ex} = \tilde{V}^{\alpha,\downarrow}_{ex}$ and $I^{\uparrow} = I^{\downarrow}$, $P = 0$. But if $\vec{\mu_1} \parallel \vec{\mu_2}$, $\vec{\mu_1}\cdot\vec{\mu_2} = \pm 1$, then we have $\Delta\tilde{V}^{\alpha}_{ex} = \tilde{V}^{\alpha,\uparrow}_{ex} - \tilde{V}^{\alpha,\downarrow}_{ex} = 2U^{\alpha}_{ex}$, which is the maximum difference in exchange potentials for primary electrons having spin directions parallel or antiparallel to the Ni^{+2} spins. This will produce the largest P values since the difference $I^{\uparrow} - I^{\downarrow}$ is the biggest. This is the basic principle which enables the determination of spin orientation within the (111) plane at normal incidence by azimuthally rotating the crystal to achieve the maximum polarization condition. When this is achieved the surface spin is parallel to the incident electron spin. Experimentally, the incident electron spin is fixed perpendicularly to the beam direction and to the scattering plane. Therefore, to keep the surface spins and the incident electron spin parallel or antiparallel one may only change the polar angle away from normal incidence in such a way that the azimuthal angle is either 60° or 240°, as shown in Fig. 1.

The actual numerical calculations for obtaining $I^{\uparrow}$ and $I^{\downarrow}$ were carried out by solving the electron multiple scattering formalism within the Renormalized Forward scattering approximation.[2] We have adapted computer programs to the requirements of this work.

Ion core phase shifts for Ni^{+2} and O^{-2} were calculated from a muffin-tin potential obtained by overlapping ionic charge densities using a computer program from the CAVLEED program package.[8] The standard Slater exchange approximation with the inclusion of Madelung corrections for ionic crystals was used. A muffin constant of 18 eV and a constant imaginary potential of 5 eV, which simulates the effect of damping, are used throughout the energy range from 10 - 110 eV. A constant potential obtained by averaging U^{α}_{ex} for a free electron is added to one $Ni^{+2\uparrow}$ ion and subtracted from an $Ni^{+2\downarrow}$ ion within the muffin-tin sphere to simulate the

antiferromagnetic ion species.[9] U_{ex}^{α} = 2.9 eV is used for $\alpha = 2/3$ and 4.35 eV is used for $\alpha = 1.0$.

Figure 2 shows the results of $I^{\uparrow}$, $I^{\downarrow}$, and P for 8 cases: a-e are for the specularly reflected beams for electron incident direction of $\theta = 30°$, $\phi = 60°$, and f-h are for $\theta = 80°$, $\phi = 60°$. f is for the specular beam, g is for the (2,-2) beam, and h is for the (0,-1) beam. The layer stacking sequences are (a) $\dot{3}\dot{1}\dot{3}\dot{2}$, (b) $\dot{3}\dot{1}\dot{3}\dot{2}$, (c) $31\dot{3}\dot{4}$, (d) $43\dot{1}\dot{3}\dot{2}\dot{3}$, (e) $\dot{1}\dot{3}\dot{2}\dot{3}$, (f) $343\dot{1}3\dot{2}$, (g) $31\dot{3}\dot{4}$, and (h) $13\dot{4}\dot{3}$, where the numbers 1, 2, 3, and 4 denote $Ni^{+2\uparrow}$, $Ni^{+2\downarrow}$, O^{-2}, and nonmagnetic Ni^{+2}, respectively. The dots appearing on top of the numbers represent repetitions of the stacking sequence into the surfaces. In short, a and b represent antiferromagnetic NiO with oxygen termination; e is similar to a and b but with Ni^{+2} termination; c and g represent one magnetic active $Ni^{+2\uparrow}$ layer on top of magnetically dead NiO underlayers and have oxygen terminations; d represents one magnetically dead layer on top of active underlayers with Ni^{+2} termination, and f is the same case for an oxygen termination. h is similar to g, but with $Ni^{+2\uparrow}$ termination. The results of our calculations show the following:

1. The variation of polarization depends crucially on the magnetization of the topmost layer. P is much higher in the case of $Ni^{+2\uparrow}$ termination, as seen by comparing a with e and h. Also, at grazing incidence f shows diminishing polarization, due simply to the fact that the topmost O^{-2} layer is nonmagnetic. These results imply that PLEED is highly sensitive to the magnetization of the topmost layer and also enables a determination of the chemical element presented on the surface via a polarization analysis.
2. At near normal incidence, the wave field penetrates deeper inside the surface and thus also probes the magnetization several layers in depth. This is illustrated in d, as the magnetic active underlayers do produce substantial polarizations in comparison with a and c.
3. Comparing the intensity and polarization profiles for the cases of $\alpha = 2/3$ and $\alpha = 1.0$, appreciable differences are found (see a and b). A larger α implies a higher polarization, in general, although at low energies the reverse can be found, due to multiple scattering. This is observed and can be a sensitive test of the exchange potential models used for the theoretical calculations.
4. The magnetic scattering strength can also be tested by varying the magnitude of magnetic moments on Ni^{+2} (i.e., changing the magnitude of ρ_S in (1)) to yield the best agreement with experimental intensity and polarization measurements.

This information will be harder to obtain in other experiments such as the spin-polarized photoemission, since the initial and final states involved in a photoexcitation process can have different spin multiplicity, which complicates the interpretation.

Finally, we observe that there is a strong angular dependence of the polarization for scattered electrons. In the case of one active layer on top, our results show polarization less than 5% at $\theta = 80°$, $\phi = 60°$, for the specularly diffracted beam (not shown in Fig. 2). But for the (2,-2) beam, substantial polarization is observed (Fig. 2g). Thus, in the experiment proper combinations of direction and energy will have to be chosen to obtain a high polarization.

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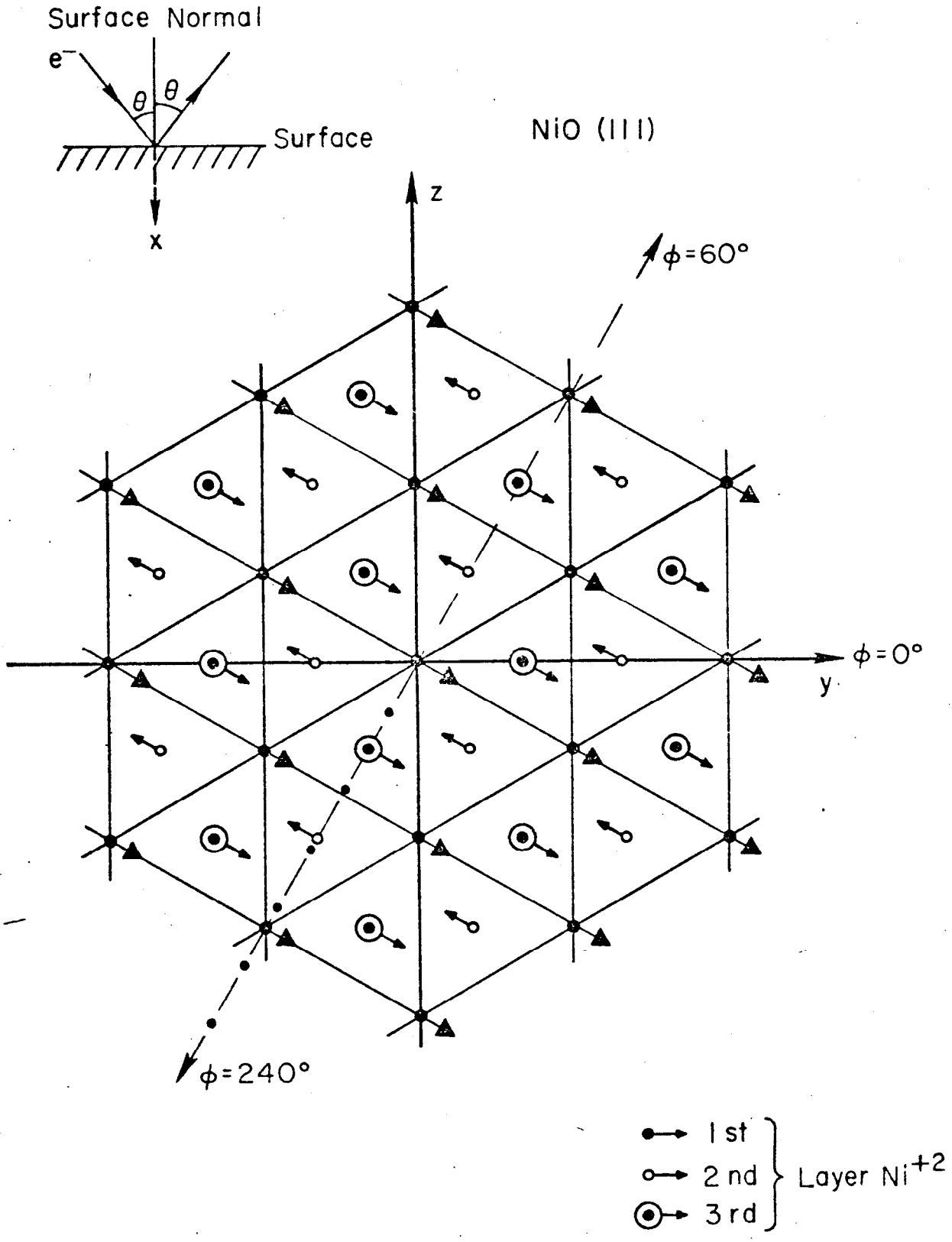
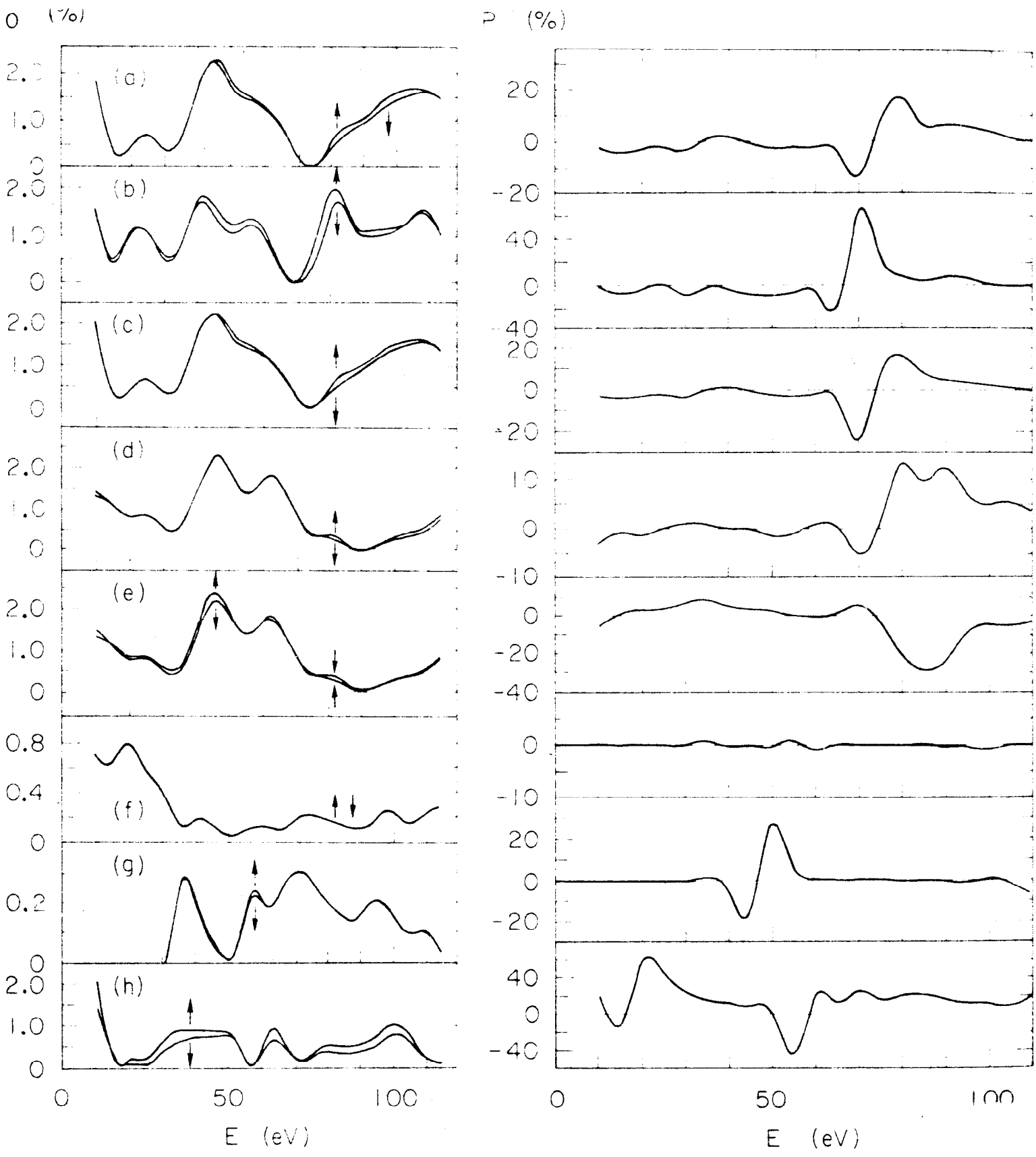
FIGURE CAPTIONS

1. Ni^{+2} sublattice in NiO (111).
2. Intensity ($I^{\uparrow}, I^{\downarrow}$) and polarization versus energy curves for incident electrons having up ($\uparrow$) and down ($\downarrow$) spin, where I_0 is the incident electron intensity. In (b), $\alpha = 1$; otherwise $\alpha = 2/3$.


Surface Normal
e⁻
θ
θ
Surface
x
NiO (111)
z
φ=60°
φ=0°
y
φ=240°
1 st
2 nd
3 rd
Layer Ni+2


I/I0 (%)
P (%)
(a)
(b)
(c)
(d)
(e)
(f)
(g)
(h)
2.0
1.0
0
0.8
0.4
0.2
20
-20
40
-40
10
-10
0
50
100
E (eV)