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Spin polarization in low-energy electron diffraction from nickel

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The computational application of a relativistic low-energy-electron-diffraction theory to Ni(111) yields practically no spin polarization at energies for which a recent reanalysis of data published in 1929 by Davisson and Germer shows significant polarization. However, large polarization values are found at very low energies in association with beam emergence thresholds. The magnitude of these resonance features and their sensitivity to the absorption potential and the surface barrier suggest that spin-polarization measurements can be expected to yield surface information also for materials of small atomic number, for which spin-orbit coupling is weak.

I. INTRODUCTION

Shortly after discovering the diffraction of slow electrons at a single-crystal surface, Davisson and Germer carried out a double scattering experiment aimed at detecting spin polarization of electrons diffracted from Ni(111).[1] Their conclusion was that no polarization was observed. Recently, however, it was pointed out by Kuyatt[2] that a correct analysis of the data of Davisson and Germer[1] implies that significant degrees of polarization were indeed observed. In particular, a peak of about 14% polarization was thus found in conjunction with an intensity maximum. Since Ni has a rather low atomic number ($Z=28$) and hence rather weak spin-orbit coupling, and since experimental asymmetries could easily produce spurious spin-polarization effects, the question remains, however, whether a genuine spin-polarization effect was observed by Davisson and Germer.[1,3]

In order to resolve this issue, I have applied a relativistic low-energy-electron-diffraction (LEED) theory[4,5] to Ni(111) for the diffraction conditions of the above experiment. A further aim of the present calculations is to obtain more detailed predictions of LEED spin polarization from Ni and to attempt to establish whether spin-polarized LEED experiments from fairly low-Z materials are worthwhile to pursue.

II. MODEL ASSUMPTIONS

A relativistic formalism for calculating intensities and spin polarization in elastic LEED from a given crystal surface as functions of the energy and orientation of the primary beam has been described elsewhere.[4,5] In its application to Ni the following specific assumptions were made. Relativistic ion core phase shifts for Ni were calculated from a muffin-tin band-structure potential obtained by overlapping atomic charge densities using the standard Slater exchange approximation with $\alpha=0.7$.[6] The relativistic phase shifts are in good agreement with nonrelativistic ones except for a small spin-orbit splitting for small l values, the difference between spin-down and spin-up phase shifts, $\delta_l^- - \delta_l^+$, being typically 0.03 for $l=1$, 0.007 for $l=2$, and less than 0.001 for $l>2$. Temperature-corrected phase shifts were obtained (cf. Ref. 5) for $T=300$ K using an effective Debye temperature of 335 K (cf. Ref. 7). Phase shifts up to $l=7$ were included in the calculations. The number of monatomic layers taken into account in the calculations was six.[8] The choice of a real inner potential of 11 eV and an imaginary potential $V_i=0.85E^{1/3}$ eV also follows Ref. 7 except for assuming $V_i=2$ eV below $E=15$ eV, where E denotes the energy of the primary beam. For a more detailed study of a very-low-energy surface resonance phenomenon associated with the emergence of the first nonspecular beam (at $E=11.15$ eV) the real inner potential was taken in its "static" limit, i.e., 13.5 eV, and the energy dependence of V_i was chosen from a recent fit to reflection coefficient experiments[9] as $V_i=0.41\ (1+\frac{1}{5}E)$.[1,4] In addition, calculations were done for $V_i=1$ and 3 eV. For the transition between the vacuum level and the (complex) inner potential, i.e., the surface barrier, several models were investigated. The real part of the surface barrier was chosen either as "nonreflecting" or as a smooth function fitted to electron-gas results.[10] For the imaginary part of the surface barrier, an abrupt step and a Gaussian function of 1-Å half width (cf. Ref. 9) were used.

III. RESULTS AND DISCUSSION

Calculations for Ni(111) for the case of normal incidence yielded intensity-energy profiles almost identical with nonrelativistically calculated ones[7,11] and in excellent agreement with experiment.[12] The spin-polarization profiles obtained for the nonspecular beams[13] exhibit only small peaks—of at most 15% polarization—which occur at energies

at which the intensity is minimal. Comparing with recent results for normal incidence on W(001),[5] it is noted that the present polarization peak values are smaller by a factor of about seven, which is in accordance with our qualitative expectation based on the low atomic number of Ni.

Specular beam results calculated for the diffraction conditions of the experiment of Davisson and Germer,[1] i.e., for the primary beam incident at 45° along the 10 azimuth, are shown in Fig. 1. The calculated intensity profile is in good agreement with the experimental one with regard to peak positions. The lack of agreement with respect to relative peak heights is not surprising, since the data were not normalized to the primary beam intensity. Above about 50 eV, the theoretical spin-polarization profile is seen to be very low. In particular, it is evident from Fig. 1 that the theoretical polarization values are substantially smaller than their experimental counterparts as obtained by Kuyatt[2] from the data of Davisson and Germer.[1] Since the polarization profile above about 50 eV was found to exhibit a sensitivity to the physical input of the calculation (cf. Sec. II), which is very small compared to the discrepancy with the experiment, and since the reliability of our theoretical method and computer code was recently verified,[14] it is concluded that the experimental polarization values above 50 eV are spurious, i.e., due to asymmetries in the apparatus.

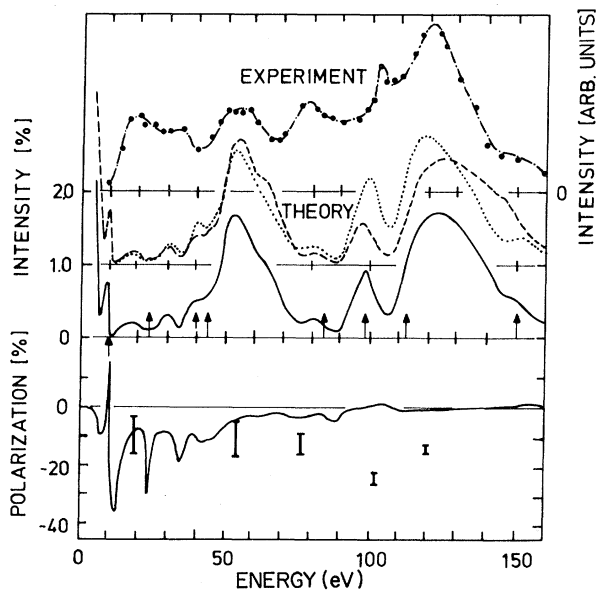

FIG. 1. Specular beam from Ni (111): theoretical intensity and spin polarization for $\theta = 45°$ (solid line); theoretical intensity for $\theta = 44°$ (dotted line) and $\theta = 46°$ (dashed line); experimental intensity (Ref. 1) (dash-dot line) for $\theta = 45°$. Vertical error bars give the polarization obtained in Ref. 2 and vertical arrows indicate external beam emergence threshold energies.

This conclusion is supported by intensity profiles calculated at $\theta = 44°$ and 46°, which are also shown in Fig. 1. For the peak near 120 eV, for example, the intensity changes—at fixed energy points—by about (5–10)% of its absolute value when θ changes by 1°. Assuming a misalignment of the axis of rotation of the second crystal (cf. Fig. 1 in Ref. 2) by 0.5°, the difference between the intensities I and I' measured for 0° and 180° rotation, respectively, would then be at least 5% of their mean value. Calculating the polarization P according to [cf. Eq. (2), Ref. 15]

$$P = [(I - I')/(I + I')]^{1/2} ,$$

one would then obtain about 16% polarization, which checks well with the experimental value. At other energies, a misalignment of 0.5° would produce spurious spin polarization of the same order of magnitude. The measured polarization at 20 eV appears, in Fig. 1, in good agreement with the theoretical value. In view of the substantial discrepancies at the other energy points this agreement seems, however, to be coincidental resulting form a fortuitous cancellation of experimental errors.

The occurrence of larger theoretical polarization values at lower energies in Fig. 1 is plausible for two reasons. First, the number of phase shifts δ_l, which contribute to the ion core scattering, increases with energy, but only δ_1 and δ_2 exhibit a significant spin-orbit splitting (cf. Sec. II). Second, absorption, which was assumed as increasing with energy, appears—from calculations performed with different V_i values at fixed energies—to be in general detrimental to LEED spin polarization.

The theoretical polarization profile in Fig. 1 exhibits, below 50 eV, several significant peaks which are correlated with beam emergence thresholds. Following earlier work,[16-18] these polarization peaks and the associated intensity minima are interpreted as surface resonance phenomena. Since surface resonances can be expected to be very sensitive to details of the potential in the surface region,[19] the energy range between 5 and 17 eV, in which the most pronounced polarization feature occurs in Fig. 1, was investigated for various choices of the uniform complex potential V_i and for various surface barriers. With regard to the latter, particular consideration was given to its imaginary part, which has so far received little attention in surface resonance studies. The calculations were done at energy intervals of 0.1 eV over the entire range and of 0.01 eV over regions of rapidly varying polarization. Results for intensity and polarization profiles are shown in Fig. 2. For a refracting but nonreflecting

barrier model, a polarization peak of -18% in conjunction with an intensity minimum is found at 12 eV. For continuous surface barrier models this feature can be seen to be drastically modified in the vicinity of the external emergence threshold of the first nonspecular beam at 11.15 eV. The correlation with a beam threshold as well as the occurrence due to the introduction of a surface barrier identifies these modifications as surface barrier resonance phenomena of the type previously reported.[16-18] Comparison of panels *A* and *B* in Fig. 2 shows that, for the same bulk imaginary potential V_i (chosen energy dependent as in Ref. 9), different models for the imaginary part V_i^s of the surface barrier, i.e., the way V_i goes towards the vacuum zero, produce substantially different intensity and polarization profiles. Though it is plausible that the barrier transfer matrix should be different for different models of V_i^s, a detailed "simple understanding" of the calculated features is not available at present. From panels *B* and *C* it can be seen that, for the Gaussian shape of V_i^s (cf. Ref. 9), the value of the bulk imaginary potential V_i also has a strong effect in particular on the polarization profile. An attempt to interpret this effect would have to consider that a change in V_i acts in two separate ways: first, by changing the substrate reflection amplitudes; and second, by changing the height of V_i^s and thereby its contribution to the barrier transfer matrix. Further calculations performed for an image potential as the real surface barrier indicate that shape and peak height of the resonance in both the intensity and polarization profile depend strongly on the real part of the surface barrier as well. Comparing the effect of different imaginary bulk potential values and of different surface barriers upon intensity profiles on the one hand and upon polarization profiles on the other, it is apparent from Fig. 2 that the polarization profiles are more sensitive. It is therefore concluded that spin-polarization measurement could, in conjunction with model calculations, provide a sensitive means of determining the bulk imaginary potential and the real and imaginary part of the surface barrier even for a low-Z material like Ni. Polarization analysis could in this respect be complementary to the recently introduced reflection coefficient analysis (cf. Ref. 9, and references therein).

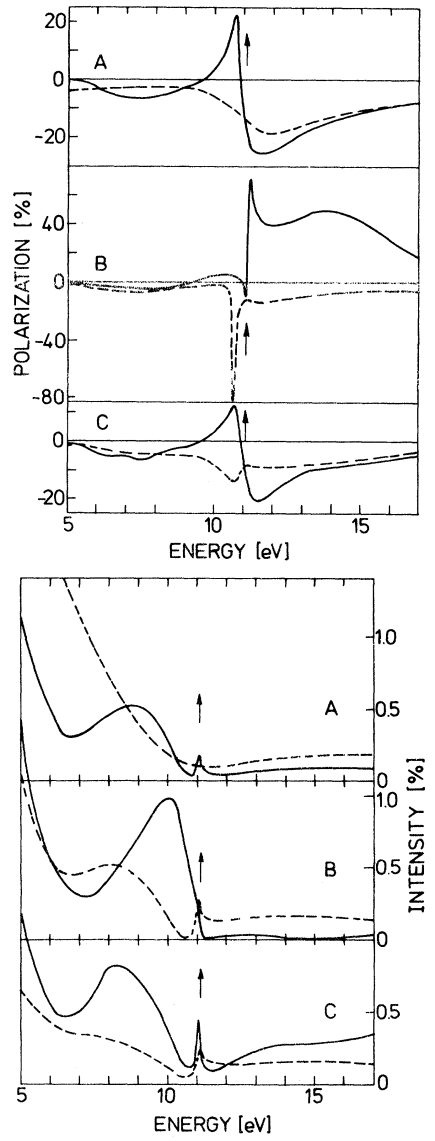

FIG. 2. (a) Fine structure of theoretical spin polarization; and (b) intensity of the specular beam from Ni(111) at $\theta = 45°$. The bulk imaginary potential V_i and the surface barrier $V_r^s + iV_i^s$ underlying the results in panels A, B, and C. of parts (a) and (b) are the following: (A) V_i from Ref. 9; dashed line: no reflection barrier; solid line: V_r^s from Lang and Kohn (Ref. 10), V_i^s of the same shape. (B) V_i from Ref. 9, V_r^s from Lang and Kohn (Ref. 10); dashed line: V_i^s Gaussian (Ref. 9); solid line: V_i^s abrupt step. (C) V_r^s from Lang and Kohn (Ref. 10), V_i^s Gaussian (Ref. 9); dashed line: $V_i = 3$ eV; solid line: $V_i = 1$ eV. Vertical arrows indicate the threshold of emergence of the first nonspecular beam.

IV. CONCLUSION

In conclusion, I would like to emphasize the two essential results of the present calculations. First, it is most unlikely that Davisson and Germer[1] did actually observe spin polarization in LEED. Second, the sizeable spin-polarization values predicted at very low energies and their sensitivity to imaginary inner potential and surface barrier indicate that spin-polarization analysis could yield surface information even for low-

Z materials, for which spin-orbit coupling is small. Spin-polarization measurements on low-Z materials should, however, not be attempted by means of a double scattering arrangement involving two crystals of the same material, as was done in Ref. 1, but rather by means of double scattering using a large-Z detector crystal (e.g., tungsten).

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[1]C. J. Davisson and L. H. Germer, Phys. Rev. 33, 760 (1929).

[2]C. E. Kuyatt, Phys. Rev. B 12, 4581 (1975).

[3]For the ferromagnetic phase of Ni, the exchange interaction of the incoming electron with the majority- and the minority-spin electrons in the solid can also give rise to LEED spin-polarization effects [cf. R. Feder, Phys. Status Solidi B 56, K43 (1973)]. Since this exchange interaction decreases with energy and is insignificant above about 100 eV, I feel that it could not account for the experimental data (Ref. 1). It is therefore not taken into account in the present theoretical study.

[4]R. Feder, Phys. Status Solidi B 49, 699 (1972).

[5]R. Feder, Phys. Rev. Lett. 36, 598 (1976).

[6]The author is grateful to J. Harris, R. O. Jones, and G. S. Painter for making this potential available. The scattering properties of such a superposition potential were recently shown to be practically the same as those for a more sophisticated self-consistent band-structure potential [S. Y. Tong, J. B. Pendry, and L. L. Kesmodel, Surf. Sci. 54, 21 (1976)].

[7]J. E. Demuth, P. M. Marcus, and D. W. Jepsen, Phys. Rev. B 11, 1460 (1975).

[8]The convergence of the present finite-crystal results for six layers is in accordance with the statement of Ref. 7 that five layers are adequate. Since the computing time required for six layers is the same as for five, six were preferred in this work.

[9]E. G. McRae and C. W. Caldwell, Surf. Sci. 57, 766 (1976).

[10]N. D. Lang and W. Kohn, Phys. Rev. B 1, 4555 (1970).

[11]The intensities of the (10) beam in Ref. 7 are almost exactly twice as large as ours over the entire energy range. Since the (10) intensities calculated for Ni (111) at normal incidence by G. E. Laramore [Phys. Rev. B 8, 515 (1973)] are very close in absolute value to ours, and since the ratio of theoretical and experimental peak intensities for the (10) beam in Ref. 7 is by about a factor of two larger than for the $(\bar{1}0)$ beam, the $(\bar{1}0)$ intensities in Ref. 7 being the same as ours, it is concluded that the (10) profile in Ref. 7 contains a scaling error and is, upon correction of this error, almost identical to ours.

[12]Comparison made with the data of J. E. Demuth and T. N. Rhodin, Surf. Sci. 42, 261 (1974), which are supplemented below 65 eV by data from R. L. Park and H. E. Farnsworth, Surf. Sci. 2, 527 (1964).

[13]At normal incidence, the specular beam is unpolarized, as can be seen from symmetry arguments and is explicitly confirmed by the numerical results.

[14]R. Feder, P. J. Jennings, and R. O. Jones, Surf. Sci. (to be published).

[15]R. Feder, Surf. Sci. 51, 297 (1975).

[16]E. G. McRae, Surf. Sci. 25, 491 (1971).

[17]P. J. Jennings, Surf. Sci. 27, 221 (1971).

[18]R. Feder, Phys. Status Solidi B 62, 135 (1974).

[19]A strong dependence of surface resonances in intensity profiles on the shape of the real part of the surface barrier was obtained by P. J. Jennings, Surf. Sci. 34, 668 (1973); and P. J. Jennings and M. N. Read, *ibid.* 41, 113 (1974).