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ANALYSIS OF THE TEMPERATURE DEPENDENT MAGNETIC SCATTERING OF FERROMAGNETIC Ni(110) SURFACE *

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ABSTRACT

The temperature dependence of the bulk and layer-by-layer surface magnetization of Ni(110) is derived using the molecular field theory. We then use these results in a dynamical polarized low-energy electron diffraction (PLEED) calculation to determine the temperature dependent polarization S of the diffracted intensities. The S vs T curves are strongly dependent on the incident electron energies and the critical exponents for surface magnitization are different from the bulk case. Multiple scattering effects pronouncely modify the results predicted by using the kinematical scattering approximations. We also examine the sensitivity of S upon the use of different spin-dependent scattering potentials of the surface atoms. These results are then compared with recent experimental data for $0.6\ T_{Curie} \leq T \leq T_{Curie}$. The usefulness of PLEED for surface magnetic structural determination are clearly demonstrated.

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The magnetic properties of solids have always been one of the most important subjects in solid state physics since the early days of quantum mechanics. Recently, due to the rapid advances of the spin polarized electron beam technology(1), it has become feasible and increasingly important to investigate the magnetic properties of solid surfaces by using polarized low energy electron diffraction (PLEED). The presence of a metal-vacuum interface has made the local environment of the surface magnetic layers appreciably different from that in the bulk. Therefore, one can not even intuitively expect that surface magnetization is just the same as bulk magnetization. PLEED is a useful technique for obtaining these informations since low energy electrons penetrate only a few layers deep into the surface and also the spin-dependent exchange-correlation scattering between the incident electron and surface electrons carries direct information about surface magnetization. In two previous papers(2, 3)(referred to as I and II), we have investigated the temperature dependent magnetic scattering of polarized electrons by the ferromagnetic Ni(110) surface near its bulk Curie temperature ($\sim$ 632 K). The basic physical principles of PLEED can be stated as follows: For a ferromagnetic surface, the magnetic scattering is determined by the exchange-correlation interaction of the incident electron spin (S_1) with the surface spin (S_2) components which are parallel ($\uparrow$) or antiparallel ($\downarrow$) to S_1. This produces a difference, $I^{\uparrow} - I^{\downarrow}$, in the diffracted intensities. The polarization S is defined as $S = (I^{\uparrow} - I^{\downarrow})/(I^{\uparrow} + I^{\downarrow})$. Therefore, by examining the S vs E (incident electron energy) and S vs T dependences, one can hopefully obtain enough understanding of surface magnetism to answer questions such as whether surface magnetization is enhanced, reduced, removed or even magnetically reconstructed and whether the surface magnetic layer exhibits the same thermal behavior as that of the bulk layer, etc. In I and II, we tackled the problem by 1) deriving the layer-by-layer surface magnetization of Ni(110) as a function of T using the molecular field theory within the Heisenberg localized spin model, 2) setting up the T dependent electron-surface scattering potential in which the exchange-correlation part had a term proportional to the layer magnetization derived in step 1), and 3) using the LEED dynamical theory for obtaining the electron-surface diffraction amplitudes by including both the single (kinematic) and multiple scattering paths for incident electrons having up and down spins. The results of I and II have shown that 1) the magnetization of surface layers are reduced in comparison with their bulk value. The temperature dependence for layers very near the surface varys as $1-t$, where $t=T/T_c$, and for bulk layers vary as $(1-t)^{\frac{1}{2}}$ as $t \rightarrow 1$, 2) near normal incidence ($\theta = 12°$), the overall S vs E curves for both the case with bulk magnetization in all layers and the case where each layer has our calculated magnetizations resemble each other except at E $\sim$ 100 eV - 150 eV where pronounced structural differences have been found, 3) at grazing incidence ($\theta = 60°$), the S - E curves between these two cases show little structural differences but an overall polarization reduction in the case of surface magnetization is observed. This correlates well with the results found in step 1),and 4) the S values decrease roughly linearly for surface magnetization near T_c, which implys a surface critical exponent of unity, and roughly as $(1-t)^{\frac{1}{2}}$ for bulk magnetization implying a critical exponent of $\frac{1}{2}$ at a few selected energy points. These are also the trends predicted by the PLEED kinematic approximation. However, serious breakdowns of such approximation do occur at energy points where S values vary rapidly. The results summarized in 1) - 4) form a useful starting

point for the investigations to be discussed in the following sections.

In this work, we examine further 1) the variation of S values obtained in I and II as θ changes locally over a small angle range, 2) the sensitivities of the Wakoh potential (4) and 3) the effect of incorporating the spin-dependence in the imaginary potential. All other physical parameters and computational procedures follow those used in I and II. We also refer readers to I and II for a detailed derivation of the layer-by-layer magnetizations.

In II, we have mentioned that the large S values calculated near 70 eV at $\theta = 12°$ is not observed in experiment for the specularly reflected beam, but remain stable as we increase the numerical accuracy and slightly vary physical parameters such as the mean free path and inner potential, etc. However, as θ varies by $\pm 2°$, the S value decreases rapidly to half its value as shown in Fig. 1. We know that there exists some uncertainty in the experimental incident angle (5) and notice also the reflectivity is extremely small ($\sim 10^{-5}$) at this energy region. The measured S values may be reduced due to the contribution of noise. A very high precision is required here and this presents difficulties in both refining the theoretical model and improving the experimental accuracy. The variation of polar angles also shifts the peak positions by a few eV and change the relative peak heights appreciably. Therefore, a precise determination of incident angle would be of great necessity in PLEED experiments.

The S - E curves obtained by using the best available band structural potential (6) (the MJW potential) and the less sophisticated Wakoh potential are shown in Fig. 2 for $\theta = 12°$, $\phi = 35.26°$ at $t = 0.6$. There is almost no structural difference between the surface and bulk case when Wakoh potential is used. In this case, below 70 eV the S values are smaller for surface magnetization than those obtained by using the MJW potential (shown in Fig. 1), although the general shape of S - E curves in both cases follow quite closely. Such an enhancement is not surprising, since the magnetic moment per Ni atom predicted by Wakoh is $0.66\mu_B$ and that by Moruzzi, Janak and Williams is $0.59\mu_B$. μ_B is the Bohr magneton. The MJW value is closer to the experimental value $0.56\mu_B$ and the results are considered more favorably.

Finally, we discuss the results of incorporating a spin dependent imaginary potential $V_i^{\uparrow,\downarrow}$ in addition to the exchange-correlation potential used in I and II for obtaining the S - E and S - t curves. It has been shown(7) that $V_i^{\uparrow,\downarrow}$ for a free electron gas can be separated into two parts, i.e., the plasmon excitations $V_{i,p}$ and the electron-hole excitations $V_{i,eh}^{\uparrow,\downarrow}$. Since plasmons are collected excitations involving both majority and minority electrons simultaneously, $V_{i,p}$ is spin-independent. On the other hand, $V_{i,eh}^{\uparrow,\downarrow}$ is spin dependent, since the electron-hole pair can be in the singlet or triplet spin states. Feder(8) proposed to evaluate $V_{i,eh}^{\uparrow,\downarrow}$ as follows:

$$\frac{V_{i,eh}^{\uparrow}}{V_{i,eh}^{\downarrow}} = \frac{n^{\downarrow}}{n^{\uparrow}} = \frac{\overline{V}_{i,eh}\left(1 - \frac{1}{2}\cdot\frac{\Delta n}{n}\right)}{\overline{V}_{i,eh}\left(1 + \frac{1}{2}\cdot\frac{\Delta n}{n}\right)} = \frac{\left(1 - \frac{1}{2}\cdot\frac{\Delta n}{n}\right)}{\left(1 + \frac{1}{2}\cdot\frac{\Delta n}{n}\right)} \quad (1)$$

where

$$\overline{V}_{i,eh} = \tfrac{1}{2}\left(V_{i,eh}^{\uparrow} + V_{i,eh}^{\downarrow}\right)$$

$$n = n^{\uparrow} + n^{\downarrow}$$

$$\Delta n = n^{\uparrow} - n^{\downarrow}$$

and

$$V_i^{\uparrow,\downarrow} = V_{i,eh}^{\uparrow,\downarrow} + V_{i,p} \qquad (2)$$

$n^{\uparrow}$ and $n^{\downarrow}$ are the number of spin up and spin down electrons of the surface atom. The ratio of $V_{i,p}/V_{i,eh}^{\uparrow,\downarrow}$ is then taken from the calculations for a free electron gas (7) in his work. Equation (1) is obtained based on the assumption that e-surface atom scattering is dominated by the S partial wave, which is a valid approximation at very low electron energies. Using Eq. (1) and (2), he observed great differences in the calculated S-E curves for Fe(110) in comparison with the case using the spin averaged $\overline{V}_{i,eh}$ term. For Ni(110), the situation is less clear since Δn of Ni is much smaller than that of Fe (magnetic moment is $0.59\mu_B$ for Ni and $2.56\mu_B$ for Fe). We shall test the effect of incorporating Eq. (1-2) here by slightly modifying Eq. (1) to include the spin thermal fluctuations, i.e.,

$$\frac{V_{i,eh}^{\uparrow}}{V_{i,eh}^{\downarrow}} \quad (T > 0) = \frac{\left(1 - \tfrac{1}{2} \cdot \frac{\Delta n}{n} \cdot m_n\right)}{\left(1 + \tfrac{1}{2} \cdot \frac{\Delta n}{n} \cdot m_n\right)} \qquad (3)$$

where m_n is the temperature dependent layer magnetization derived in I and II. In principle $V_{i,eh}^{\uparrow,\downarrow}$ should be layer dependent. We take an averaged value m_n out of the first 4 layers, since these layers give the most contribution to the reflected intensities.

Our calculated S-E curves with and without the inclusion of spin dependence in V_i are shown in Fig. 3 at $t = 0.6$ for specularly reflected beam at $\theta = 12°$, $\phi = 35.26°$. The overall shape in both cases follow fairly closely except at $E \sim 50$ eV and $E \sim 85$ eV. But in the first case the absolute S values at $E = 20$ eV is $\sim -2\%$ and at $E = 125$ eV is $\sim 3\%$. In the second case, these numbers are $\sim -4\%$ and $\sim 1\%$, respectively. The experimental values are $\sim -4\%$ and $\sim 2\%$. The inclusion of $V_{i,eh}^{\uparrow,\downarrow}$ does not seem to improve the agreement between theory and experiment. Moreover, the comparison of calculated and experimental S-t curves does not seem to indicate an improvement after the inclusion of $V_{i,eh}^{\uparrow,\downarrow}$ than the results obtained in I and II. At 125 eV, the S values decrease rather slowly as $t \to 1$, which does not show roughly a linear dependence. We therefore conclude that the spin dependence of the imaginary potential is much less important in the case of Ni(110) than Fe(110), 2) a more vigorous derivation is needed for determining $V_{i,eh}^{\uparrow,\downarrow}$ for

transition metals which will not employ such a drastic approximation as in Eq. (1), if a detailed comparison between calculations and experimental data is planned. Some recent derivations(9) have also shown that such spin dependence in the imaginary part of the scattering potential is negligible except at very low energies for Ni. We hope to clarify this problem in a forthcoming paper.

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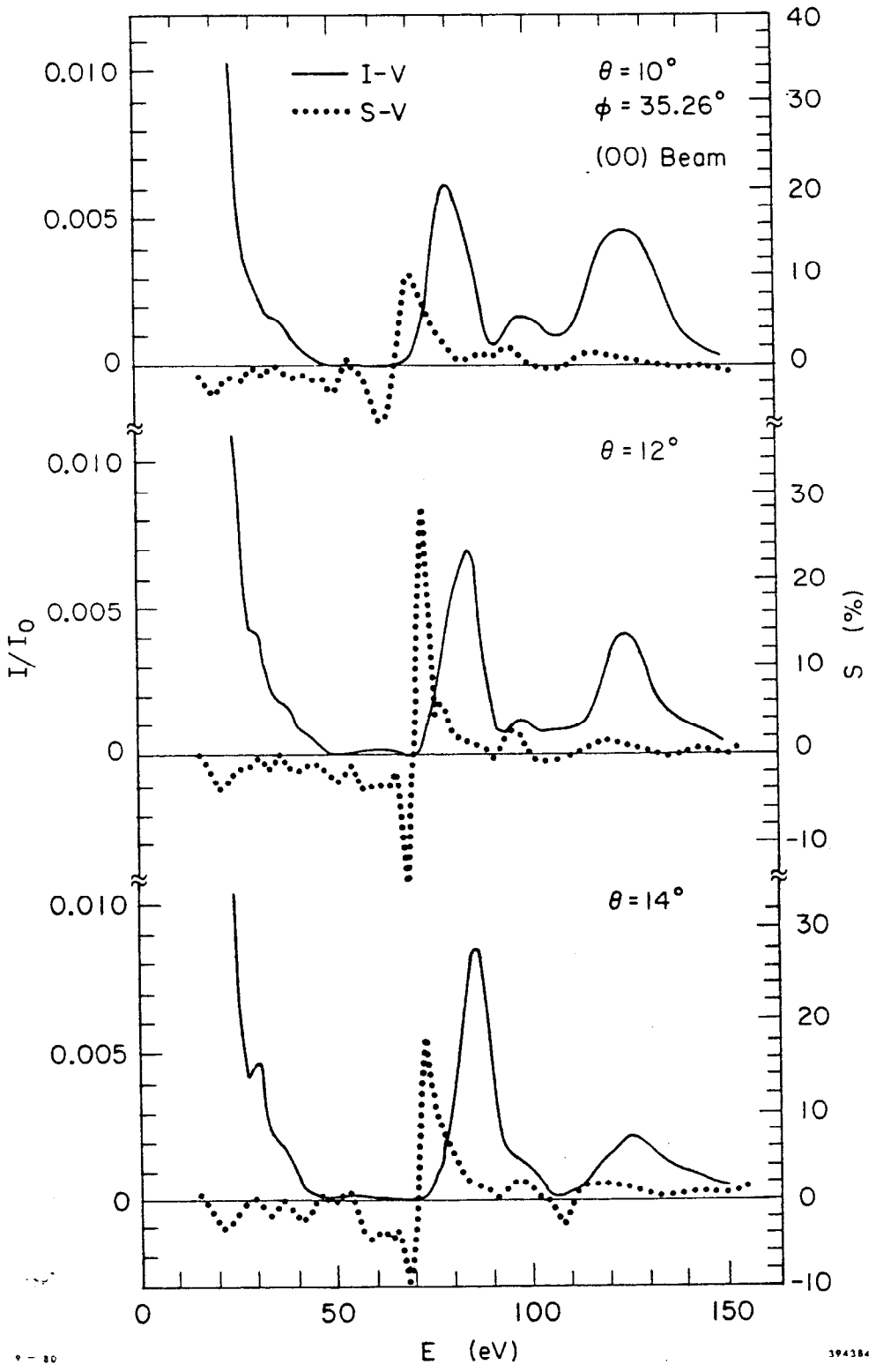

Fig. 1. I-E and S-E curves as a function of incident polar angles.

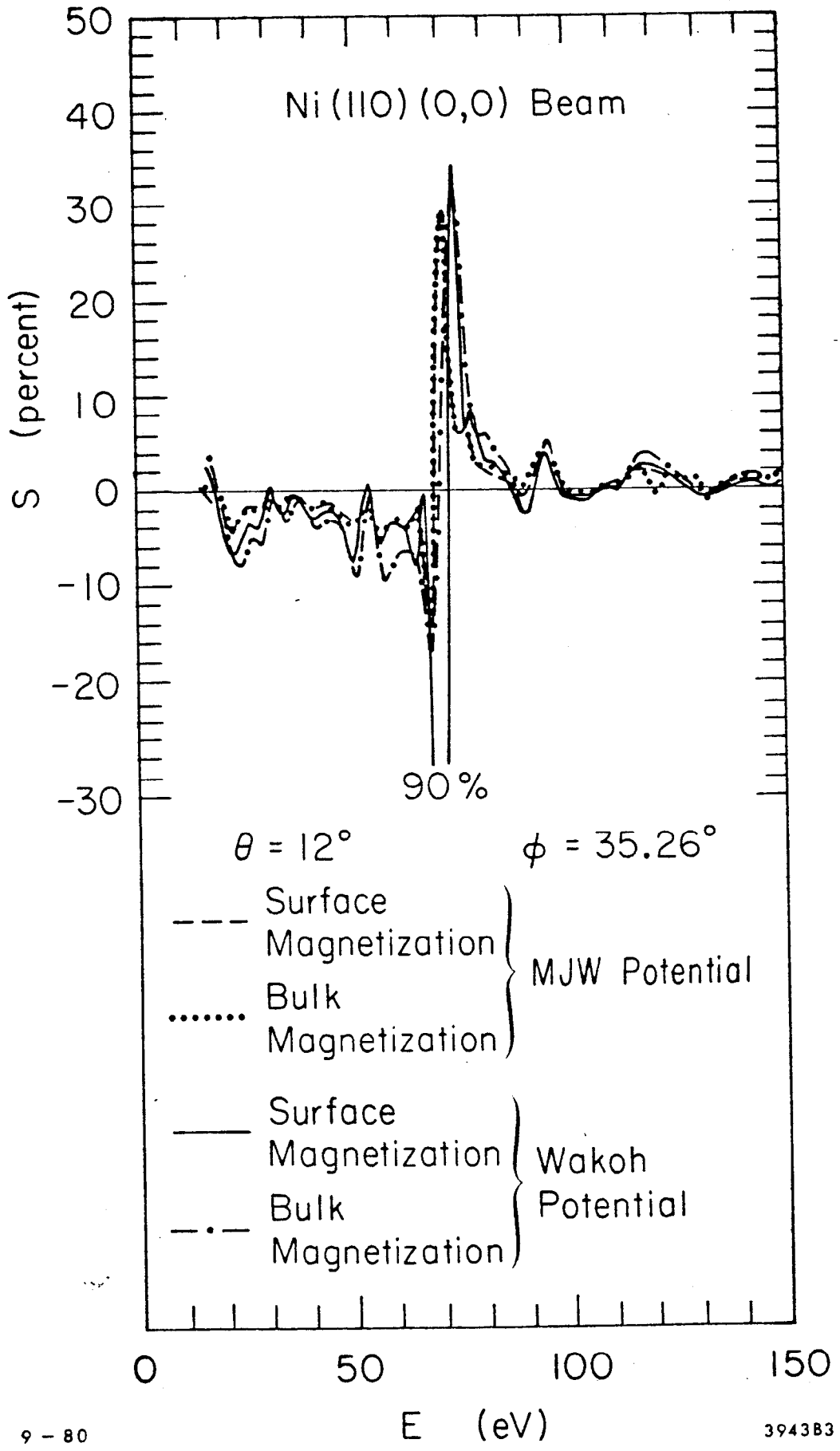

Fig. 2. S-E curves obtained by using the MJW potential and the Wakoh potential.

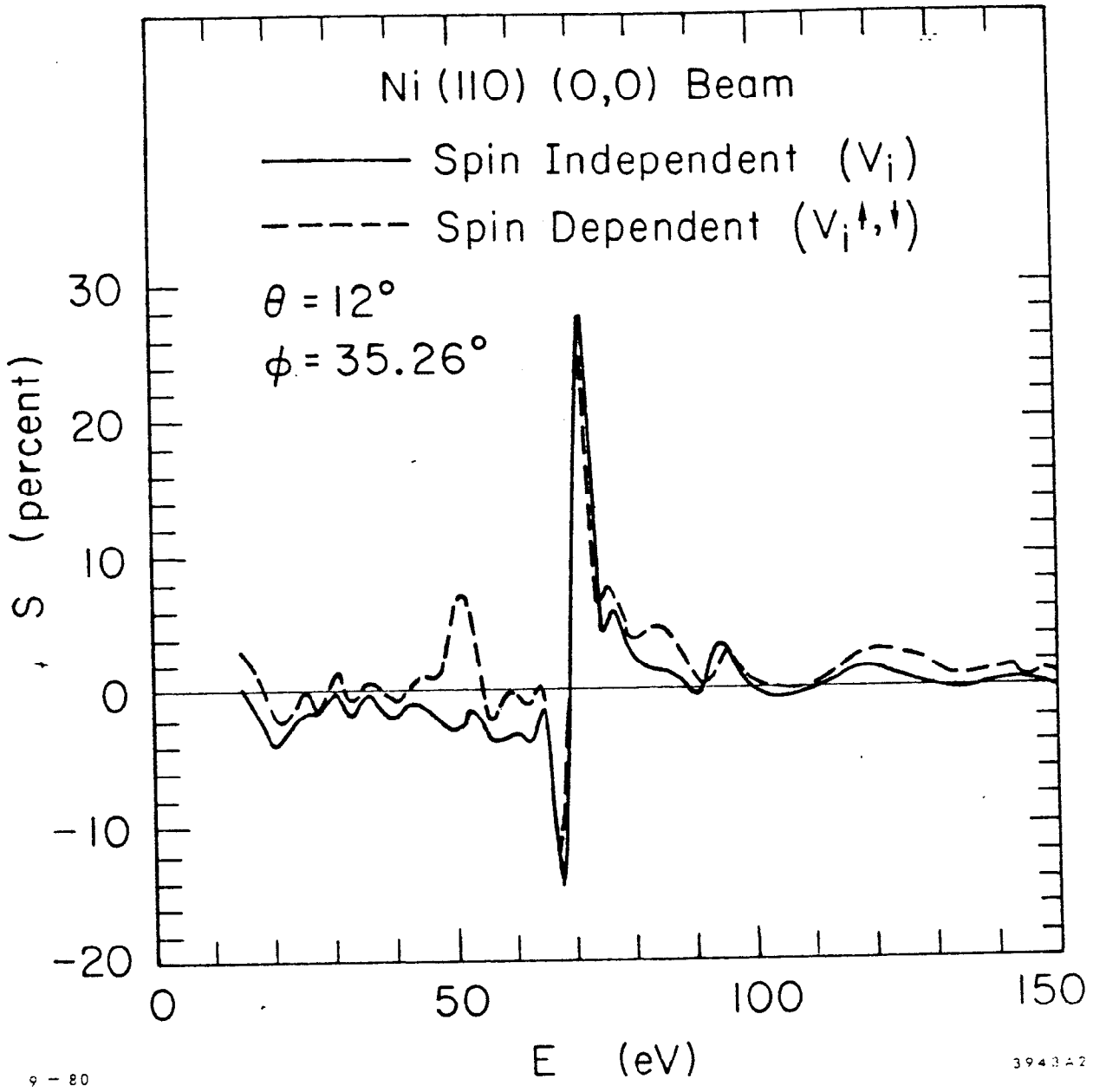

Fig. 3. S-E curves obtained with and without the inclusion of spin dependence in V_i.

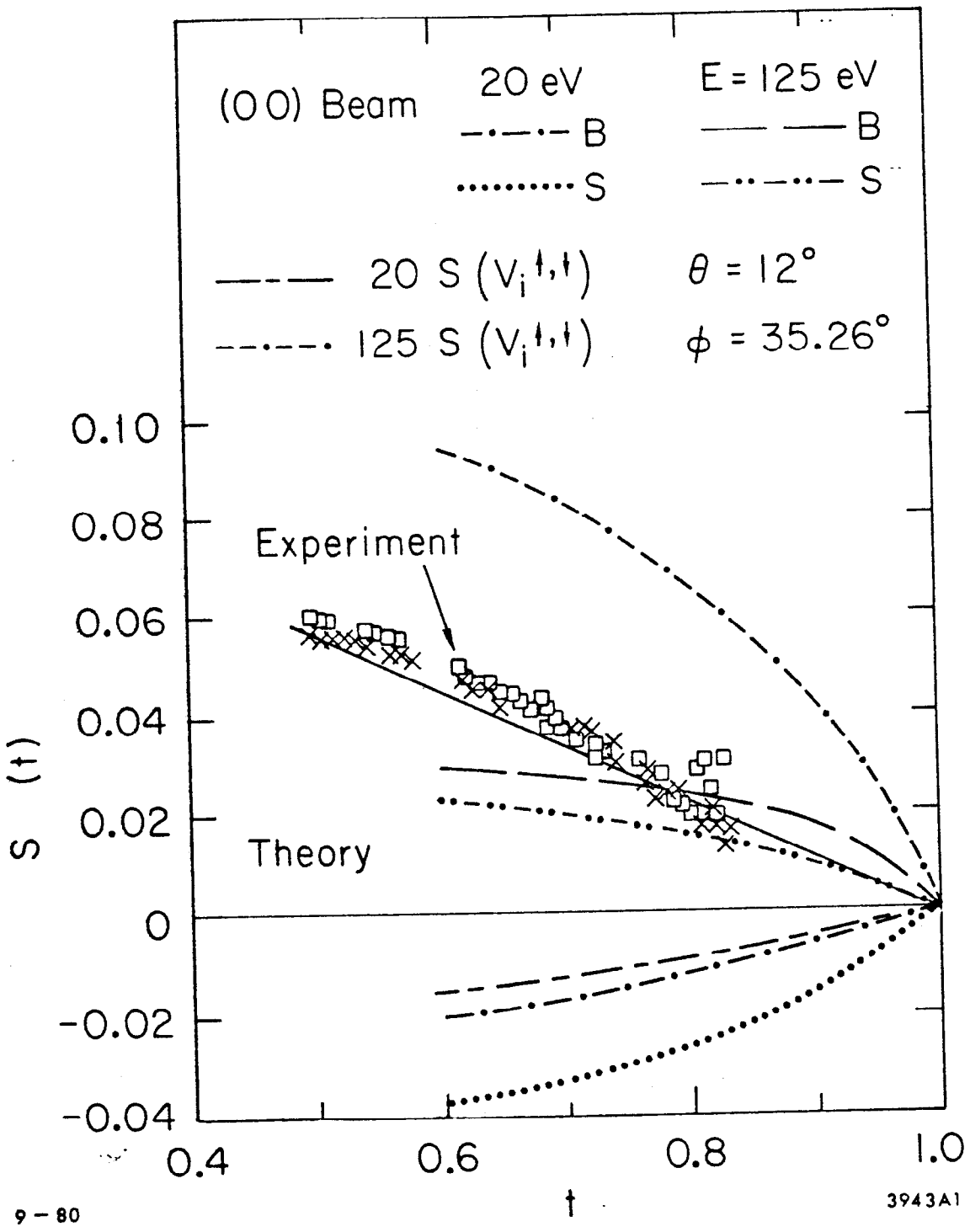

Fig. 4. S-t curves obtained with and without the inclusion of spin dependence in V_i.