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Spin-wave theory of spin-polarized electron energy loss spectroscopy (SPEELS) measurements in 5 ML Fe film deposited on W(110)

S. MAMICA*, H. PUSZKARSKI

Surface Physics Division, Institute of Physics, Adam Mickiewicz University,
ul. Umułtowska 85, 61-614 Poznań, Poland

Detection of spin waves with higher wave vector values is now possible with spin-polarized electron energy loss spectroscopy (SPEELS), a method recently reported to have been applied for detecting spin waves in a range of wave vector values covering in principle the whole Brillouin zone. This paper presents a comparison of spin-wave spectra resulting from our theoretical investigations (within the model based on a bilinear Hamiltonian expressed in second-quantization formalism) with the corresponding SPEELS results obtained recently for 5 ML Fe film deposited on W(110). By considering the mixed bcc-fcc film structure we were able to explain details of the reported SPEELS spectra, indicating the surface character of the modes associated with the observed peaks.

Key words: *spin waves; SPEELS; ultrathin Fe film*

1. Introduction

Due to the recent dynamic development of magnetoelectronics, properties of spin waves in magnetic thin film systems have been intensively studied both experimentally and theoretically. The standard experimental methods of probing spin waves, i.e. ferromagnetic resonance (FMR) and Brillouin light scattering (BLS), only allow investigation of waves with low wave vector values (wave vector near the Brillouin zone centre). This limitation does not apply to spin-polarized electron energy loss spectroscopy (SPEELS) [1–4]. Besides allowing penetration of the whole Brillouin zone, SPEELS has an advantage of being especially sensitive to surface spin waves. Recent studies by Vollmer et al. on Co and Fe ultra-thin films [5, 6] are of particular interest in this context.

The paper presents the results of our calculations of ultra thin film spin wave energy spectra, providing a basis for a tentative interpretation of the SPEELS spectrum obtained for 5 ML Fe/W(110) and reported in [6].

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*Corresponding author, e-mail: mamica@amu.edu.pl

2. Essentials of SPEELS experiment on 5 ML Fe deposited on W(110)

The inelastic electron scattering occurring in a SPEELS experiment results in energy and momentum transfer from the scattered electrons to the studied sample. The incident electron beam is spin-polarized, the polarization being either antiparallel (↑) or parallel (↓) to the magnetization of the sample. The scattering itself can occur in two ways: either an incident electron is reflected, passing a part of its energy and momentum to electrons in the sample, or it knocks out an electron of the sample to take its place. In the latter case, if the spin of the incident electron is antiparallel to the magnetization of the sample, the magnetization will decrease by $g\,\mu_B$, producing a spin excitation (such as a Stoner excitation or a spin wave). The electron knocked out of the sample will join the scattered beam, resulting in its spin polarization asymmetry. The essence of SPEELS is the measurement of the scattered intensity as a function of two parameters: the energy loss (E_{loss}) and the wave vector component parallel to the surface ($\mathbf{k}_{||}$). The asymmetry spectrum measured in function of E_{loss} and $\mathbf{k}_{||}$ contains information on spin excitations that have occurred in the scattering process. On the other hand, as the scattered electrons are monochromatic and of low energy (in the order of 10 eV), their penetration range into the sample is as low as a few atomic layers; therefore, the information obtained principally concerns the surface region of the studied sample.

The SPEEL measurements reported in [6] were performed on an ultrathin (5 ML) Fe layer set on a W(110) substrate by the molecular beam epitaxy (MBE) at room temperature. Upon preparation, the sample was magnetized in-plane along the easy-magnetization direction (<110> in Fe/W(110) thin films). The chosen electron scattering plane was perpendicular to the magnetization direction. The resulting SPEEL intensity spectrum, as well as the asymmetry spectra corresponding to four wave vector values ($\mathbf{k}_{||} = -0.17$ Å^{-1}, -0.35 Å^{-1}, -0.69 Å^{-1} and -1.03 Å^{-1}) are shown in [6], Fig. 5. Two regions can be distinguished in the asymmetry spectrum: above 500 meV, with asymmetry characteristic of Stoner excitations, and below 500 meV, with a very wide line extending from about 100 meV to 500 meV and showing two clearly separated peaks at 215 meV and 310 meV. The spectrum shows no significant dispersion, as the positions of the peaks remain the same in all four spectra obtained for the four different wave vector values. On the other hand, SPEEL asymmetry increases with the wave vector value (from ca. 0.1 for $\mathbf{k}_{||} = -0.17$ Å^{-1} to ca. 0.2 for $\mathbf{k}_{||} = -1.03$ Å^{-1}). The obtained wide line is attributed by the authors to a spin wave excitation, and the notch separating the two peaks is associated with vibration losses due to adsorption species deposited on the sample surface during measurements (which is of importance because of long measurement time).

Key information necessary for proper interpretation of the spectrum obtained is that about the structure of the studied sample. The structure of ultrathin Fe layers was studied, among others, in [7], reporting the results of STM investigation of Fe films of the thickness ranging from 1 ML to 5 ML, set on a Cu(001) substrate by the MBE method. In contrast to the 'bulk' Fe, which shows the α (bcc) structure at temperatures below 1185 K, thin-film Fe (of thickness up to 4 ML) has the fcc structure. The thickness threshold, above which reconstruction to the bcc structure occurs, is approximately 4–5 ML. Therefore, ultra-thin Fe layers of the thickness close to the threshold value are assumed to have a mixed structure [7] with alternating bcc and fcc phases, and the SPEEL spectrum discussed above can be expected to contain information on spin waves occurring concurrently in both structure types. Assuming this point of view, we think the two peaks in the asymmetry spectrum can be associated with excitation of two different spin waves, and the observed asymmetry increase with the wave vector value might suggest their surface character. A theoretical elaboration of this idea is presented below.

3. Theoretical results

In order to verify our hypothesis, we have calculated the energy spectra of spin waves in a thin film of mixed bcc–fcc structure and surface cut (110). The calculations were performed within the framework of the Heisenberg localized spin model, assuming an exchange (nearest neighbour only) and Zeeman Hamiltonian in the standard form:

$$H = -2J \sum_{(l\mathbf{j};l'\mathbf{j}')} \hat{\mathbf{S}}_{l\mathbf{j}} \cdot \hat{\mathbf{S}}_{l'\mathbf{j}'} - g\mu \sum_{l\mathbf{j}} \mathbf{H}^{\mathrm{eff}} \cdot \hat{\mathbf{S}}_{l\mathbf{j}} \tag{1}$$

$\mathbf{H}^{\mathrm{eff}}$ comprising both external and demagnetizing fields. The sums extend over different pairs of neighbouring spins, $l\mathbf{j}$ defining the spin position; l is the layer number and $\mathbf{j}$ denotes the two-dimensional vector defining the position of the spin in the l-th layer. We diagonalize the Hamiltonian (1) by applying the procedure described in [8].

Figure 1 shows the numerically determined energy spectra of spin waves in a thin film of thickness L = 5 ML and exchange constant $2SJ$ = 36 meV. The spectra corresponding to the fcc and the bcc structures are shown in Figs. 1a, b, respectively. Both spectra were calculated for surface cut (110), along the characteristic path in the respective 2D Brillouin zone (see the inset in each plot). The solid lines represent the energy of individual modes, and the shaded area denotes the hypothetical band region. In both the fcc(110) and the bcc(110) structures the Brilloun zone features regions in which the two lowest modes are of surface nature (see Fig. 1c). In the fcc(110) structure, the second surface mode appears between points Δ and X to vanish between Y and Σ; in the bcc(110) structure, the second surface mode appears in the vicinity of point C to vanish around point Σ. Indicated in Figure 1, the lowest surface mode energy values are 310 meV and 216 meV in the fcc(110) and bcc(110) structures, respectively. These values exactly correspond to the position of the peaks in the SPEEL asymmetry spectra obtained in the above-discussed experiment. Note also that in both structures zero-dispersion regions, i.e. those in which the spin wave energy is independent of the wave vector value, are found in the Brillouin zone: region X-S in fcc(110) and region D-Y in bcc(110). Therefore, we suggest the occurrence of two non-dispersive peaks in the SPEEL asymmetry spectrum might be due to excitation of two surface spin-wave modes associated with the fcc and the bcc structures.

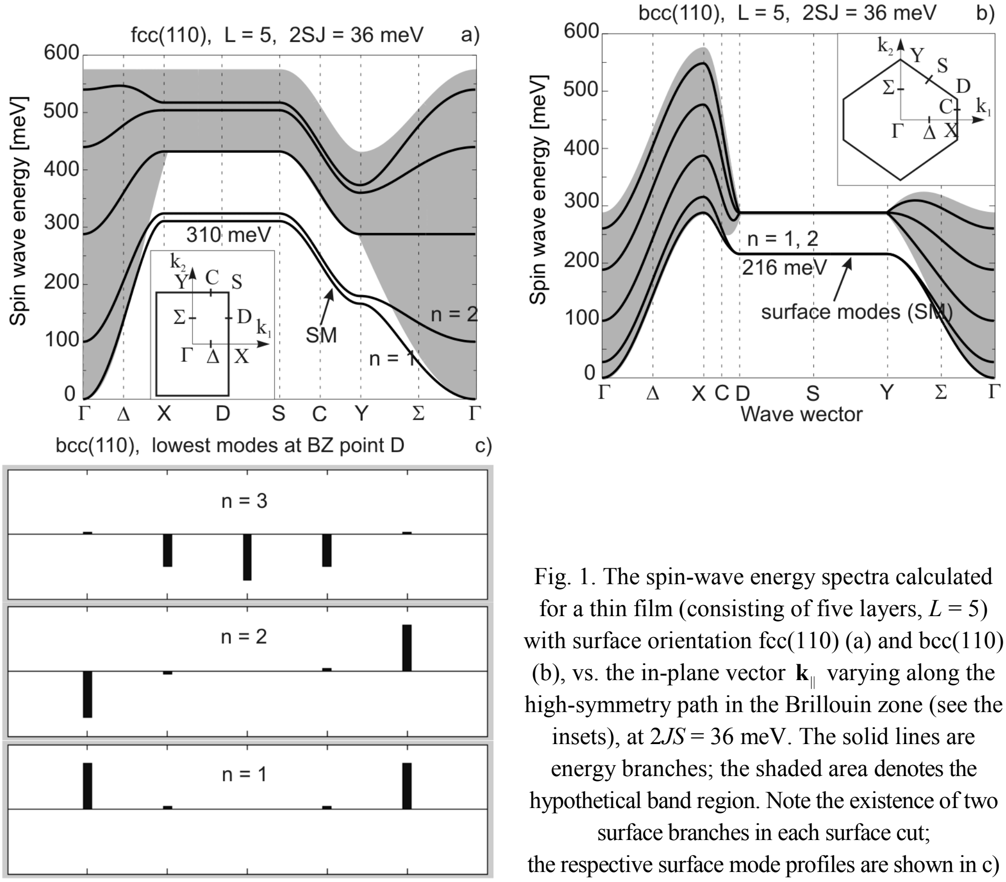

Fig. 1. The spin-wave energy spectra calculated for a thin film (consisting of five layers, $L = 5$) with surface orientation fcc(110) (a) and bcc(110) (b), vs. the in-plane vector $\mathbf{k}_{\|}$ varying along the high-symmetry path in the Brillouin zone (see the insets), at $2JS = 36$ meV. The solid lines are energy branches; the shaded area denotes the hypothetical band region. Note the existence of two surface branches in each surface cut; the respective surface mode profiles are shown in c)

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