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Theory of Spin-Polarized Auger Electrons from Ferromagnetic Materials

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Our previous theory of spin-polarized $L_{23}M_{23}M_{23}$ Auger electrons from ferromagnetic materials is improved by taking account of the life time broadening Γ_i in the Auger initial state and the spin-orbit interaction in the 2p state. Experimental data of Auger electrons from $Fe_{83}B_{17}$ are re-analysed by using revised parameter values for the exchange interactions (the exchange constant J_2 between 3d and 2p spins and J_3 between 3d and 3p spins), which are essentially important in the spin polarization of Auger electrons. It is shown that the effect of J_2 is strongly affected by Γ_i. A possibility of another mechanism for the spin polarization is also discussed.

§1. Introduction

Spin-polarized Auger electron spectroscopy is a newly developing field in the study of magnetic materials. The spin polarization of Auger electrons from ferromagnetic samples is expected to provide us with important information on the spin-dependent electronic states and their interactions in the material. Mainly due to technical problems, however, precise experimental data were not obtained until quite recently. The first successful observation of spin-polarized LMM and MMM Auger electrons has recently been made by Landolt and Mauri[1,2] by using a ferromagnetic glass sample of $Fe_{83}B_{17}$. According to their results, the $M_{23}M_{45}M_{45}$ Auger electrons, as well as $L_3M_{45}M_{45}$ and $L_3M_{23}M_{45}$ Auger electrons, exhibit the *positive* spin polarization, where the positive spin polarization means that the Auger electron spin polarization is parallel to the ferromagnetic spin direction. Since these transition processes include the 3d electron transition, the observed spin polarization can be interpreted,[3] at least qualitatively, as originating from the exchange splitting of the 3d band of Fe. For the $L_3M_{23}M_{23}$ Auger electrons, on the other hand, Landolt and Mauri observed two considerably large peaks of spin polarization of the order of $\pm 10\%$, although this Auger process does not include directly the 3d electron transition. The positive and negative spin polarization peaks are located at the Auger electron kinetic energies corresponding to the singlet and triplet final states of the 3p hole pair, respectively.

For the mechanism of the spin polarization of $L_3M_{23}M_{23}$ Auger electrons, Bennemann[3] proposed an interpretation based on the multiplicities of the 3d electron and core hole spins. In his theory, however, the role of the ferromagnetic ordering of the 3d spins, which should be responsible for the spin polarization of the Auger electron, is not clearly shown. Recently, the present authors[4,5] presented a model in order to explain the experimental data. Reference 4 is referred to hereafter as I. In I, the 3d spins were approximated by well-localized spins with the magnitude $S^{3d}=1$, and their ferromagnetic ordering was treated by the molecular field approximation. The exchange interactions between 3p spins, between 3d and 3p spins, and between 3d and 2p spins, were shown to be important in the spin polarization of the $L_{23}M_{23}M_{23}$ Auger electrons. In this theory, however, the effect of the life time of the 2p hole in the initial state of the Auger transition was not taken into account. The spin-orbit couplig in the 2p state and the orbital contribution to the multiplets of the two 3p holes were also disregarded, for

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simplicity. The purpose of the present paper is to improve our previous theory I, and also to consider another mechanism which may affect the spin polarization.

In §2 and 3 we improve our model by taking accout of the life time effect of the 2p hole. Furthermore, the spin-orbit interaction in the 2p state and the orbital effect on the multiplets of two 3p holes are considered in §4. In §5 we investigate a possibility of another mechanism. Section 6 is devoted to the discussion.

§2. Formulation

We consider a system which consists of the 2p, 3p, 3d electrons and an incident primary electron. In the initial state of the $L_3M_{23}M_{23}$ Auger transition, a $2p_{3/2}$ hole is created by the Coulomb interaction V_p between the primary electron and the 2p electron. We call this state *Auger initial state.* By the $L_3M_{23}M_{23}$ Auger interaction V_A, the system goes to the final state which contains two 3p holes and an Auger electron. We call this state *Auger final state.* We describe the Hamiltonian of the system in the Auger initial state and that in the Auger final state as H_i and H_f, and denote their eigenvalues and eigenstates, respectively, as E_i, $|i>$ and E_f, $|f>$. When the primary electron has the energy $\varepsilon_{n_pk_p}$ and the spin σ_p, where n_p is the band index and $\boldsymbol{k}_p$ is the wave vector, the number of emitted Auger electron N_A is expressed as follows:

$$N_A=\sum_f \left| \sum_i \frac{\langle f|V_A|i\rangle\langle i|V_p a^+_{n_p,k_p,\sigma_p}|0\rangle}{E_0+\varepsilon_{n_pk_p}-E_i+i\Gamma_i/2} \right|^2 \times \frac{\Gamma_f/2\pi}{(E_0+\varepsilon_{n_pk_p}-E_f)^2+(\Gamma_f/2)^2}, \quad (2.1)$$

where $|0>$ is the ground state of the system consisting of the 2p, 3p and 3d electrons (excluding the primary electron), E_0 is the energy of $|0>$, Γ_i and Γ_f represent, respectively, the energy widths of the Auger initial state and the Auger final state. Here, Γ_i is mainly due to the L_3MM Auger decay (the life time effect of the 2p hole) and Γ_f is due to the $M_{23}M_{45}M_{45}$ Auger decay (the life time effect of the 3d hole pair), although the effect of a finite experimental resolution is also included effectively in Γ_f.

In this section, we formulate the Auger electron spectrum with the same model as that in I except for the existence of Γ_i. The model is shown in Fig. 1. The 3d states are approximately treated as localized spins with the magnitude $S^{3d}=1$, and the interaction between the localized 3d spins is taken into account by the molecular field approximation. The 3d spin is assumed to couple with the 2p hole spin by the exchange interaction J_2 in the Auger initial state, and with the 3p hole spin by the exchange interaction J_3 in the Auger final state. Furthermore, the 3p hole pair is assumed to couple each other by the exchange interaction J_0. Here, we disregard the spin-orbit interaction in the 2p state and the orbital contribution to the multiplets of the two 3p holes, but their effects will be studied in §4.

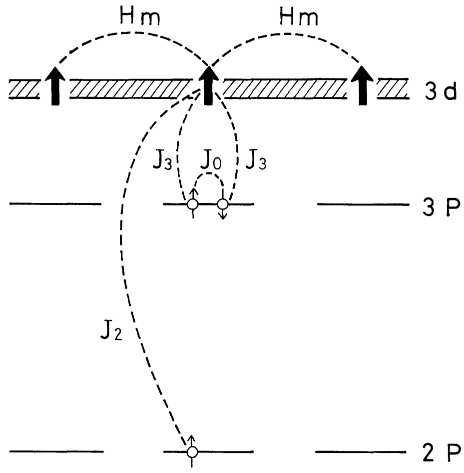

Fig. 1. Schematic representation of our model system.

The state $|0>$ is expressed as

$$|0\rangle=|1,1\rangle|g\rangle, \quad (2.2)$$

where $|1, 1>$ and $|g>$ represent, respectively, the 3d spin state $|S^{3d}=1, S^{3d}_z=1>$ and the stae where all the 2p and 3p levels are occupied. Here and hereafter, we describe explicitely the 2p, 3p and 3d states only on the single atomic site at which the 2p hole is created by the primary electron, since the Auger transition is an essentially intraatomic process. The energy E_0 is given by

$$E_0=E_g-H_m,$$

where E_g is the energy of the state $|g>$ and H_m is the molecular field acting on the 3d spin under consideration.

When we assume that the two electrons (n_1, $\boldsymbol{k}_1$, σ_1) and (n_2, $\boldsymbol{k}_2$, σ_2) are created by the scattering between the primary electron and a 2p electron through $V_{\rm p}$, the Hamiltonian of the Auger initial state is expressed as

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$$H_{\rm i}=E_{\rm g}-\varepsilon_{\rm 2p}+\varepsilon_{n_1k_1}+\varepsilon_{n_2k_2}-H_{\rm m}S_z^{\rm 3d}-J_2\boldsymbol{S}^{\rm 3d}\cdot\boldsymbol{s}^{\rm 2p}. \tag{2.3}$$

Here, $\varepsilon_{\rm 2p}$ is the 2p core level and $\boldsymbol{s}^{\rm 2p}$ is the 2p hole spin, where the direction of $\boldsymbol{s}^{\rm 2p}$ is taken in the opposite direction to that of the removed 2p electron. The eigenstates of $H_{\rm i}$ can easily be obtained as linear combinations of the following basis functions:

$$|n_1\boldsymbol{k}_1\sigma_1,\ n_2\boldsymbol{k}_2\sigma_2;\ {\rm 2p}m\sigma;\ S_z^{\rm 3d}\rangle=a^+_{n_1,k_1,\sigma_1}a^+_{n_2,k_2,\sigma_2}a_{{\rm 2p},-m,-\sigma}|1,\ S_z^{\rm 3d}\rangle|g\rangle. \tag{2.4}$$

On the other hand, the Hamiltonian of the Auger final state is given by

$$H_{\rm f}=E_{\rm g}-2\varepsilon_{\rm 3p}+\varepsilon_{n_1k_1}+\varepsilon_{n_2k_2}+\varepsilon-H_{\rm m}S_z^{\rm 3d}-J_3\boldsymbol{S}^{\rm 3d}\cdot(\boldsymbol{s}_1^{\rm 3p}+\boldsymbol{s}_2^{\rm 3p})-J_0\boldsymbol{s}_1^{\rm 3p}\cdot\boldsymbol{s}_2^{\rm 3p}, \tag{2.5}$$

where $\varepsilon_{\rm 3p}$ is the 3p level, ε is the kinetic energy of the Auger electron, and $\boldsymbol{s}_1^{\rm 3p}$ and $\boldsymbol{s}_2^{\rm 3p}$ are the spins of the 3p holes. We can diagonalize $H_{\rm f}$ by using the linear combination of the basis functions

$$|n_1\boldsymbol{k}_1\sigma_1,\ n_2\boldsymbol{k}_2\sigma_2,\ \varepsilon{\rm p}m\sigma;\ L^{\rm 3p}L_z^{\rm 3p},\ S^{\rm 3p}S_z^{\rm 3p};\ S_z^{\rm 3d}\rangle=a^+_{n_1,k_1,\sigma_1}a^+_{n_2,k_2,\sigma_2}a^+_{\varepsilon{\rm p},m,\sigma}|L^{\rm 3p}L_z^{\rm 3p},\ S^{\rm 3p}S_z^{\rm 3p}\rangle|1,\ S_z^{\rm 3d}\rangle, \tag{2.6}$$

where

$$|L^{\rm 3p}L_z^{\rm 3p},\ S^{\rm 3p}S_z^{\rm 3p}\rangle=\frac{1}{\sqrt{2}}\sum_{m_1m_2}\sum_{\sigma_1\sigma_2}\langle 1m_1 1m_2|L^{\rm 3p}L_z^{\rm 3p}\rangle\left\langle\frac{1}{2}\,\sigma_1\,\frac{1}{2}\,\sigma_2\right|S^{\rm 3p}S_z^{\rm 3p}\Big\rangle a_{{\rm 3p},-m_1,-\sigma_1}a_{{\rm 3p},-m_2,-\sigma_2}|g\rangle, \tag{2.7}$$

where $\langle 1m_1 1m_2|L^{\rm 3p}L_z^{\rm 3p}\rangle$ and $\langle 1/2\ \sigma_1 1/2\ \sigma_2|S^{\rm 3p}S_z^{\rm 3p}\rangle$ are the Clebsch-Gordan coefficients.

We approximately write $V_{\rm p}$ and $V_{\rm A}$ as follows:

$$V_{\rm p}=v_{\rm p}\sum_{n_1n_2}\sum_{k_1k_2}\sum_{m\sigma_2}a^+_{n_1,k_1,\sigma_{\rm p}}a^+_{n_2,k_2,\sigma_2}a_{{\rm 2p},m,\sigma_2}a_{n_{\rm p},k_{\rm p},\sigma_{\rm p}}, \tag{2.8}$$

and

$$V_{\rm A}=\sum_{\varepsilon\sigma}V_{{\rm A}\sigma}(\varepsilon),$$

with

$$V_{{\rm A}\sigma}(\varepsilon)=v_{\rm A}\sum_{mm'\sigma'}a^+_{\varepsilon{\rm p},m,\sigma}a^+_{{\rm 2p},m',\sigma'}a_{{\rm 3p},m',\sigma'}a_{{\rm 3p},m,\sigma}, \tag{2.9}$$

where $v_{\rm p}$ and $v_{\rm A}$ are assumed to be constant. When the primary electron is not spin-polarized, the number of the Auger electrons with energy ε and spin σ is expressed as

$$N_\sigma(\varepsilon)=\frac{1}{2}\sum_{\sigma_{\rm p}}\sum_{f}\left|\sum_{i}\frac{\langle f|V_{{\rm A}\sigma}(\varepsilon)|i\rangle\langle i|V_{\rm p}a^+_{n_{\rm p},k_{\rm p},\sigma_{\rm p}}|0\rangle}{E_0+\varepsilon_{n_{\rm p}k_{\rm p}}-E_{\rm i}+{\rm i}\Gamma_{\rm i}/2}\right|^2\frac{\Gamma_{\rm f}/2\pi}{(E_0+\varepsilon_{n_{\rm p}k_{\rm p}}-E_{\rm f})^2+(\Gamma_{\rm f}/2)^2}. \tag{2.10}$$

Then the intensity and the spin polarization of the Auger electrons with energy ε are given by

$$I(\varepsilon)=N_\uparrow(\varepsilon)+N_\downarrow(\varepsilon), \tag{2.11}$$

$$P(\varepsilon)=\frac{N_\uparrow(\varepsilon)-N_\downarrow(\varepsilon)}{N_\uparrow(\varepsilon)+N_\downarrow(\varepsilon)}. \tag{2.12}$$

The expression (2.10) of $N_\sigma(\varepsilon)$ can easily be extended to the case of finite temperature by replacing $|0>$ and E_0 as $|1,\ S^{\rm 3d}>|g>$ and $E_g-S_z^{\rm 3d}H_m(T)$, respectively, and by taking the ensemble average over $S_z^{\rm 3d}$. Here, $H_{\rm m}(T)$ is the molecular field at temperature T, whose expression is given in I.

We have assumed in I that the 2p holes with ↑ and ↓ spins are created with equal probability by the spin-unpolarized primary electron (except for the spin-flip effect by J_2). This is directly followed when we assume that the density of states of the excited state $(n, \boldsymbol{k}, \sigma)$ [see eq. (2.4)] is independent of the spin σ. On this assumption our calculation in §3 and 4 will also be made, but a consideration beyond this assumption will be given in §5.

§3. Numerical Calculations

Our model includes six parameters J_0, J_2, J_3, H_m, Γ_i and Γ_f, and they are estimated as follows: The value of H_m at zero temperature is estimated to be 0.135 eV by using the Curie temperature $T_c=1042$ K of pure iron and J_0 is estimated to be 6.5 eV from the experimental peak separation in $I(\varepsilon)$. For convenience, we show in Fig. 2 the experimental spectra, which exhibit two main peaks in $I(\varepsilon)$ and a positive and a nagative peaks of the order of $\pm 10\%$ in $P(\varepsilon)$. (The hatched region represents the uncertainty coming from different estimations of the backgroud, as well as the statistical error in experiments.) The value of the width Γ_f is estimated to be 6.0 eV from the experimental spectral width. For the value of the width Γ_i, we use a theoretical result $\Gamma_i=0.36$ eV obtained by Krause and Oliver.[6] Reference 6 is referred to hereafter as KO. Finally we estimate $J_2=0.14$ eV and $J_3=0.5$ eV so that the largest values of $P(\varepsilon)$ become of the order of $\pm 10\%$.

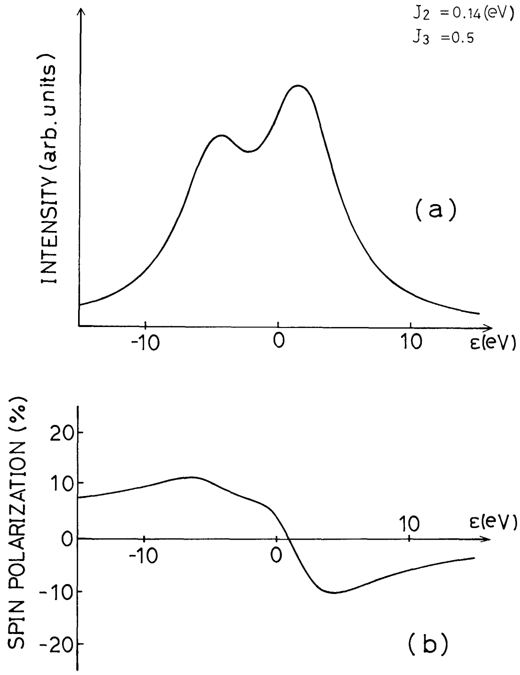

Fig. 3. Intensity (a) and spin polarization (b) calculated by using $J_0=6.5$ eV, $J_2=0.14$ eV, $J_3=0.5$ eV, $\Gamma_i=0.36$ eV, $\Gamma_f=6.0$ eV and $S^{3d}=1$.

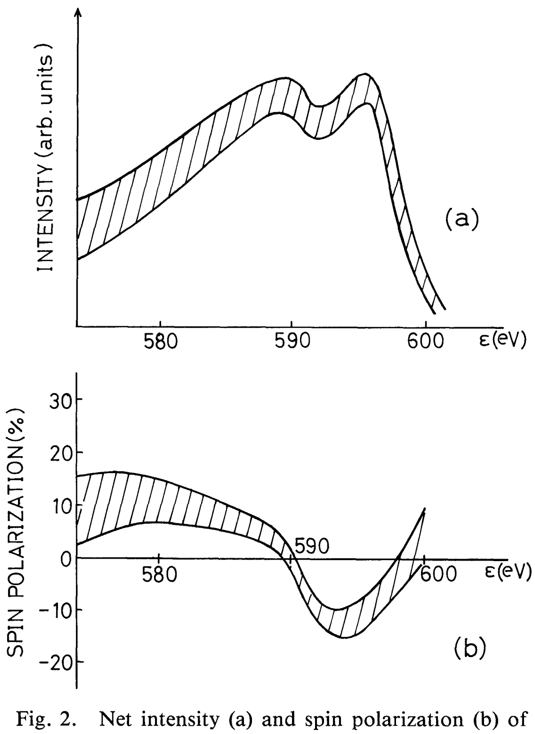

Fig. 2. Net intensity (a) and spin polarization (b) of $L_3M_{23}M_{23}$ Auger electrons from $Fe_{83}B_{17}$. These are obtained from the experimental data[1] by subtracting the background.

The results for $I(\varepsilon)$ and $P(\varepsilon)$ are shown in Fig. 3, where ε is measured with $2\varepsilon_{3p}-\varepsilon_{2p}-\varepsilon_{vac}$ (ε_{vac} being the vacuum level) as origin. When we consider several simplifying assumptions in our theory and the large uncertainty range in the experimental data, these results are found to agree satisfactorily with the experimetal data in Fig. 2. As we investigated in I, both effects of the exchange interactions J_2 and J_3 are essentially important in the spin polarization. The exchange interaction J_3 in the final state affects only the 3p spin triplet final state and gives a positive peak and a negative peak of spin polarization as shown in Fig. 4(a), where J_3 is varied with vanishing J_2. Through the exchange interaction J_3, the 3p spin triplet

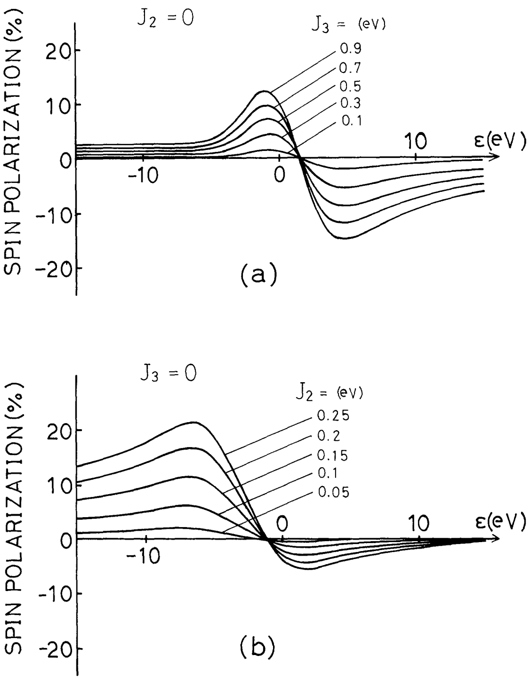

Fig. 4. Spin polarization calculated for various values of J_3 with vanishing J_2 in (a), and for various values of J_2 with vanishing J_3 in (b). Other parameters are taken as J_0= 6.5 eV, Γ_i=0.36 eV and Γ_f=6.0 eV.

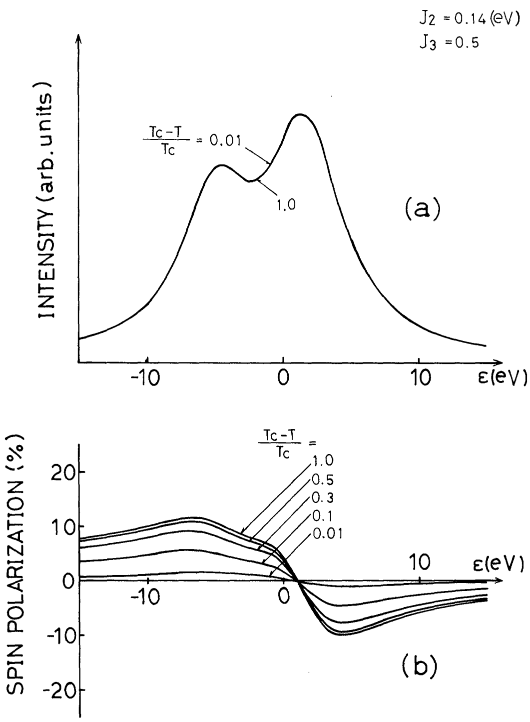

Fig. 5. Temperature variation of the intensity (a) and the spin polarization (b). Parameters are the same as those in Fig. 3.

final state splits into the 3p-3d quintet (around $\varepsilon\sim5.8$ eV), triplet (around $\varepsilon\sim4.8$ eV) and singlet (around $\varepsilon\sim4.3$ eV) final states. The 3p-3d quintet final state gives the negative spin polarization and the 3p-3d triplet and singlet final states give the positive spin polarization. The negative peak of the experimental spin polarization is considered to originate mainly from the 3p-3d quinted final state.

On the other hand, through the exchange interaction J_2, the 3p singlet final state gives the large positive spin polarization and the triplet final state gives only the small negative spin polarization as shown in Fig. 4(b), where J_2 is varied with vanishing J_3. The off-diagonal term of the 3d-2p exchange interaction is written as $(J_2/2)\ (S^{3d}_+ s^{2p}_- + S^{3d}_- s^{2p}_+)$, by which the ↓ spin of the 2p hole can flip to the ↑ spin with the simultaneous flip of the 3d spin from $S^{3d}_z=1$ to 0, but the ↑ spin cannot flip at zero temperature. Thus the probability of the 2p hole having ↑ spin is more than that of the 2p hole having ↓ spin. By this spin flip mechanism, the 3p singlet and triplet final states give, respectively, the large positive and small negative spin polarizations. The positive peak of the experimental spin polarization is considered to originate mainly from the 3p singlet final state. The positive peak coming from J_3 is considered not to be resolved from that coming from J_2 because of the broadening Γ_f.

Next, we calculate the temperature variation of $I(\varepsilon)$ and $P(\varepsilon)$, and the results are shown in Fig. 5. The spin polarization $P(\varepsilon)$ decreases monotonically to zero when the temperature approaches T_c and this fact can easily be understood because we attribute the spin polarization to the exchange interaction between an average magnetic moment (i.e., ferromagnetic moment) of the 3d spin and core hole spins.

Instead of $S^{3d}=1$ which corresponds to the Bohr magneton number $n_B=2.0$, we also calculate $I(\varepsilon)$ and $P(\varepsilon)$ at zero temperature by using $S^{3d}=3/2$ (i.e., $n_B=3.0$). Since the Bohr magneton number of iron, n_B(Fe), is not exactly 2.0 [n_B(Fe)$\sim$2.2 in pure iron], it is con-

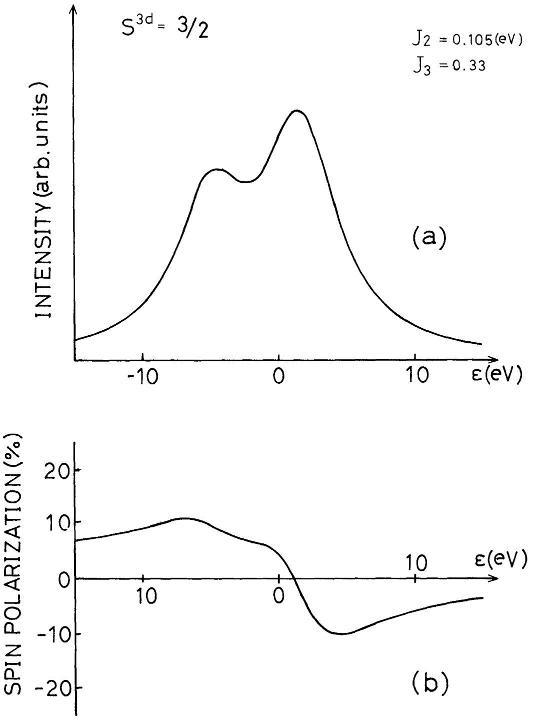

Fig. 6. Calculated results of the intensity (a) and the spin polarization (b) similar to Fig. 3, but with $S^{3d}=3/2$, $J_2=0.105$ eV and $J_3=0.33$ eV.

sidered that the calculation of the spin polarization with $S^{3d}=3/2$ is necessary in order to check the propriety of our model. The results are shown in Fig. 6 and we can obtain much the same results as those in Fig. 3 only by reducing the exchange interactions to $J_2=0.105$ eV and $J_3=0.33$ eV so as to compensate for the increase of S^{3d}.

For the energy width of the Auger initial state, we have so far used the theoretical value $\Gamma_i=0.36$ eV which is given by KO. Here we investigate the effect of the variation of Γ_i to the spin polarization. In the limit of $\Gamma_i\to 0$, eq. (2.10) reduces to the following simplified expression:

$$N_\sigma(\varepsilon)=\frac{1}{2}\sum_{\sigma_p}\sum_{f}\sum_{i}|\langle f|V_{A\sigma}(\varepsilon)|i\rangle \times\langle i|V_p a^{+}_{n_p,k_p,\sigma_p}|0\rangle|^2 \times\frac{\Gamma_f/2\pi}{(E_i-E_f)^2+(\Gamma_f/2)^2}, \quad (3.1)$$

which corresponds to the expression that we used in I. Figure 7 shows the spin polarization

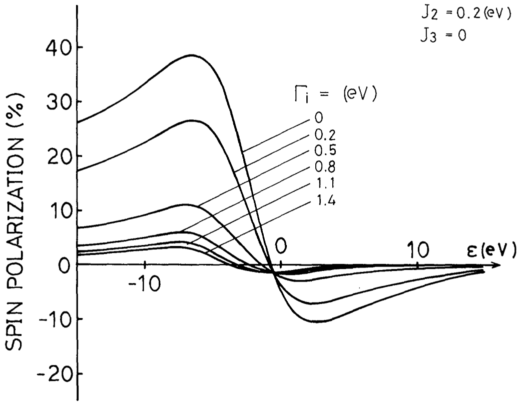

Fig. 7. Spin polarization calculated for various values of Γ_i with $J_0=6.5$ eV, $J_2=0.2$ eV, $J_3=0$, $\Gamma_f=6.0$ eV and $S^{3d}=1$ at zero temperature.

calculated for various values of Γ_i with $J_2=0.2$ eV and $J_3=0$ (the contribution of J_3 to the spin polarization being not affected by Γ_i). With $\Gamma_i=0$, the 3p singlet final state gives the positive spin polarization of about 40%. However, the spin polarization decreases rapidly with increasing Γ_i. The magnitude of Γ_i represents the strength of the Auger decay of the 2p hole, and thus the decrease of the spin polarization with increasing Γ_i signifies that the Auger transition occurs before the 2p hole spin flips due to the exchange interaction J_2. For the value of Γ_i, a theoretical estimation of $\Gamma_i\sim 1.3$ eV, which is much larger than that by KO, has also been reported by Chen *et al.*[7] If we use this value of Γ_i, we must take a much larger value of J_2 in order to reproduce the experimental result. In this connection, some disccusion will be given in §6.

§4. Effect of Spin-Orbit Interaction in the 2p State

In this section we improve our model by taking account of the spin-orbit interaction in the 2p state. In the expression (2.3) of the Hamiltonian H_i, ε_{2p} is replaced by

$$\varepsilon_{2p}+\lambda \boldsymbol{l}\cdot \boldsymbol{s}^{2p}, \quad (4.1)$$

where λ is the spin-orbit coupling constant and l is the orbital angular momentum of the 2p hole. Then the 2p level splits into $2p_{3/2}$ and $2p_{1/2}$ levels, so that the $L_{23}M_{23}M_{23}$ Auger Spectrum also splits into $L_3M_{23}M_{23}$ and $L_2M_{23}M_{23}$ Auger spectra. Experimentally, the $L_2M_{23}M_{23}$

Auger intensity is very weak because of the decay of the $2p_{1/2}$ hole into the $2p_{3/2}$ hole, so that its spectral structure is not observed clearly. Therefore, we also confine our calculation to the $L_3M_{23}M_{23}$ Auger process. Since the value of $\lambda(\sim 20\text{ eV})$ is much larger than Γ_i and J_2, the total angular momentum of the 2p hole, j^{2p}, is a good quantum number, and H_i is diagonalized by using the basis functions

$$|n_1k_1\sigma_1, n_2k_2\sigma_2; 2p j^{2p} j_z^{2p}; S_z^{3d}\rangle = a^+_{n_1,k_1,\sigma_1} a^+_{n_2,k_2,\sigma_2} \sum_{m\sigma} \langle 1m \frac{1}{2}\sigma | j^{2p} j_z^{2p}\rangle a_{2p,-m,-\sigma} |1, S_z^{3d}\rangle |g\rangle, \quad (4.2)$$

instead of eq. (2.4). In eq. (4.2), $\langle 1m1/2\sigma| j^{2p}j_z^{2p}\rangle$ is the Clebsch-Gordan coefficient (j^{2p} being taken as 3/2).

In the Auger final state, we also take account of the orbital contribution to the L-S term energy of the 3p hole pair. Then, in the expression (2.5) of the Hamiltonian H_f, the exchange coupling term $-J_0 s_1^{3p}\cdot s_2^{3p}$ is replaced by the L-S term energy $E(L^{3p}, S^{3p})$. For the multiplets ^{1}S. ^{1}D and ^{3}P which are represented by the eigenstates (2.6), the L-S term energy E takes the following values:

$$E(^1S)=F_0+10F_2,$$
$$E(^1D)=F_0+F_2,$$
$$E(^3P)=F_0-5F_2,$$

where F_0 and F_2 are the Coulomb integrals for the 3p hole pair.

The eigenvalues and eigenstates of H_i and H_f thus obtained are substituted into eqs. (2.10)-(2.12), and the calculated results are shown in Fig. 8, where ε is measured with $2\varepsilon_{3p}-(\varepsilon_{2p}+\lambda/2)+F_0-\varepsilon_{vac}$ as origin. In this calculation, the value of F_2 is chosen as 1.07 eV from the experimental peak separation in $I(\varepsilon)$, and J_2 and J_3 are taken to be 0.35 eV and 0.6 eV, respectively. The other quantities Γ_i, Γ_f, H_m and S^{3d} are fixed to be the same values as those used in the calculation of Fig. 3.

In Fig. 8, the two main peaks in $I(\varepsilon)$ correspond to ^{3}P and ^{1}D final states, and a new small peak at $\varepsilon\sim -10$ eV (which in not observed clearly in experimental data) corresponds to the ^{1}S final state. The essential results of the present calculation are found to be almost unchanged from those of Fig. 3 except the difference in the estimated value of J_2, and the agreement of the calculated spectra with experimental data is still statisfactory. For the value of J_2, we find that in order to obtain the positive spin polarization of the order of 10% we have to take $J_2\sim 0.35$ eV, which is considerably larger than the previous value 0.14 in Fig. 3. This result comes from that the spin flip of the 2p hole due to the exchange interaction J_2 is partly compensated by the spin flip

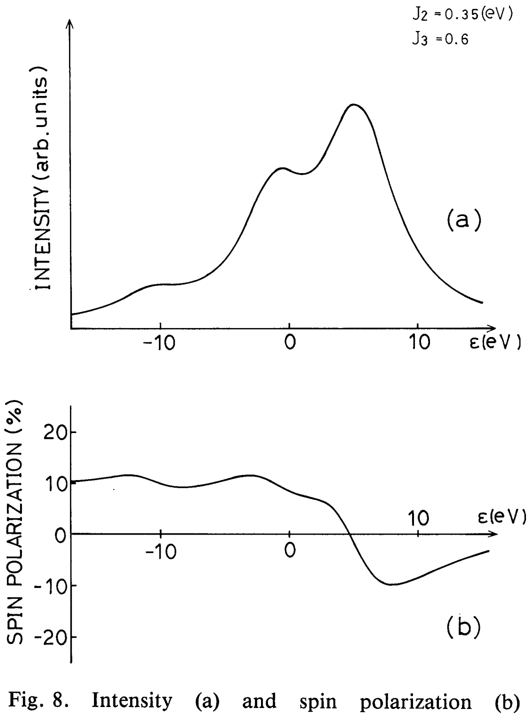

Fig. 8. Intensity (a) and spin polarization (b) calculated at zero temperature by taking account of the spin-orbit interaction in the 2p state. Parameters are taken as $F_2=1.07$ eV, $J_2=0.35$ eV, $J_3=0.6$ eV, $\Gamma_i=0.36$ eV, $\Gamma_f=6.0$ eV and $S^{3d}=1$.

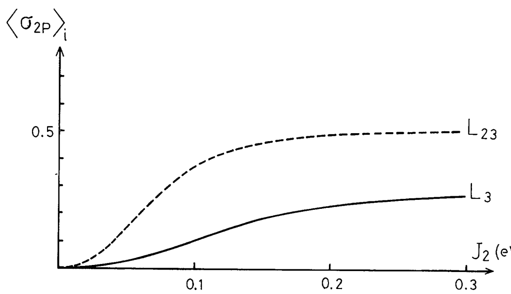

Fig. 9. The quantity $\langle\sigma_{2p}\rangle_i$ calculated with the spin-orbit interaction (solid curve) and without the spin-orbit interaction (dashed curve).

due to the off-diagonal part of the spin-orbit interaction $(\lambda/2)(l_+s_-^{2p}+l_-s_+^{2p})$. To see this effect, we calculate the following quantity:

$$\langle\sigma_{2p}\rangle_i=2\sum_{i\sigma_p}\langle i|S_z^{2p}|i\rangle|\langle i|V_p a^+_{n_p,k_p,\sigma_p}|0\rangle|^2$$
$$/\sum_{i\sigma_p}|\langle i|V_p a^+_{n_p,k_p,\sigma_p}|0\rangle|^2, \qquad (4.3)$$

which represents the average value of the z-component of the 2p hole spin in the Auger initial state (where Γ_i is taken to be 0) at zero temperature. The result is shown in Fig. 9, where the solid (L_3) and dashed (L_{23}) curves represent the results obtained with and without the spin-orbit interaction, respectively. We can find that the spin-orbit interaction suppresses the increase of $\langle\sigma_{2p}\rangle_i$ due to the exchange interaction J_2.

§5. Possibility of Another Mechanism

We have so far assumed that the density of states of the electronic state $(n, \boldsymbol{k}, \sigma)$ to which the 2p electron is excited by the primary electron is independent of the spin σ. However, this assumption is not valid when the 2p electron is excited to the 3d band, which has the exchange splitting in the ferromagnetic state. In this case the excitation of the 2p electron with ↓ spin to the 3d band with ↓ spin (i.e., the minority spin) can occur more strongly than that of the 2p↑ electron to the 3d↑ band, because the 3d↓ band has more unoccupied states than the 3d↑ band. Therefore, the 2p hole spin can be polarized in the Auger initial state, and we expect to have Auger electron spin polarization even when the exchange interactions J_2 and J_3 are absent.[2)]

Since the 2p electron can be excited both to the 3d band and the other bands which have no exchange splitting, we define the quantity r by

$$r=\frac{T_{3d\downarrow}-T_{3d\uparrow}}{T_{tot}}, \qquad (5.1)$$

where $T_{3d\sigma}$ is the transition probability of the 2p electron (with σ spin) to the 3d band with σ spin, and T_{tot} is the total transition probability of the 2p electron (with ↑ and ↓ spins). With the value of r as a parameter, we calculate $P(\varepsilon)$ from eqs. (2.10) and (2.12) by disregarding the exchange interactions J_2 and J_3. The quantities

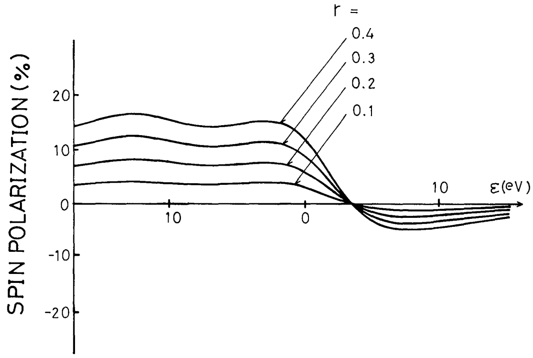

Fig. 10. Spin polarization calculated for various values of r at zero temperature. Parameters are taken as $J_2=J_3=0$, $\Gamma_i=1.4$ eV and $\Gamma_f=6.0$ eV.

Γ_i and Γ_f and taken as 1.4 eV and 6.0 eV, respectively, and the spin-orbit interaction in the 2p state is taken into account. The result is shown in Fig. 10. By this 2p→3d excitation mechanism, the singlet final state contributes to the positive spin polarization while the triplet final state contributes only the small negative spin polarization. These spin polarizations increase with increasing r. As found from comparison between Fig. 10 and Fig. 4(b), the effect of r is similar to that of J_2. This is because both of r and J_2 cause the spin polarization of the 2p hole in the Auger initial state, which is the origin of the Auger electron spin polarization.

As shown here, we can generally say that for the positive spin polarization of the singlet final state there coexist two mechanisms coming from r and J_2. The value of r is proportional to the exchange splitting of the 3d band, as well as to the density of states of the 3d band. Further, it depends on the kinetic energy of the incident primary electron ε_{pr}; r is very large when ε_{pr} is close to the binding energy of the 2p electron, but r decreases with increasing ε_{pr}. In the experiment by Landolt and Mauri,[1)] ε_{pr} is taken as 2900 eV, which is much larger than the 2p binding energy, so that the value of r will be very small (presumably smaller than 0.1). Thus we expect that the contribution of J_2 is much larger than that of the 2p→3d excitation mechanism.

§6. Discussion

In this paper, we have extended our

previous theory I by taking account of the life time broadening Γ_i in the Auger initial state, the spin-orbit interaciton in the 2p state, and so on. In I, we estimated the exchange interactions $J_3=0.5$ eV and $J_2=0.05$ eV from the analysis of the Auger electron spin polarization $P(\varepsilon)$. The value of J_3 is estimated from the analysis of the negative peak of $P(\varepsilon)$, which is not much modified in the present improved theory, and we conclude that J_3 is $0.5\sim0.6$ eV. However, the positive peak of $P(\varepsilon)$, from which the value of J_2 is estimated, is found to be very much sensitive to Γ_i. It is also found that the spin-orbit interaction in the 2p state tends to suppress the effect of J_2. Thus we have revised the previous estimation of J_2; by assuming $\Gamma_i=0.36$ eV, which was given by KO, we have obtained $J_2=0.35$ eV. This estimation seems to be reasonable as mentioned below.

Experiments of the L_3 X-ray photoelectron spectroscopy (XPS) provide us with some information on Γ_i and J_2. Fuggle and Alvarado[8] studied systematically the experimental line width of L_1, L_2 and L_3 XPS for various elements with atomic number $Z=10\sim35$. They found that the observed line width is in considerable agreement with the theoretical result by KO, but in transition metals the experimental value is much larger than the theoretical one. They interpreted the origin of this anomalous line broadening in transition metals as the exchange coupling between the 3d and core hole spins. For the L_3 XPS of iron, the difference between the experimental and theoretical line width is about 0.4 eV, which is consistent with our value $J_2=0.35$ eV.

Theoretical calculations of the 3d-2p and 3d-3p multiplet splitting in iron have been made only for the free atom, but no estimation has been made for the metallic system. We obtain the following theoretical estimation for J_2 and J_3 for the free atom of iron:

$$J_2\sim0.8 \text{ eV and } J_3\sim3.2 \text{ eV},$$

by using the exchange integrals[9] $G^1(n\text{p}, 3\text{d})$ and $G^3(n\text{p}, 3\text{d})$ with $n=2$ and 3, and by averaging the energy separation between spin singlet and triplet states over the P, D and F orbital states. In the metallic system, these values are reduced by the larger extension of the 3d wave function, as well as by the screening effect due to conduction electrons. However, the ratio J_3/J_2 will not be very much modified. In our estimation, the value of J_3/J_2 is smaller than this atomic value, but seems to be situated within a reasonable range.

Although our estimation $J_2\sim0.35$ eV and $J_3\sim0.6$ eV with $\Gamma_i\sim0.36$ eV is considered to be most reasonable, we cannot completely exclude the possibility of different estimation. The value of Γ_i does not seem to be very well established. For instance, Chen *et al.*[7] obtained a theoretical value about 1.3 eV. As we have shown in §3, the estimation of J_2 depends strongly on what value is assumed for Γ_i. Furthermore, the 2p→3d excitation mechanism coexists with the mechanism of the exchange interaction J_2 for the positive spin polarization of the singlet final state. As we have mentioned in §5, the exchange interaction mechanism is expected to be predominant in the experiment by Landolt and Mauri,[1] but there exists some ambiguity because it is difficult to estimate theoretically the precise value of r. Since the value of r depends on the energy of the primary electron, ε_{pr}, it is very interesting to compare the experimental data with different values of ε_{pr}. Moreover, if the spin-polarized Auger measurement becomes possible to be made with the 2p electron excitation by the monochromatic light, the effects of the two mechanisms will be able to be measured separately.

Very recently, Landolt *et al.*[2] have also observed the spin polarized Auger electrons from ferromagnetic nickel, and its analysis is an interesting problem left in future investigations.

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