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Abstract. The diagonal and off-diagonal elements of the optical conductivity tensors of ferromagnetic Ni, Co and Fe have been calculated using the direct interband transition model from the self-consistent spin-polarized band structures. At low photon energies (< 3 eV), most of the interband transitions making peaks in both the diagonal and off-diagonal elements involve the localized 3d character in the minority-spin bands with the majority-spin bands only contributing structureless backgrounds. At higher photon energies, both the majority- and minority-spin bands construct separate peaks with the minority-spin peak being located at higher energies. The energy differences between the two peaks for Ni, Co and Fe are 0.3 eV, 0.8 eV and 1.5 eV respectively, which agree well with the spin-exchange splittings determined from angle-resolved photoemission measurements. For Ni and Co significant differences have been found in energy positions of the interband peaks between the calculated and experimental spectra. An empirical self-energy correction model has been applied, in which the sizes of the energy shifts of the excited-state quasiparticle states from those of the ground state are proportional to the density of d character in each state and the energy difference between each state and the Fermi level. The self-energy-corrected spectra for Ni and Co have been brought into good agreement with the experimental spectra.

1. Introduction

Optical studies have been providing a great deal of assistance in investigating the electronic structures of solids. The optical response functions (e.g. dielectric function and optical conductivity) of solids which can be measured by various optical techniques (e.g. ellipsometry) contain information on the optical transitions between one-electron energy levels below and above the Fermi level E_F in the band structures of solids. Also, the optical response functions can be theoretically calculated if the band structures are known in the whole Brillouin zone (BZ), which can be calculated by various schemes. By comparing the calculated optical response functions with the experimental results the validity of the band structures of various solid systems can be estimated. Also, particular bands in certain parts of the BZ can be identified as contributing to certain absorption structures in an optical response function.

The band structures, in general, are calculated using the local density approximation (LDA), in which the exchange–correlation potential of an electron system is a simple functional of the local electron density. The LDA has been a good approximation for solid systems with homogeneous and slowly varying electron density and remarkable in

explaining the ground-state properties [1]. Also, calculations of optical response functions from the ground-state band structures using the direct interband transition model produced good quantitative agreement with the experimental spectra for some metallic elements and compounds [2, 3] in the energy region where the optical absorptions are dominated by the interband transitions involving itinerant s–p bands located near E_F. However, when well-localized states (e.g. 3d) are involved in the optical transitions it has been found that calculated optical response functions from the ground-state band structures usually disagree with experimental results [4–7], the disagreements being basically due to significantly modified potentials compared to those in the ground state that excited electron–hole pairs feel, resulting in significant differences between the ground-state and excited-state quasiparticle solutions. For a localized electron system the many-body interaction between an excited electron–hole pair and the rest of the system is also describable in terms of a single-particle exchange–correlation mechanism as in the LDA, and is believed to cause finite shifts of the excited-state quasiparticle energies from the corresponding ground-state energies.

In the excited state the exchange–correlation process can be described by a non-Hermitian, non-local, and energy-dependent self-energy operator [8] in an integral equation called the Dyson equation, while in the ground state of the LDA systems it is described by a real, local, and energy-independent potential in the Schrödinger equation. For a homogeneous electronic charge distribution as in the LDA the difference in the eigenvalues between the two equations due to the difference in the exchange–correlation process between the excited and ground states can be described by a complex self-energy shift ($\Sigma = \Sigma_1 + i\Sigma_2$), which is a local but energy-dependent quantity. The real and imaginary parts of the self-energy shift represent the shift of the quasiparticle energies from the ground-state ones and the lifetime of the quasiparticle states respectively. The magnitude of the self-energy shift is expected to approach zero near E_F to make the exchange–correlation process in the excited state approach that in the ground state. Although, in principle, it is necessary to go beyond the LDA to describe excited-state properties, due to difficulties in exact calculations of the self-energy it is sometimes worthwhile to employ a rather simple empirical model to estimate the self-energy based on the ground-state band structures.

In this work, the optical response functions of ferromagnetic transition-metal elements Ni, Co and Fe have been calculated from the spin-polarized band structures. The linearized-augmented-plane-wave (LAPW) method [29] has been used to calculate the spin-polarized band structures of the elements and the optical conductivity tensors have been calculated from the band structures by only counting contributions from momentum- and spin-conserved interband transitions. The three ferromagnetic elements have unfilled 3d bands, which are well-localized in energy and space compared to neighbouring s–p bands and cause ferromagnetism at room temperatures due to net magnetic moments from the population differences between the exchange-split spin-up and spin-down bands. The 3d bands are distributed across E_F with the centre of mass of both spin-up and spin-down bands located just below E_F [4], so the interband transitions involving them are expected to contribute to the optical response functions from low photon energies and can be identified using the band structures. Also, by comparing the calculated optical spectra with the experimental spectra the differences in the electronic structure between the ground and excited state can be identified from the discrepancies between the two spectra, particularly in the energy positions of the absorption peaks. The energy differences between the ground- and excited-state spectra can be explained in terms of the self-energy shifts due to changes in the exchange–correlation contribution to the single-particle energy spectra in the excited state, which is bigger for more localized states.

An empirical self-energy correction model has been introduced to estimate the shifts of the excited-state quasiparticle energies from the corresponding ground-state values, in which the energy shift for a quasiparticle state is assumed to be affected by both the energy position relative to E_F and the amplitude of the 3d character of each ground-state band. The self-energy-corrected optical spectra for Ni and Co produce better agreements with the experimental spectra.

2. Calculational details

The self-consistent spin-polarized band structures for FCC Ni, HCP Co, and BCC Fe have been calculated using the LAPW method based on the muffin-tin approximation for the crystal potential. The exchange–correlation contribution to the crystal potential was estimated from the local spin-density approximation and the scalar-relativistic approximation for the Dirac equation [10] was used for the spin-polarized calculations. The spin–orbit coupling was added perturbatively after the spin-polarized bands and their wavefunctions were obtained from self-consistent iterations. The lattice parameters used in the calculations were from experimental data [11]. The differences in the electron population between the majority- and minority-spin bands obtained from the calculations are 0.60, 1.56 and 2.29 for Ni, Co and Fe respectively, which are in fair agreement with the experimental data [11] (0.606, 1.72 and 2.22 respectively).

The optical response of solid systems with cubic or HCP crystal structure and magnetized along the z-axis can be described by an optical conductivity tensor of the form

$$\begin{pmatrix} \sigma_{xx} & i\sigma_{xy} & 0 \\ -i\sigma_{xy} & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$$

where each tensor element has real and imaginary parts, e.g. $\sigma_{xx} = \sigma_{xx}^{(1)} + i\sigma_{xx}^{(2)}$. In the absence of magnetization, $\sigma_{xx} = \sigma_{yy} = \sigma_{zz}$ for cubic crystal structure and for HCP structure the diagonal elements have two independent components, $\sigma_\perp$ ($= \sigma_{xx} = \sigma_{yy}$) and $\sigma_\parallel$ ($= \sigma_{zz}$), representing components orthogonal and parallel to the z-axis (or c-axis) respectively. The off-diagonal element σ_{xy} is non-zero in the presence of a magnetic moment due to spin ordering along the z-axis and is known to affect magneto-optic properties such as the Kerr effect [12]. For the diagonal elements the real part represents the absorption of photons while for the off-diagonal elements the imaginary part represents the absorption.

Calculations of the diagonal and off-diagonal elements of the optical conductivity tensors for the ferromagnets Ni, Co and Fe were performed by integrating momentum- and spin-conserved interband transitions [12, 13]. For the BZ integration the linear-energy-tetrahedron method [14] was used, in which the energy eigenvalues were evaluated at the four corners of elementary tetrahedra in the irreducible BZ of each crystal structure and the electric-dipole matrix elements were calculated using the wavefunctions at the centres of the tetrahedra. The electric-dipole matrix elements were assumed to be constant within a tetrahedron and equal to the matrix element calculated at the centre. The numbers of tetrahedra generated for the calculations of the optical transitions from the spin–orbit band structures were 6144 in 1/16 of the BZ for FCC Ni, 4608 in 1/8 of the BZ for HCP Co and 1536 in 1/16 of the BZ for BCC Fe. For a direct comparison with the experimental spectra the calculated optical conductivity spectra were convoluted with an energy-dependent Lorentzian broadening function [15] of width equal to the imaginary part of the self-energy Σ_2 for the lifetimes of the excited states. Theoretical calculations for Ni [16, 17] showed a parabolic behaviour of Σ_2 for quasiparticle states near E_F (< 10 eV), So, a parabolic expression, $\Sigma_2(E) = 0.05E^2$ with E being the photon energy in eV, was adopted in the present calculations.

3. Analyses and discussions

Figure 1 shows the averaged real part of the diagonal elements of the optical conductivity tensor of Ni calculated from the spin-polarized band structures. The spectra excluding the effect of the quasiparticle lifetimes agree well with the results of previous calculations [12, 13]. It is seen that the optical absorption below 3 eV is dominated by the contribution from the interband transitions in the minority-spin bands, while the interband transitions in the majority-spin bands only provide structureless background. These absorption structures are mainly due to transitions between occupied d character and unoccupied p character. Due to the unfilled nature of the minority-spin d bands with t_{2g} symmetry, the amplitude of the minority-spin p character is strong just above E_F through p–d hybridization, leading to the intensity of the d→p transitions in the minority-spin bands being larger than that in the majority-spin bands. At higher energies above 3 eV, both the majority- and minority-spin bands contribute absorption peaks at about 5.5 and 5.8 eV respectively. These two peaks are mainly due to the interband transitions between the s–d character in the band 1 below E_F and the p character in the band 6 above E_F. Due to a rather small energy separation between the minority- and majority-spin peaks (about 0.3 eV) compared to heavy lifetime broadening (about 1 eV) for the excitation energies of about 5 eV estimated from the imaginary part of the self-energy the sum of the two contributions produces a single broad peak at about 5.6 eV. Due to the quite small exchange splitting [13] of band 1 compared to that of band 6 the energy difference between the two peaks (0.3 eV) can approximately represent the average exchange splitting of band 6 near E_F. The exchange splitting for the occupied bands near E_F for Ni determined from angle-resolved photoemission (ARPES) measurements [18, 19] is also 0.3 eV. It is also seen that the inclusion of the spin–orbit coupling does not cause a significant change in the optical spectrum except at low energies where the spin–orbit coupling produces a resolved absorption peak at about 0.3 eV.

The calculated optical conductivity of Ni is compared with the experimental data [20] in figure 2. It is seen that each interband peak in the calculated spectrum has a corresponding one in the experimental spectrum. However, the peaks in the calculated spectrum are located at higher energies than those in the experimental spectrum. The discrepancies are known to be due to the final-state effect, in which a major modification in the exchange–correlation contribution to a single-particle potential in the excited state compared to that in the ground state leads to shifts in the quasiparticle energy spectrum from the ground-state values as well as finite lifetimes in the excited state. This self-energy shift is expected to be bigger for more localized-electron systems. In the band picture, a localized 3d hole in the valence bands is mainly screened by neighbouring 3d electrons at the same atomic site. So, the hole has to move with a screening cloud of neighbouring localized electrons [17] so that the effective mass of the hole becomes larger than the corresponding ground-state value without screening, leading to a shrinking of the bandwidth of the 3d bands toward their centre of mass located near E_F. A direct way for detecting the self-energy shift in band states is ARPES measurements for quasiparticle states below E_F [18, 19, 21] and angle-resolved inverse photoemission (ARIPES) measurement for quasiparticle states above E_F [22], in which the measured dispersions along some symmetry directions are compared with the ground-state band structures to estimate the energy shifts of particular bands between the excited and ground states. In optical studies changes in energy gap between the excited-state and ground-state energy spectra can be estimated by comparing the experimental spectra with the calculated spectra from the ground-state band structures.

An empirical model for estimating the shift in the energy spectrum between the excited and ground states has been introduced, in which the excited-state quasiparticle energies
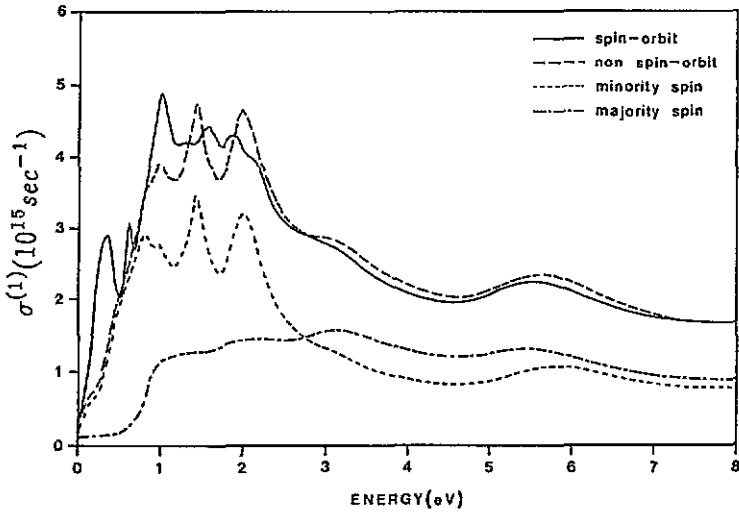
Figure 1. The averaged real part of the diagonal elements of the optical conductivity tensor, $\sigma^{(1)} = (\sigma^{(1)}_{xx} + \sigma^{(1)}_{yy} + \sigma^{(1)}_{zz})/3$, calculated for ferromagnetic FCC Ni. The short-dashed and dot-dashed lines represent contributions from the minority- and majority-spin bands respectively, calculated from the band structure without the spin–orbit coupling, and the long-dashed line represents the sum of the two contributions. The solid line represents the result including the spin–orbit coupling.
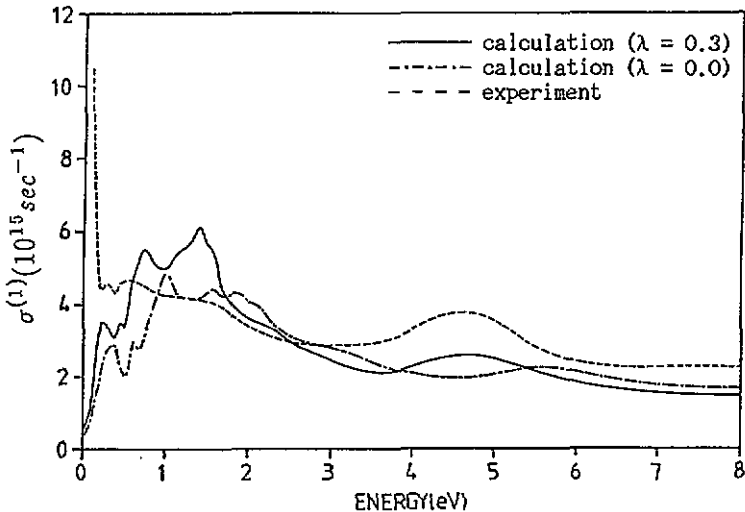
Figure 2. A comparison of the self-energy-corrected ($\lambda = 0.3$) optical conductivity spectrum with the uncorrected ($\lambda = 0.0$) spectrum and the experimental spectrum for ferromagnetic FCC Ni.

$E(n, k)$ differ from the corresponding ground-state values $E_0(n, k)$ by the real part of the self-energy shift, proportional to $E_F - E_0(n, k)$, i.e.

$$E(n, k) = E_0(n, k) + \Sigma_1(n, k) = E_0(n, k) + \lambda_{nk}[E_F - E_0(n, k)] \qquad (1)$$

for the states near E_F, where λ_{nk} is a parameter proportional to the exchange–correlation strength of the electronic system [23]. A linear behaviour of Σ_1 was obtained for Ni for quasiparticle states near E_F (< 10 eV) from theoretical calculations [16, 17] and was also obtained for nearly-free-electron metals (Li, Na, Al) with the self-energy shifts smaller by less than 50% compared to Ni [24]. Here, λ_{nk} was assumed to be non-zero for states with d character and proportional to the amplitude of the d character $N_d(n, k)$ of each eigenstate at (n, k) in the ground-state band structures so that

$$\lambda_{nk} = \lambda N_d(n, k) \tag{2}$$

where λ is a constant proportional to the exchange–correlation strength of the d states, which is expected to be bigger for more-localized electron systems. λ was determined to make the self-energy-corrected spectrum agree with the experimental spectrum. In calculating the optical conductivities including the self-energy shift the electric-dipole matrix elements for the quasiparticle states were assumed to be the same as those calculated from the ground-state band structures because the quasiparticle wavefunctions are usually not much different from the corresponding ground-state ones [24].

In figure 2 the self-energy-corrected optical conductivity spectrum of Ni with $\lambda = 0.3$ is compared with the ground-state spectrum ($\lambda = 0$) and the experimental spectra. It is seen that the self-energy-corrected spectrum shows a good agreement with the experimental spectrum for the structures at about 0.8, 1.5 and 4.6 eV. The largest energy shift was made for the 4.6 eV structure, shifted by 1.0 eV from its ground-state energy position.

Figure 3 shows the calculated optical conductivities of HCP Co. Each calculated spectrum for the two components ($\sigma_{\parallel}$ and $\sigma_{\perp}$) shows only two interband structures at low-energy range (< 2 eV), one at the same energy and the other separated by about 0.5 eV, and the average of the two spectra shows three structures as in the experimental spectrum shown in figure 4. So, the averaged spectrum in figure 3 has been used to evaluate the self-energy correction in Co as shown in figure 4. As in the case of Ni, the low-energy interband structures below 3 eV are dominated by transitions in the minority-spin bands [13]. Also, the broad peak at about 5.6 eV in the ground-state ($\lambda = 0$) spectrum is contributed by both the majority-spin bands peaked at about 5.2 eV and the minority-spin bands peaked at about 6.0 eV. As in the case of Ni, the energy difference of 0.8 eV can be approximated as the average exchange splitting between the majority- and minority-spin bands near E_F and it agrees well with the result (0.85 eV) of an ARPES measurement [25]. It is seen that the corrected spectrum with $\lambda = 0.2$ shows a good agreement over the whole energy range with the experimental data [20] for both the energy positions and the linewidths of the structures. The 5 eV peak in the corrected spectrum, which shows a largest shift of 0.6 eV from its ground-state energy position, agrees with the experimental spectrum in energy position, linewidth and magnitude. The smaller self-energy shift in Co (0.6 eV) compared to the shift in Ni (1.0 eV) for their 5.6 eV peaks is due to the exchange–correlation strength in Co being weaker than that in Ni, due to the Co 3d states being less localized than those of Ni.

Figure 5 shows the calculated optical conductivity spectrum of BCC Fe compared with the experimental spectrum. As in the case of Ni and Co, the low-energy structrues below 3 eV are dominated by transitions in the minority-spin bands [13]. At higher enrgies, the minority-spin bands contribute the structure at about 5.0 eV and the majority-spin bands contribute the structure at about 6.5 eV. The two structures are mainly due to transitions between bands 1 and 6 as in the case of Ni and are well-resolved from each other due to a larger energy separation between the two structures than the corresponding ones in Co and Ni. As in Ni and Co the energy difference of 1.5 eV between the two structures can
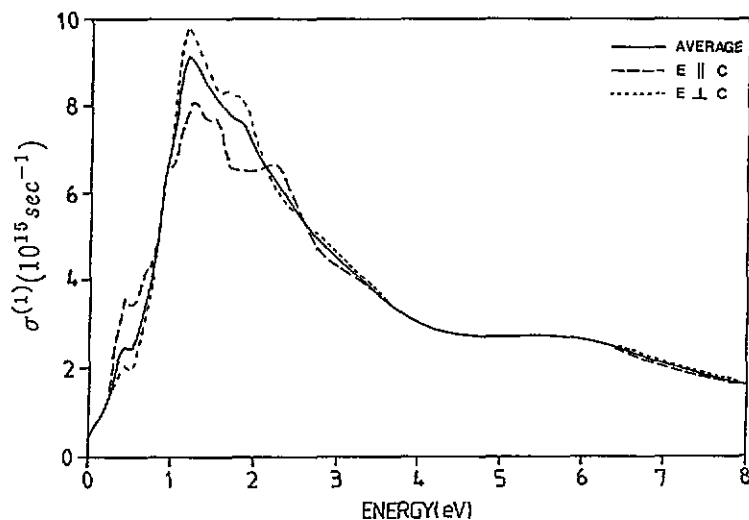
Figure 3. Calculated real parts of the diagonal elements of the optical conductivity tensor for ferromagnetic HCP Co.
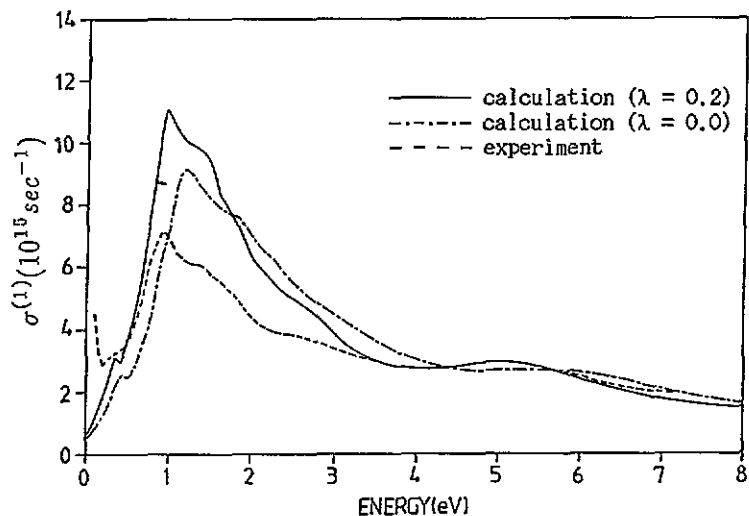

Figure 4. A comparison of the self-energy-corrected ($\lambda = 0.2$) optical conductivity spectrum with the uncorrected ($\lambda = 0.0$) spectrum and the experimental spectrum for ferromagnetic HCP Co.

be approximated as the average exchange splitting of d bands near E_F and it agrees well with the ARIPES result [22] of 1.8 eV and ARPES results [26, 27] of 1.5 eV. Also, the energy positions of the interband structures in the calculated spectrum agree within 0.1 eV with the corresponding ones in the experimental spectrum [20], which means that the quasiparticle energy spectrum in Fe does not differ much from the ground-state one and that the 3d states in Fe are relatively more itinerant than those of Co and Ni.

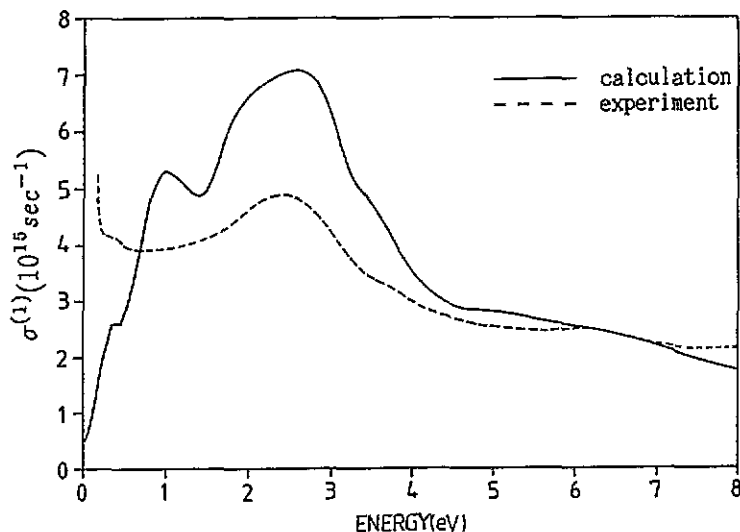Figures 6, 7 and 8 show the imaginary parts of the off-diagonal components of the optical

Figure 5. A comparison of the averaged real part of the diagonal elements of the optical conductivity tensor with the experimental spectrum for ferromagnetic BCC Fe.

conductivity tensors for Ni, Co and Fe respectively. Inclusion of spin–orbit coupling causes minor changes in the spectra at low energies as in the case of diagonal elements. Again, the self-energy-corrected spectrum for Ni in figure 6 with the same parameter as the diagonal component ($\lambda = 0.3$) shows a better agreement with the experimental spectrum [28] for the structures at about 1.5 and 3 eV, which shift from their ground-state positions by about 0.5 and 1 eV respectively. For Co the self-energy-corrected spectrum in figure 7 with weaker exchange–correlation strength ($\lambda = 0.2$) than in Ni also shows a good agreement with the experimental spectrum [28]. The structure at about 1.5 eV in the self-energy-corrected spectrum is shifted from its ground-state position by about 0.4 eV. For Fe the calculated spectrum in figure 8 contains no self-energy correction as in figure 5. Overall agreement is good between the calculated and experimental spectrum [28] except for the energy position of the structure at about 2 eV, which differs by about 0.3 eV. According to the results of ARPES measurements the 3d bands in Ni shifted from their ground-state positions by up to 1 eV with the reduction in the bandwidth of about 30% [18], while for Co the reduction in the bandwidth was about 20% [24] and for Fe the experimental data nearly agreed with the ground-state band structures [27]. The unoccupied bands of Fe were investigated by an ARPES measurement, in which the bandwidths of the unoccupied 3d bands were reduced by about 10% toward E_F [22]. These results agree with the present calculation results, in which the self-energy shifts for Ni (with maximum shift of about 1 eV) are bigger by about a factor of 1.5 than those for Co (with maximum shift of about 0.6 eV) and by a factor of 3 than those for Fe (with maximum shift of about 0.3 eV).

4. Summary

The calculated optical conductivities of ferromagnetic Ni, Co and Fe show that the minority-spin bands dominate the interband absorption structures in the low-energy region (< 3 eV). These structures are mainly due to d→p transitions. At higher energies, the majority-spin bands as well as the minority-spin bands contribute absorption structures mainly due to
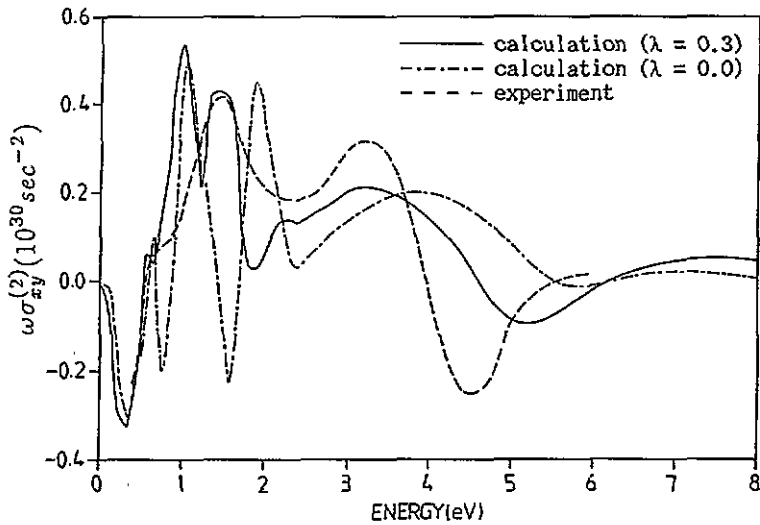
Figure 6. A comparison of the calculated off-diagonal element of the optical conductivity tensor with ($\lambda = 0.3$) and without ($\lambda = 0.0$) self-energy correction with the experimental spectrum for ferromagnetic FCC Ni.
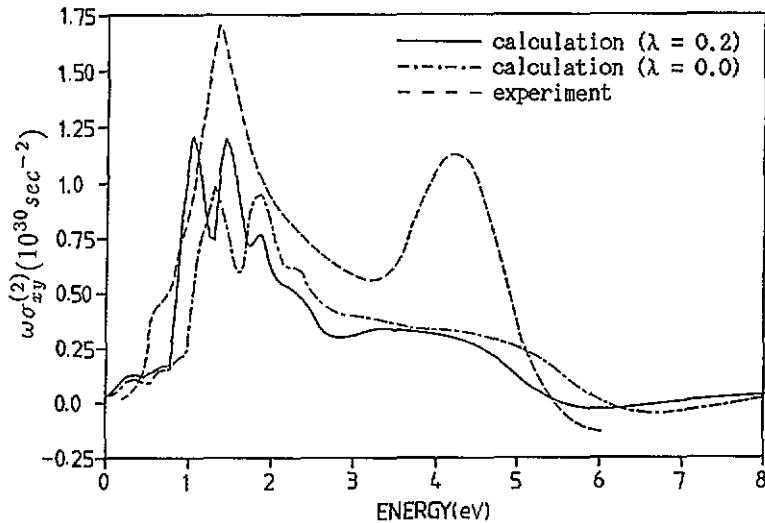

Figure 7. A comparison of the calculated off-diagonal element of the optical conductivity tensor with ($\lambda = 0.2$) and without ($\lambda = 0.0$) self-energy correction with the experimental spectrum for ferromagnetic HCP Co.

sd→p transitions with the minority-spin peaks located at energies higher by 0.3, 0.8 and 1.5 eV for Ni, Co and Fe respectively. These energy differences are due to average exchange splittings in the spin-polarized band structures and agree well with the values determined experimentally using ARPES and ARIPES. Due to the localized nature of the 3d bands the calculated optical conductivities disagree with the experimental spectra and the disagreement is the biggest in Ni and the smallest in Fe, which shows a qualitative relationship between
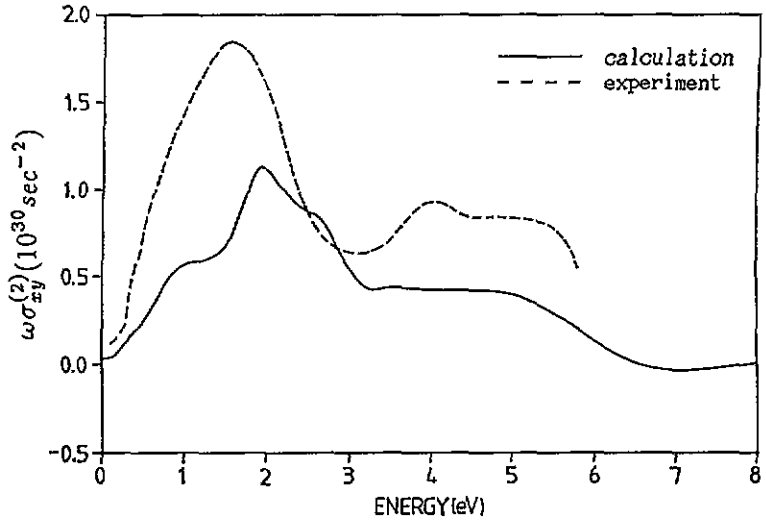
Figure 8. A comparison of the calculated off-diagonal element of the optical conductivity tensor with the experimental spectrum for ferromagnetic BCC Fe.

the degree of localization and the self-energy shift for the 3d bands. A self-energy-correction model has been applied in which the energy shifts for the quasiparticle states are proportional to a product of the density of d character and the energy difference relative to E_F of each state. The self-energy-corrected optical conductivities for Ni and Co show good agreement with the experimental spectra. On the other hand, the magnitudes of the spin-exchange splittings for the three ferromagnets were found to remain almost unchanged in the excited state.

Acknowledgments

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