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Spin-polarized first-principles calculation of momentum densities of Fe

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Abstract. We perform first-principles calculations on the momentum densities in Fe. The ridge and valley appear on the Σ and Δ lines, respectively, on the (001) plane. This anisotropic distribution of the momentum densities is found to originate from the difference between symmetries of the $\Sigma(C_{2v})$ and $\Delta(C_{4v})$ lines. The calculated one-dimensional momentum densities of the majority spin have a broader distribution than those of the minority spin, which is expected to be due to the fact that the distribution in the real space of the majority spin is narrower than that of the minority spin.

1. Introduction
Electron momentum densities are detected by experiments of positron annihilations and Compton scattering and provide useful information on electronic structures [1-2]. In positron annihilation experiments, two-dimensional angular correlation of annihilation radiation (2D-ACAR) and Doppler broadening annihilation radiation (DBAR) spectra detect two-dimensional and one-dimensional momentum densities, respectively. Recently, spin-polarized positron annihilation experiments attracted scientific interests since they can be applied to studies of spintronics and magnetic materials [3-4]. Spin-polarized DBAR spectra have been observed and thus the study of the momentum densities for the majority and minority spins becomes important [3-4].

In this paper, we perform calculations of momentum densities of the spin-polarized material, Fe. First, we find the prominent anisotropy of the momentum densities on the (001) plane; the momentum densities on the Δ line are smaller than those on the Σ line. We analyze the anisotropy based on the group theory [1,5] and find that the Δ and Σ lines have high (C_{4v}) and low (C_{2v}) symmetries, respectively. This difference in symmetry is the origin of the anisotropy. Next, we find that the momentum distribution of the majority spin is broader than that of the minority spin, which is consistent with experimental results of DBAR [3]. This difference is expected to originate from the fact that distribution of the majority spin densities in the real space is narrower than that of the minority spin densities [6].
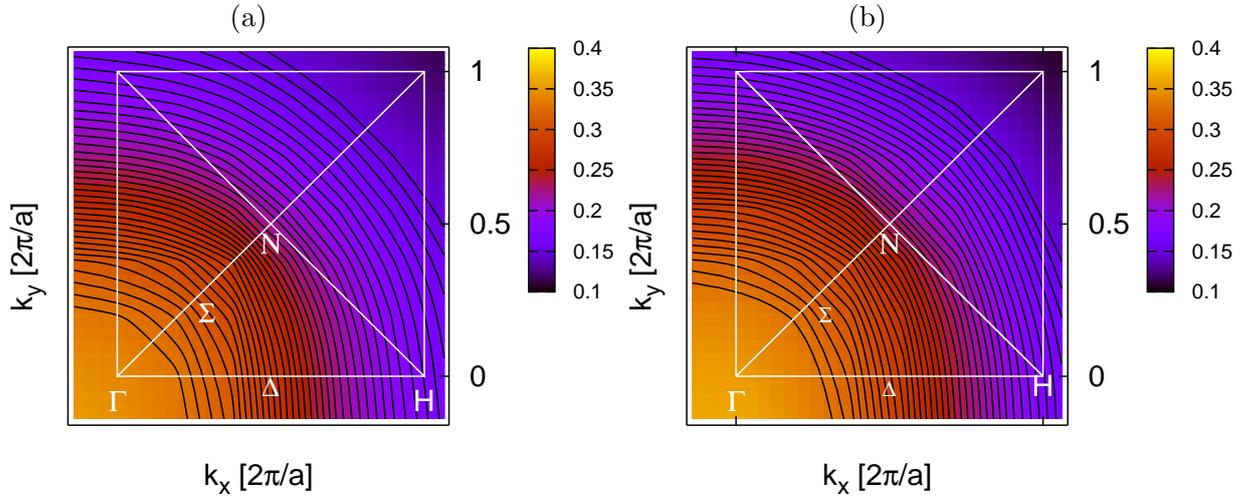
Figure 1. Momentum densities on the (001) plane of the majority spin (a) and minority spin (b).The values of the contour lines are in the arbitrary units (a.u.).

2. Method

The Bloch wave function, $\Psi_n^{\mathbf{k}}$, is given by

$$\Psi_n^{\mathbf{k}}(\mathbf{r}) = \psi_n^{\mathbf{k}}(\mathbf{r}) \exp(i\mathbf{k} \cdot \mathbf{r}), \tag{1}$$

where n and $\mathbf{k}$ is the band index and the wavenumber, respectively, and $\psi_n^{\mathbf{k}}(\mathbf{r})$ is the periodic function. The electron momentum density for the momentum $\mathbf{p}$ in the first Brillouin zone (FBZ) is given by [1]

$$\rho(\mathbf{p}) = \sum_n^{occ.} \left| \int_{cell} \psi_n^{\mathbf{p}}(\mathbf{r}) d\mathbf{r} \right|^2. \tag{2}$$

When the momentum is outside the FBZ ($\mathbf{p}' = \mathbf{p} + \mathbf{G}$), the momentum density is given by

$$\rho(\mathbf{p}') = \sum_n^{occ.} \left| \int_{cell} \psi_n^{\mathbf{p}}(\mathbf{r}) \exp(i\mathbf{G} \cdot \mathbf{r}) d\mathbf{r} \right|^2, \tag{3}$$

where $\mathbf{G}$ is a reciprocal lattice vector. The momentum densities deduced from positron annihilation experiments include the positron wavefunction effect but we do not consider this effect in Eqs.(2) and (3). The density is also affected by electron-positron correlation and electron-electron correlation which is imperfectly included in the density functional theory (DFT) calculations. Indeed a previous study suggests these effects on the 2D-ACAR by comparing experimental and calculational results [7]. However, since these effects are small, we neglect these effects in our study.

We perform DFT calculations to obtain the Block wave function $\Psi_n^{\mathbf{k}}(\mathbf{r})$. We use the spin-polarized generalized gradient approximation. The cutoff energies of the wave function and charge density are 25.0 Ry and 225.0 Ry, respectively. The number of the sampling k points is $20 \times 20 \times 20$. The lattice constant is deduced from a structure optimization calculation (2.845 Å).

3. Results and discussion

3.1. Three-dimensional momentum densities

We calculate momentum densities of the majority and minority spins on the (001) plane (Figure 1). We find that the ridge appears on the Γ-N (Σ) line and the valley appears on the Γ- H (Δ) line
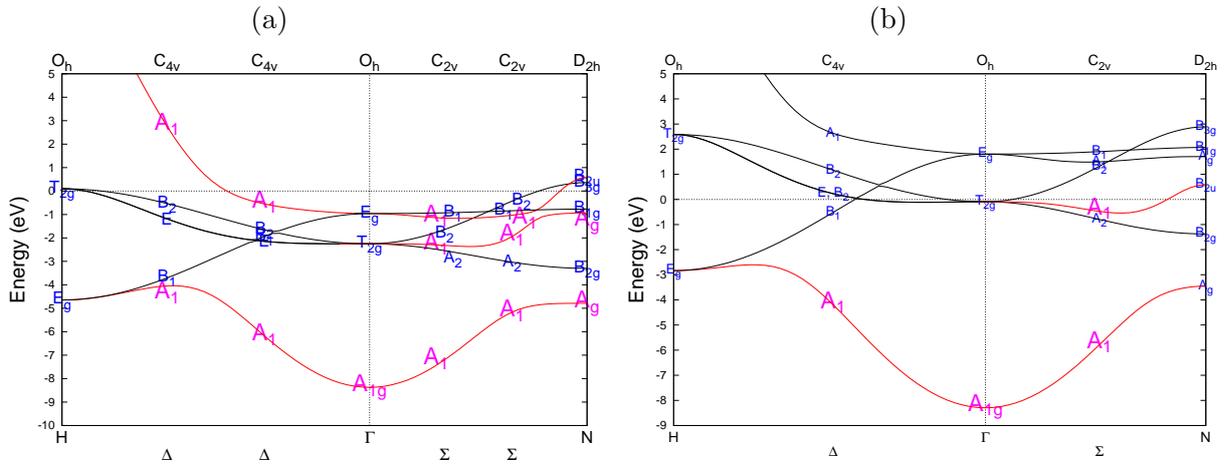
Figure 2. Band structure of the majority spin(a) and minority spin(b). The red lines represent totally symmetric occupied bands and black lines do non-totally-symmetric and/or unoccupied bands. The band energies are measured from the Fermi energy.
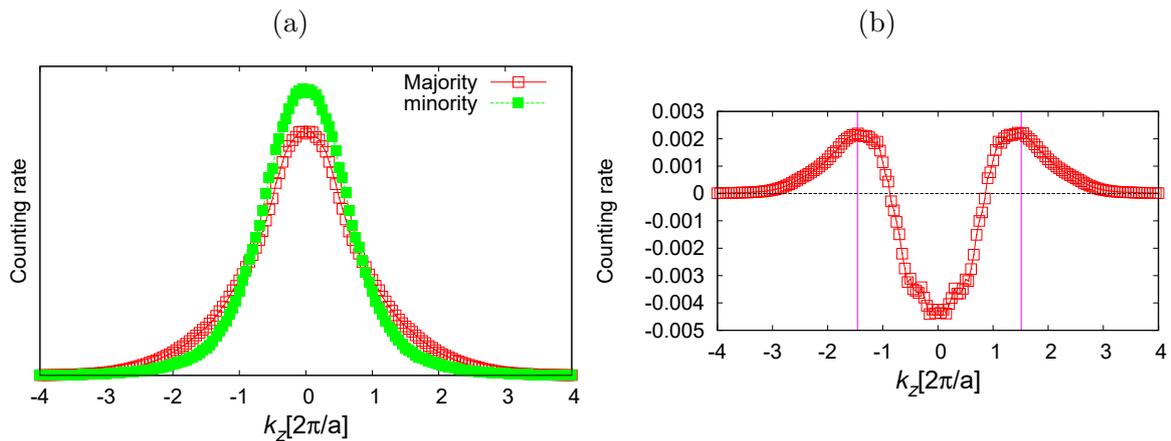

Figure 3. One dimensional momentum densities of the majority spin and the minority spin (a), and difference between majority spin and minority spin (b).

in both cases of the majority and minority spins.

We next analyze the anisotropy by using the group theory. The band structures with the irreducible representations are shown in Figure 2. In the case of the majority (minority) spin, we find three (two) totally symmetric occupied bands on the Σ line, and only one or two (one) totally symmetric occupied bands on the Δ line. Therefore, the Σ line has more totally symmetric occupied bands than the Δ line. This difference in the number of the irreducible representation originates from the fact that the Δ line (C_{4v}) has higher symmetry than the Σ line (C_{2v}). Since only the totally symmetric representation contributes to the momentum density, the momentum density on the Σ line is expected to be larger than that on the Δ line and this expectation is consistent with our calculational results mentioned above.

3.2. One-dimensional momentum densities
Next, we calculate one-dimensional momentum densities which are spatially averaged [3]. We find that the momentum distribution for the majority spin is broader than that for minority

spin (**Figure 3**). This feature is consistent with the result of the experiment of DBAR [3]. When p = 0, the sign is minus and we find that the positive peak appears at $p = 1.4$ in the $2\pi/a$ unit in FIG.3 (b).

In a previous study, it was reported that the distribution of the majority spin in the real space is narrower than that of the minority spin [6]. This difference in the real-space distribution is expected to be the origin of the difference in the momentum density distribution.

4. Conclusion

In this study, we perform calculations of the spin-polarized momentum densities of Fe using the DFT. We first find the prominent anisotropy of the momentum densities on the (001) plane; the ridge and valley appear on the Σ and Δ lines, respectively. This anisotropy originates from the fact that the symmetry of the Σ line (C_{2v}) is lower than that of the Δ line (C_{4v}). We also find that the one-dimensional momentum densities of the majority spin is broader than that of the minority spin. The difference in the distributions of the momentum densities is expected to originate from the fact that the distribution in space of the majority spin density is narrower than that of the minority spin density.

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