Kunitomo HIRAI

Department of Physics, Nara Medical University, Kashihara 634

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On the basis of an electronic structure calculation, spin density wave states of fcc Fe and Cr are discussed with particular attention to the difference between them. The wave vector at which the unenhanced spin susceptibility of nonmagnetic fcc Fe or Cr becomes maximum is shown to correspond well to the observed wave vector of spin density wave. It is found that a nesting of the Fermi surface hardly contributes to determining the wave vector of the susceptibility maximum for fcc Fe, which exhibits a remarkable contrast to Cr. Another reasoning of the susceptibility maximum is extended from a real space viewpoint. Difference in characteristics of the spin density wave state between fcc Fe and Cr is further illustrated by the electronic structure calculation of spin density wave states with finite magnetic moments.

§1. Introduction

In transition metals electronic structure and electron correlation play decisive roles in determining their magnetism. Although these two factors are both important, in some problems electron correlation can be treated less rigorously than electronic structure or *vice versa*. Magnetism at ground state presumably corresponds to the former case: electron correlation is treated within a mean-field approximation like a local density functional (LDF) one. The stable magnetic structure in 3d transition metals has been discussed in this way and it has been shown that the observed magnetic structure of 3d transition metals can be well explained through investigations of their electronic structures. Energy difference between magnetic structures has been realized to arise mainly from kinetic energy of 3d electrons. The present paper follows the same way to discuss the spin density wave (SDW) states of fcc Fe and (bcc) Cr.

The SDW state of fcc Fe has recently been reported by Tsunoda in his series of X-ray and neutron diffraction experiments for γ Fe precipitates in a Cu matrix.^{1)~3)} Most of the γ Fe precipitates have been found to have distorted lattices and complex magnetic structures similar to an antiferromagnetic one of the first kind of the fcc lattice;¹⁾ the first kind antiferromagnetic structure was formerly considered to be the magnetic structure of γ Fe precipitates.⁴⁾ In some of the γ Fe precipitates such as γ FeCo alloy precipitates, however, it has been found that the lattice distortion is suppressed and the magnetic structure is not the complex one but SDW.^{2),3)} The complex magnetic structure is considered to be stabilized by the lattice distortion,⁵⁾ and hence the magnetic structure of fcc Fe precipitates can be concluded to be SDW as long as the lattice remains cubic.

The SDW state of Cr, which was regarded as the only example of SDW states in transition metals, has been extensively investigated in both experimental and theoretical aspects.⁶⁾ Theoretically, the electronic structure of nonmagnetic Cr has been studied in detail to explain the mechanism by which the SDW state is stabilized. It is generally admitted that a special feature of the Fermi surface of Cr, namely, the nesting of the Fermi surface plays a decisive role in determining the ordering wave vector of SDW,⁷⁾ which was quantitatively supported by the calculation of unenhanced spin susceptibility of nonmagnetic Cr.⁸⁾

The purpose of this paper is to elucidate characteristics of the SDW state of fcc Fe in comparison with those of Cr. The focus of interest is whether the SDW of fcc Fe can be ascribed to the nesting mechanism or not. The present author previously predicted a possibility of the SDW ground state of fcc Fe in the discussion about systematic change of the stable magnetic structure in transition metals.⁹⁾ The SDW ground state was turned out to appear when the valence falls in an intermediate region between ferromagnetic and antiferromagnetic regions; the ferromagnetic region spreads from an area of a nearly-filled band while the antiferromagnetic one spreads around that of a half-filled band. There is thus no direct relation between the prediction of the SDW ground state of fcc Fe and the nesting of the Fermi surface. The discussion was based on unenhanced spin susceptibility calculation of nonmagnetic state and energy calculation of SDW states with finite magnetic moments by means of a real space method for calculating electronic structure of SDW states. These calculations, however, were intended for qualitative discussion and we took account of wave vectors only along the line $a^*(q, 0, 0)$ but not those along the line $a^{*}(1, q, 0)$, on which the observed wave vector of SDW of fcc Fe lies; where $a^{*}=2\pi/a$ and a denotes the lattice constant. We therefore reexamine these calculations to have a quantitatively reliable discussion about the SDW of fcc Fe.

In the previous letter¹⁰ we showed a part of the results of unenhanced spin susceptibility calculation and reported that the wave vector Q_0 at which the unenhanced spin susceptibility $\chi(Q)$ becomes maximum corresponds well to the observed wave vector of SDW. Calculated $\chi(Q)$ has a maximum at $Q_0 = a^*(1, q_0, 0)$ with $q_0 \sim$ 7/48 for fcc Fe and at $Q_0 = a^* (q_0, 0, 0)$ with $q_0 \sim 46/48$ for Cr, while the observed wave vector is $a^*(1, 0.123, 0)$ for fcc Fe₉₇Co₃ precipitates²⁾ and $a^*(0.95, 0, 0)$ for Cr.⁶⁾ Although Q_0 is nothing but the ordering wave vector of SDW when the magnetic moments are infinitesimal,¹¹⁾ it is fairly probable that the ordering wave vector of SDW with finite magnetic moments is not far from Q_0 .

We discuss in this paper the difference in unenhanced spin susceptibility between fcc Fe and Cr in more detail. As mentioned above, an effect of the nesting of the Fermi surface is the point at issue. We compare steepness of $\chi(Q)$ around Q_0 and Fermi energy dependence of $\chi(Q)$ of fcc Fe with those of Cr. We estimate a contribution in $\chi(Q)$ from energy bands near the Fermi surface to draw a definite conclusion as to the effect of the nesting of the Fermi surface. In addition, we investigate another mechanism of SDW than the nesting one by introducing non-local spin susceptibilities. We then discuss which mechanism is adequate to the SDW of fcc Fe or that of Cr.

In the latter part of this paper we have discussions based on electronic structure

of SDW states with finite magnetic moments, whereas we have discussions based on that of nonmagnetic state in the former part. We calculate the electronic structure of helical SDW states of fcc Fe and Cr in a self-consistent manner by using a tight-binding method and investigate the stable SDW state by comparing energies of these states. On the basis of the investigation of the stable SDW state and the magnitude of local magnetic moments, characteristics of the SDW are discussed with particular reference to the difference between fcc Fe and Cr.

The outline of this paper is as follows. In § 2 we show calculated unenhanced spin susceptibilities of fcc Fe and Cr. The difference between them is discussed. In § 3 we discuss an origin of the SDW of fcc Fe in terms of non-local spin susceptibilities. We show in § 4 results of electronic structure calculation for helical SDW states with finite magnetic moments. The stable SDW states of fcc Fe and Cr are investigated. Finally we summarize our discussion and conclusions in § 5.

§ 2. Unenhanced spin susceptibility

The unenhanced spin susceptibility is defined as susceptibility of nonmagnetic state with no account of the enhancement due to electron correlation and therefore can be obtained directly from the electronic structure of nonmagnetic state. We calculate the electronic structure of nonmagnetic state by the first-principle tightbinding method¹²⁾ with a minimal basis set, that is, one *s*, three p, and five *d* orbitals per atom; the potential parameters are those obtained self-consistently for the experimental lattice constant by the linear muffin-tin orbital (LMTO) method with the LDF formalism. With eigenvalues $\varepsilon_{k,\mu}$ and eigenvectors $|k, \mu\rangle$ of nonmagnetic state thus obtained in the tight-binding method, unenhanced spin susceptibility against staggered magnetic field with a wave vector $Q, \chi(Q)$ is calculated as

$$\chi(\boldsymbol{Q}) = 2\mu_{\rm B}^{2} \sum_{\boldsymbol{k}} \sum_{\mu,\nu} |\langle \boldsymbol{k} + \boldsymbol{Q}, \nu | \boldsymbol{k}, \mu \rangle|^{2} \frac{f(\varepsilon_{\boldsymbol{k},\mu}) - f(\varepsilon_{\boldsymbol{k}+\boldsymbol{Q},\nu})}{\varepsilon_{\boldsymbol{k}+\boldsymbol{Q},\nu} - \varepsilon_{\boldsymbol{k},\mu}}, \qquad (1)$$

where $f(\varepsilon)$ is the Fermi distribution function. We take the temperature to be zero and then $f(\varepsilon)$ is reduced to the step function $\theta(E_{\rm F}-\varepsilon)$, where $E_{\rm F}$ is the Fermi energy. The summation is accordingly restricted to the case $\varepsilon_{k,\mu} \leq E_{\rm F} < \varepsilon_{k+Q,\nu}$ or $\varepsilon_{k,\mu} > E_{\rm F}$ $\geq \varepsilon_{k+Q,\nu}$.

Wave vectors we consider are those along the symmetry lines in the Brillouin zone including those on the symmetry points. Considering the symmetry of $\chi(Q)$ in Q space, we suppose that most states are covered by taking account of these wave vectors, though we do not reject the possibility that $\chi(Q)$ may become maximum at other wave vectors having lower symmetry.

For the sake of accuracy, we perform the *k* summation of Eq. (1) by dividing the Brillouin zone into cubes of volume $(a^*/48)^3$; the number of *k* points in the irreducible 1/48 Brillouin zone is 10569 for fcc and 5525 for bcc. The summation of such large number of *k* points ensures that the numerical error of $\chi(Q)$ is less than 1%.

Now we show results for fcc Fe and Cr. In Fig. 1(a), we show the calculated $\chi(Q)$ of fcc Fe in the vicinity of X point of the fcc Brillouin zone, that is, for Q along

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Fig. 1. Calculated χ(Q) of (a) fcc Fe and (b) Cr. Solid lines are χ(Q) for their Fermi energies determined by n_e=8 for Fe and n_e=6 for Cr; broken lines are those for slightly lower E_F (or less n_e: (a) n_e=7.92, (b) n_e=5.94) and dotted lines are those for slightly higher E_F (or more n_e: (a) n_e=8.08, (b) n_e=6.07). The position of the maximum of χ(Q) is indicated by an arrow.

the symmetry lines $Q = a^*(1, q, q)$ $(0 \le q \le 1/4)$, $Q = a^*(q, 0, 0)$ $(3/4 \le q \le 1)$ and $Q = a^*$ (1, q, 0) $(0 \le q \le 1/4)$. In Fig. 1(b), we show the calculated $\chi(Q)$ of Cr in the vicinity



Fig. 2. Calculated \(\chi(Q; E_F)\) of (a) fcc Fe and (b) Cr as a function of E_F. Each line represents \(\chi(Q; E_F)\) for \(Q\) along (a) \(a^*(1, q, 0)\) and (b) \(a^*(q, 0, 0)\).

of H point of the bcc Brillouin zone, that is, for Q along the symmetry lines Q $=a^{*}(1-q, q, q) \ (0 \le q \le 1/4), \ Q = a^{*}(q, 0, q)$ 0) $(3/4 \le q \le 1)$ and $Q = a^*(1-q, q, 0)$ (0) $\leq q \leq 1/4$). Each curve in these figures represents $\chi(Q)$ for various $E_{\rm F}$'s near that for Fe or for Cr, in other words, for various valences, $n_{\rm e}$'s, around eight for Fe or around six for Cr. As mentioned above, $\chi(Q)$ has a maximum at Q_0 $=a^{*}(1, q_{0}, 0)$ with $q_{0} \sim 7/48$ for fcc Fe and at $Q_0 = a^*(q_0, 0, 0)$ with $q_0 \sim 46/48$ for Cr. We notice from Fig. 1(a) that the value of q_0 for fcc Fe increases slightly when the Fermi energy $E_{\rm F}$ rises, or equivalently when the valence n_e increases. Such behavior of q_0 against n_e agrees qualitatively with the observed concentration dependence of q_{obs} in fcc FeCo alloy precipitates.³⁾ Similarly, we notice from Fig. 1(b) that the value of q_0 for Cr

increases when the valence n_e increases. This behavior of q_0 against n_e agrees well with the observed concentration dependence of q_{obs} in Cr alloys.⁶⁾ The $E_{\rm F}$ dependence of q_0 can be also found in Fig. 2, where $\chi(Q; E_F)$ is plotted as a function of E_F for various **Q**'s. We confirm from Fig. 2 the above-mentioned behavior of q_0 against E_F or $n_{\rm e}$.

Let us discuss the difference in $\chi(\mathbf{Q})$ between fcc Fe and Cr. We find in Fig. 1 a sharp rise around Q_0 in $\chi(Q)$ of Cr but not such a significant rise in $\chi(Q)$ of fcc Fe. The difference between fcc Fe and Cr becomes clearer by comparing the $E_{\rm F}$ dependence of $\chi(\mathbf{Q}; E_{\rm F})$ shown in Fig. 2; $\chi(\mathbf{Q}; E_{\rm F})$ of Cr exhibits one definite peak for $\mathbf{Q} = a^*$ (1, 0, 0) and this peak splits into two when Q deviates from $a^*(1, 0, 0)$, while that of fcc Fe does not exhibit such peaks. Both the rise around Q_0 in $\chi(Q)$ and the shift of the peak in $\chi(Q; E_{\rm F})$ accompanied by the change of Q for Cr can be ascribed to the nesting of the Fermi surface: for Q close to the nesting vector, the denominator in Eq. (1), $\varepsilon_{k+Q,\nu} - \varepsilon_{k,\mu}$, approaches zero in a wide area of **k** near the Fermi surface. Thus we can barely find characteristics indicating the nesting of the Fermi surface in $\chi(Q)$ of fcc Fe, whereas we can easily find them for Cr.



WAVE VECTOR

Fig. 3. Contribution in $\chi(Q)$ from energy bands lying in the vicinity of the Fermi surface for (a) fcc Fe and (b) Cr. Short broken, dotted-broken, long broken, and dotted lines correspond to the cases $\Delta = 0.005$, 0.01, 0.02 and 0.04(Ry), respectively. The solid line is the $\chi(Q)$ itself, which is subtracted by ten so as to be placed in the same figure.

In order to determine whether the nesting of the Fermi surface has an effect on the maximum of $\chi(\mathbf{Q})$ of fcc Fe or not, we investigate a contribution in $\chi(Q)$ from energy bands lying in the vicinity of the Fermi surface, that is, from energy eigenvalues $\varepsilon_{\boldsymbol{k},\mu}$ and $\varepsilon_{\boldsymbol{k}^+\boldsymbol{Q},\nu}$ in Eq. (1) such that $|E_{\rm F} - \epsilon_{\boldsymbol{k},\mu}| \leq \Delta$ and $|E_{\rm F}$ $-\varepsilon_{k+Q,\nu} \leq \Delta$. Here the parameter Δ is varied so that the contribution from the Fermi surface manifests itself. In practice we take $\Delta = 0.005, 0.01, 0.02$ and 0.04 (Ry); it is to be noted that the d band width is about 0.4 Ry for fcc Fe and 0.5 Ry for Cr. The result is shown in Fig. 3. It is found that the contribution of Cr corresponds roughly to the rise around Q_0 discussed above even when \varDelta is small. As for Cr, energy bands near the Fermi surface are thus concluded to have an important effect on the determination of Q_0 . The contribution of fcc Fe, in contrast to Cr, is found to be almost independent of Q when \varDelta is small. We therefore reach the conclusion that the nesting of the Fermi surface has only a minor effect on the maximum of $\chi(Q)$ of fcc Fe.

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In the next section we discuss another origin of the maximum of $\chi(Q)$ of fcc Fe and hence a mechanism of stabilizing the SDW of fcc Fe. Contrary to the case of the nesting of the Fermi surface, the origin of the maximum of $\chi(Q)$ is discussed in a real space picture with the help of non-local spin susceptibilities.

§ 3. Non-local spin susceptibility

Local and non-local spin susceptibilities are defined as the susceptibility for the induced magnetic moment M_i at the *i*th site when the magnetic field h_j is applied locally at the *j*th site; that is,

$$\chi_{ij} = (M_i/h_j)_{h_j \to 0}$$
 (2)

In terms of χ_{ij} , the unenhanced spin susceptibility $\chi(Q)$ is expressed in principle as

$$\chi(Q) = \sum_{j} \chi_{ij} \exp(iQ(R_j - R_i)) = \sum_{\delta} \chi_{0\delta} \exp(iQR_{\delta}), \qquad (3)$$

where \mathbb{R}_i is the position vector of the *i*th site and δ represents the displacement between the *j*th and *i*th sites. In the tight-binding method χ_{ij} is calculated by

$$\chi_{ij} = (2\mu_{\rm B}^2/\pi) {\rm Im} \int^{E_{\rm F}} d\omega \sum_{m,n} G_{im,jn}(\omega) G_{jn,im}(\omega) , \qquad (4)$$

where $G_{im,in}(\omega)$ is the site off-diagonal element of the Green function of nonmagnetic state, which is given by



Fig. 4. Calculated $\chi_{\delta}(Q)$ of (a) fcc Fe and (b) Cr. Solid lines show the correct $\chi(Q)$ calculated by Eq. (1). Broken, dotted-broken and dotted lines correspond to the cases $\delta = (4 \ 4 \ 0)$, $(4 \ 0 \ 0)$ and $(2 \ 2 \ 0)$, respectively.

$$G_{im,jn}(\omega) = \sum_{\boldsymbol{k},\mu} C_m(\boldsymbol{k},\mu) C_n^*(\boldsymbol{k},\mu) \frac{\exp(i\boldsymbol{k}(\boldsymbol{R}_i - \boldsymbol{R}_j))}{\omega - \varepsilon_{\boldsymbol{k},\mu}}$$
(5)

with $C_m(\mathbf{k}, \mu)$ denoting the *m*th $(m=s, p_x, \dots, d_{xy}, \dots)$ orbital component of the eigenvector $|\mathbf{k}, \mu\rangle$. Here we confine ourselves to the case of zero temperature.

We calculate $\chi_{0\delta}$ with δ up to the neighbor (4 4 0) (in units of a/2) for both fcc and bcc lattices; the neighbor (4 4 0) is the 17th neighbor in an fcc lattice and the 12th one in a bcc lattice. In the calculation we perform the **k** summation of Eq. (5) with the same number of **k** points as the calculation of $\chi(Q)$. Replacing the summation over the whole lattice sites in Eq. (3) by the summation up to the shell of the neighbor δ , we can obtain an approximate estimate of $\chi(Q)$, $\chi_{\delta}(Q)$; that is,

$$\chi_{\delta}(\boldsymbol{Q}) = \sum_{\delta'(\boldsymbol{R}_{\delta'} \leq \boldsymbol{R}_{\delta})} \chi_{0\delta'} \exp(i\boldsymbol{Q}\boldsymbol{R}_{\delta'}) , \qquad (6)$$

where $R_{\delta} = |\mathbf{R}_{\delta}|$. In Fig. 4 we show the obtained $\chi_{\delta}(\mathbf{Q})$ of various δ 's for fcc Fe and Cr, together with a correct $\chi(\mathbf{Q})$ calculated by Eq. (1). It is found that $\chi_{\delta}(\mathbf{Q})$ can reproduce a general feature of $\chi(\mathbf{Q})$ well even by a summation of a relatively small number of neighboring shells, which is consistent with a similar discussion for $\chi(\mathbf{Q}) = \mathbf{0}$, or equivalently for the density of state $\rho(E_{\rm F})$.¹³



Fig. 5. The δ dependence of $\chi_{0\delta}$ (lower figure) and $\chi_{\delta}(\mathbf{Q})$ (upper figure) for (a) fcc Fe and (b) Cr. In the lower figures, we omit (a) $\chi_{0\delta}$ for δ of the first neighbor in an fcc lattice and (b) that of the first and second ones in a bcc lattice. In the upper figures, small marks represent $\chi_{\delta}(\mathbf{Q})$ and a large mark represents the correct value of $\chi(\mathbf{Q})$ for \mathbf{Q} along (a) $a^*(1, q, 0)$ and (b) $a^*(q, 0, 0)$. Each figure of a different q is specified by the kind of mark and is shifted by one for every change of q.

Let us discuss the maximum of $\chi_{\delta}(Q)$ in comparison with that of $\chi(Q)$. For fcc Fe, $\chi_{(440)}(Q)$ has a maximum around $Q = a^*(1, 8/48, 0)$, while both $\chi_{(220)}(Q)$ and $\chi_{(400)}(Q)$ have a maximum at $Q = a^*(1, 0, 0)$. Although the maximum of $\chi_{(440)}(Q)$ is not so clear as that of the correct $\chi(Q)$, as is seen in Fig. 4. their positions of maximum are rather close to each other; the correct $\chi(Q)$ has a maximum around $Q = a^*(1, 7/48, 0)$. For Cr, $\chi_{\delta}(Q)$ has a maximum at Q $=a^{*}(1, 0, 0)$ even for $\delta = (4 \ 4 \ 0)$ and there seems no indication that $\chi_{\delta}(Q)$ comes to have a maximum around $Q = a^*(46/48)$, 0, 0) at which the correct $\chi(Q)$ has a maximum. To make this clear, we investigate the convergence of $\chi_{\delta}(Q)$ with respect to δ . Figure 5 shows $\chi_{0\delta}$ and $\chi_{\delta}(Q)$ as a function of δ . It is found for Cr that $\chi_{0\delta}$ nearly converges to zero and $\chi_{\delta}(Q)$ settles to a certain value for δ within the 9th and 12th neighbor shells. The disagreement between this value and the correct $\chi(Q)$ is particularly large for the case q = 46/48, which is the position of the maximum of $\chi(Q)$. It

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Fig. 6. Figure similar to Fig. 2, except that $\chi(Q; E_F)$ is replaced by $\chi_{(440)}(Q; E_F)$.

may therefore be concluded that $\chi_{\delta}(Q)$ cannot reproduce the maximum of $\chi(Q)$ even for δ of a fairly distant neighboring shell. The maximum of $\chi(Q)$ of Cr cannot be explained in a real space picture referring to neighbors, but in a reciprocal k space picture, that is, by the nesting of the Fermi surface, which is consistent with the discussion in § 2.

Returning to fcc Fe, we find from Fig. 5 that $\chi_{0\delta}$ of fcc Fe roughly converges to zero, though the convergence is slow compared with that of Cr. Accordingly $\chi_{\delta}(Q)$ of fcc Fe is gradually approaching a certain value for δ up to the 17th neighbor shell. We expect that the disagreement between $\chi_{\delta}(Q)$ and the correct $\chi(Q)$ is due mainly to this slow convergence of $\chi_{0\delta}$ and that $\chi_{\delta}(Q)$ can

correctly reproduce the maximum of $\chi(Q)$ when the convergence is attained for a more distant δ . In fact, $\chi_{\delta}(Q)$ for δ of the 17th neighbor (4.4.0) reproduces at least the position of the maximum of $\chi(Q)$, as is mentioned above. We thus reach the conclusion that the maximum of $\chi(Q)$ of fcc Fe can be explained in a real space picture.

In Fig. 6 we show figures similar to Fig. 2 discussed in § 2; we show $\chi_{(440)}(Q; E_F)$ in place of $\chi(Q; E_F)$. It is found that for fcc Fe the E_F dependence of $\chi(Q; E_F)$ can be generally reproduced by $\chi_{(440)}(Q; E_F)$, though the change with respect to Q is not fully reproduced. We again expect that an improvement will be brought about by $\chi_{\delta}(Q)$ of a more distant δ . As for Cr, it is found that the peak of $\chi(Q; E_F)$ due to the nesting of the Fermi surface cannot be reproduced by $\chi_{(440)}(Q; E_F)$, as is naturally expected.

We thus confirm that the maximum of $\chi(Q)$ can be ascribed to the nesting of the Fermi surface for the case of Cr but to a mechanism describable in a real space picture for the case of fcc Fe. Here we discuss this mechanism in brief, recalling that the maximum of $\chi(Q)$ can be reproduced by $\chi_{(440)}(Q)$ for fcc Fe. We can write $\chi_{(440)}(Q)$ for $Q = a^*(1, q, 0)$ as

$$\chi_{(440)}(Q) = K_0 + K_2 \cos(2\pi q) + K_4 \cos(4\pi q), \qquad (7)$$

where $K_0 = \chi_{0(000)} - 4\chi_{0(110)} + \cdots$, $K_2 = 2\chi_{0(200)} - 8\chi_{0(211)} + \cdots$ and $K_4 = 2\chi_{0(400)} - 8\chi_{0(411)} + \cdots$. We note that $\chi_{0\delta}$ for δ of the nearest neighbor, $\chi_{0(110)}$ gives a constant term in $\chi_{\delta}(Q)$ of $Q = a^*(1, q, 0)$. This is a peculiarity of the symmetry line $Q = a^*(1, q, 0)$; the state specified by a wave vector on this line is described as a stacking of antiferromagnetic planes with a magnetic coupling between adjacent planes modified by q, and the contribution of $\chi_{0(110)}$ between adjacent planes always cancels out. The maximum of $\chi_{\delta}(Q)$ can be easily solved from Eq. (7) and is turned out to be determined by

competition between K_2 and K_4 , or by total balance among $\chi_{0\delta}$'s. When $\chi_{\delta}(\mathbf{Q})$ has a maximum around $\mathbf{Q} = a^*(1, q, 0)$ of $q \neq 0$, there must be a large negative K_4 (correctly speaking, $|K_2| < -4K_4$); in other words,the contribution from $\chi_{0\delta}$ for δ of a relatively distant neighbor such as $\chi_{0(400)}$ must exceed that from $\chi_{0\delta}$ for δ of a near neighbor such as $\chi_{0(200)}$. In the present case, $\chi_{0(422)}$ has a large negative value (see Fig. 5) and plays an important role in determining the maximum of $\chi_{\delta}(\mathbf{Q})$. The mechanism discussed here is thus analogous to that operating in insulator helical magnets like MnO₂,^{14),15)} and is essentially the same as we presented previously in the discussion about the possibility of the SDW ground state in fcc Fe.

§4. Helical SDW

We have so far discussed the SDW states in transition metals on the basis of electronic structure of nonmagnetic state. Although an ordering wave vector of SDW has been expected to be not far from Q_0 , we have to calculate electronic structure of SDW states with finite magnetic moments to obtain the ordering wave vector correctly. Up to the present, an electronic structure calculation of SDW states has never been carried out except for the calculation by means of a real space method.⁹⁾ This is because the size of matrices to be solved is fairly large for SDW states of a long period in orthodox band calculation methods. We can now manage to calculate the electronic structure of SDW states in a simplified model explained below. On the basis of calculated electronic structure of SDW states, we discuss in this section the stable SDW state and the magnitude of local magnetic moments of fcc Fe and Cr.

As is well known, there are a few types of SDW, for example, helical one, sinusoidal one and so on. Experimentally, the SDW of Cr is a sinusoidal one⁶⁾ and that of fcc Fe is conjectured to be a helical one.³⁾ Nevertheless we take helical SDW states only into consideration. The calculation for sinusoidal SDW states is more difficult than that for helical SDW states, because in sinusoidal SDW states the magnitude of a magnetic moment at each atomic site is modulated and hence the number of electrons at each atomic site is modulated.¹⁶⁾ As for helical SDW states, the direction of a magnetic moment at each atomic site is modulated but the magnitude of a magnetic moment at each atomic site is modulated but the magnitude of a magnetic moment, as well as the number of electrons, is the same for every atomic site.

We calculate electronic structure of helical SDW states with a simple model Hamiltonian based on the first-principle tight-binding method. Although tightbinding parameters in spin-polarized system are in principle to be obtained by potential parameters determined self-consistently in the local spin density functional formalism, we make the following simplification to reduce difficulties of computation. We first assume that most of the tight-binding parameters are the same as those of the nonmagnetic state except for the energy levels of d orbitals. This assumption is naturally justifiable when the magnitude of local magnetic moments is small, as is seen in the calculation of antiferromagnetic Cr.¹⁷⁾ We next introduce parameters Uand J which reflect electron correlation effect; U represents the intra-atomic Coulomb integral between d orbitals and J represents the exchange one. We then adopt a

Hartree-Fock approximation to determine the spin-dependent shift of the energy levels of d orbitals in a self-consistent manner. It is to be noted that for helical SDW states the parameter which we vary is a single one $U_{\mathbb{R}} \equiv (U+4J)/5$, since there is no charge modulation in helical SDW states. Details of the derivation of the model Hamiltonian is referred to Ref. 9).

The Hamiltonian for helical SDW states which we take is accordingly written as the sum of the tight-binding one of nonmagnetic state, H_{non} and the parametrized one for the electron correlation in d orbitals; that is,

$$H_{\rm SDW} = H_{\rm non} + \sum_{i} \sum_{m \in d} \sum_{\sigma, \sigma'} (\mathcal{D}_i)_{\sigma\sigma'} a^{\dagger}_{im\sigma} a_{im\sigma'}$$

$$\tag{8}$$

with

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$$D_{i} = -U_{\rm R} M_{di} \frac{1}{2} \begin{bmatrix} \cos \theta_{i} & \sin \theta_{i} \exp(-i\phi_{i}) \\ \sin \theta_{i} \exp(i\phi_{i}) & -\cos \theta_{i} \end{bmatrix} , \qquad (9)$$

where $a_{im\sigma}$ ($a_{im\sigma}^{\dagger}$) is the annihilation (creation) operator for an electron of spin σ in the *m*th orbital on the *i*th site. The direction of the magnetic moment at the *i*th site is described by the polar angle θ_i and the azimuthal one ϕ_i , and we can choose the conditions $\theta_i = QR_i$ and $\phi_i = 0$ without loss of generality for a helical SDW with a single wave vector Q. The *d*-component of the magnitude of the magnetic moment at the *i*th site, M_{di} , which is common for every atomic site in the case of helical SDW states (that is, $M_{di} = M_d$ irrespective of *i*), is determined self-consistently by the following equations:

$$M_{di} = \sum_{m \in d} \left[\cos \theta_i (\langle a_{im \uparrow}^{\dagger} a_{im \uparrow} \rangle - \langle a_{im \downarrow}^{\dagger} a_{im \downarrow} \rangle) + \sin \theta_i (\exp(-i\phi_i) \langle a_{im \uparrow}^{\dagger} a_{im \downarrow} \rangle + \exp(i\phi_i) \langle a_{im \downarrow}^{\dagger} a_{im \uparrow} \rangle) \right]$$
(10)

and

$$\langle a_{im\sigma}^{\dagger}a_{im\sigma'}\rangle = (-1/\pi) \operatorname{Im} \int^{E_{\rm F}} d\omega \langle im\sigma | (\omega - H_{\rm SDW})^{-1} | im\sigma' \rangle .$$
⁽¹¹⁾

The Hamiltonian H_{SDW} can be readily solved in the basis set consisting of $|\boldsymbol{k}m\sigma\rangle$, $|\boldsymbol{k}+Qm\sigma\rangle$, ..., where the number of these basis vectors depends on the period of SDW.

In practice we calculate the electronic structure of commensurate helical SDW states of $Q = a^*(1, q, 0)$ with q = 0, 1/8, 1/4 in an fcc lattice and $Q = a^*(q, 0, 0)$ with q = 1, 15/16, 7/8 in a bcc lattice. The size of the matrix to be solved is $36L_{\text{SDW}}$ for the fcc SDW and $18L_{\text{SDW}}$ for the bcc SDW, where L_{SDW} denotes the number of layers of which one period of SDW consists; for example, the matrix is 576×576 for the fcc SDW with $Q = a^*(1, 1/8, 0)$ and also 576×576 for the bcc SDW with $Q = a^*(15/16, 0, 0)$. We note that the electronic structure calculation of helical SDW states with a large L_{SDW} requires much computation time even by this simplified model and that it is still difficult to perform the calculation by the LMTO method or another.

As for an arbitrary parameter U_{R} , we can estimate a value of U_{R} from the first-principle LMTO calculation for the antiferromagnetic states of fcc Fe or Cr. For example, we can tentatively choose U_{R} such that the magnitude of local magnetic moments of the antiferromagnetic state calculated by the present model coincides



Fig. 7. Magnitude of local magnetic moments of (a) the states AF, H(1/8) and H(1/4) of fcc Fe and (b) the states AF, H(15/16) and H(7/8) of Cr. The cases of $n_e=7.92$, 8 and 8.08 are shown for fcc Fe and those of $n_e=5.92$, 5.96 and 6 are shown for Cr. The value indicated in figures represents the value of $U_{\rm R}$ (mRy).



Fig. 8. Energy of the SDW states of (a) fcc Fe and (b) Cr. The energy is measured from that of the corresponding nonmagnetic state. Others are the same as Fig. 7.

with that by the LMTO method, which was reported to be about 1.6 $\mu_{\rm B}$ for fcc Fe¹⁸⁾ and 0.3 $\mu_{\rm B}$ for Cr¹⁷⁾ in the case of the experimental lattice constant. Nevertheless we do not determine a specific value of $U_{\rm R}$ but discuss changes of the magnitude of local magnetic moments and the energy with respect to a change of $U_{\rm R}$ to illustrate the

difference between fcc Fe and Cr. Discussion concerning the value of U_{R} and in addition the validity of the present model will be published elsewhere together with details of the calculation.

Now let us discuss results of the calculation. For the sake of simplicity, we abbreviate the fcc SDW states of $Q = a^*(1, q, 0)$ with q = 0, 1/8 and 1/4 as states AF, H(1/8) and H(1/4), respectively and the bcc SDW states of $Q = a^*(q, 0, 0)$ with q = 1, 15/16 and 7/8 as states AF, H(15/16) and H(7/8), respectively. We show in Fig. 7 the magnitude of local magnetic moments, M and in Fig. 8 the energy, E of these SDW states, where E is measured from the energy of the nonmagnetic state with the same $n_{\rm e}$. For fcc Fe we present cases of the valence $n_{\rm e}=7.92$, 8 and 8.08. For Cr we present cases of $n_{\rm e}=5.92$, 5.96 and 6; for the case that $n_{\rm e}$ is more than 6, we have an almost only solution of the state AF for a small $U_{\rm R}$.

In the first place, we look over the change of M with respect to the change of $U_{\rm R}$ for every case of $n_{\rm e}$. The change of M is rather moderate for fcc Fe compared with that for Cr; we note here that we choose values of $U_{\rm R}$ at intervals of 4 mRy for fcc Fe and of 1 mRy for Cr. There is almost no essential difference between the cases $n_{\rm e} = 7.92$, 8 and 8.08 for fcc Fe, whereas there is an obvious difference between the cases $n_{\rm e} = 5.92$ and 6 for Cr. As for the change of M between SDW states, it is found for fcc Fe that M of the state AF is the largest of the three when $U_{\rm R}$ is small and that M of the state H(1/4) becomes the largest when $U_{\rm R}$ becomes large. On the other hand, it is found for Cr that M of the state AF is always the largest except for the case of $U_{\rm R} = 0.075$ Ry and $n_{\rm e} = 5.92$, where the states AF and H(15/16) becomes large and finally the state H(15/16) cannot hold a finite M.

In the next place we discuss the state having the lowest energy. It is found first that the state having the largest *M* does not always have the lowest energy. For fcc Fe, the state H(1/8) has the lowest energy of the three for all cases of $U_{\rm R}$ and $n_{\rm e}$. However, the energy difference between the states H(1/8) and H(1/4) becomes smaller, regardless of $U_{\rm R}$, when $n_{\rm e}$ increases. We therefore expect that q of the wave vector $a^*(1, q, 0)$ of the lowest energy state increases continuously between 1/8 and 1/4. As for Cr, the state H(15/16) is found to be the lowest energy state of the three for every case of $n_{\rm e}$ =5.92, 5.96 or 6, when $U_{\rm R}$ is so small that M of the state AF is around 0.3 $\mu_{\rm B}$. Nevertheless, we expect that q of the wave vector $a^*(q, 0, 0)$ of the lowest energy state is between 7/8 and 15/16 for $n_e = 5.92$, around 15/16 for $n_e = 5.96$, and between 15/16 and 1 for $n_e=6$, judging from the energy difference between the three states. As U_{R} becomes large and accordingly M becomes large, q approaches 1 and the state AF gets to have the lowest energy for every case of $n_{\rm e}$. It is to be emphasized that the wave vector of the lowest energy SDW state when M is small agrees with the wave vector at which the unenhanced spin susceptibility becomes maximum for both fcc Fe and Cr. We however need further calculations for a state with an intermediate value of q between 0, 1/8 and 1/4 for the fcc SDW and between 1, 15/16 and 7/8 for the bcc SDW to determine the wave vector of the lowest energy state accurately.

We here refer to the difference in the SDW states between fcc Fe and Cr. As is seen above, the SDW of fcc Fe is rather stiff but the SDW of Cr is soft against the

change of $U_{\rm R}$ or $n_{\rm e}$; the magnitude of magnetic moments or the wave vector of the lowest energy SDW state does not change much for fcc Fe but it changes much for Cr. Above all, the behavior against the change of $U_{\rm R}$ and hence against that of M is different between fcc Fe and Cr: when M becomes large, the wave vector of the lowest energy SDW state remains almost the same position for fcc Fe, while it approaches rapidly to the wave vector of the antiferromagnetic state for Cr. This rapid change of the wave vector for Cr may be due to the fact that the SDW of Cr is ascribed to the nesting of the Fermi surface. We suppose that features which the Fermi surface of nonmagnetic state possesses fade out and the nesting of the Fermi surface becomes obscure when M becomes large. In this connection, we may add the following fact: in the case that the SDW state H(15/16) or H (7/8) of Cr has the lowest energy, the SDW state gain a certain amount of energy, for example, about 0.08 mRy for the state H(15/16) or $n_{\rm e}$ =5.96 (see Fig. 8), once having a solution of a finite M. The explanation of this fact in view of the nesting of the Fermi surface will be presented in a future publication.

§ 5. Concluding remarks

We have discussed in the former half of this paper the SDW states of fcc Fe and Cr on the basis of the unenhanced spin susceptibility $\chi(Q)$ and the non-local spin susceptibilities $\chi_{0\delta}$'s of nonmagnetic state. We have obtained for Cr substantial evidences pointing that the nesting of the Fermi surface plays a decisive role in determining the maximum of $\chi(Q)$ and hence the wave vector of SDW. Above all, the typical shift of peaks observed in the $E_{\rm F}$ dependence of $\chi(Q)$ and the estimate of the contribution from energy bands lying in the vicinity of the Fermi surface are conclusive evidences. In contrast to Cr, we have not obtained an evidence pointing that the nesting of the Fermi surface plays such a decisive role for fcc Fe. We have then tried to discuss the origin of the $\chi(Q)$ maximum of fcc Fe in terms of $\chi_{0\delta}$, in other words, a real space expansion of $\chi(Q)$. It has been found that the real space expansion of $\chi(Q)$ up to the 17th neighbor (4.4.0) of an fcc lattice can reproduce the maximum position of $\chi(Q)$ of fcc Fe. This fact enables us to conclude that the $\chi(Q)$ maximum of fcc Fe is determined by balance among $\chi_{0\delta}$'s, or by competition between $\chi_{0\delta}$'s for δ of a near neighbor and those of a slightly distant neighbor. The origin of the SDW of fcc Fe thus has been shown to be different from that of Cr.

Now we briefly recall the previous discussion in which we predicted the possibility of the SDW ground state of fcc Fe. As mentioned in § 1, the difference between the previous discussion and the present one consists essentially in the kind of wave vectors. In the previous discussion, we investigated SDW states with a wave vector $Q = a^*(q, 0, 0)$ to show that the condition for the appearance of SDW is given by $\chi_{0\delta}$ for a near neighbor δ such as $\chi_{0(110)}$ and $\chi_{0(200)}$. Since behavior of these $\chi_{0\delta}$'s with respect to the filling of d band is simple, we could connect the appearance of SDW with the number of d electrons as follows: the most stable state changes continuously from an antiferromagnetic state to a ferromagnetic state via an SDW one when the number of d electrons changes from five to ten. In the present case of $Q = a^*(1, q, 0)$, however, the condition for the appearance of SDW is given by $\chi_{0\delta}$ for δ of a distant

neighbor, the behavior of which is rather complex. It is therefore not easy to express the appearance of SDW adequately by connecting with a quantity with a physical meaning, though the number of d electrons is really a decisive factor in the appearance of SDW. At any rate, the mechanism of the appearance of SDW which we presented previously has been proved to be valid.

In the latter half of this paper we have shown that helical SDW states with finite magnetic moments have really lower energy than the antiferromagnetic state; that the wave vector of the helical SDW state having the lowest energy nearly equals to that obtained from the maximum of the unenhanced spin susceptibility when the magnitude of local magnetic moments is small. We have investigated characteristics of the helical SDW states in view of the magnitude of local magnetic moments and the state of the lowest energy. The change of the state of the lowest energy when the magnitude of local magnetic moments becomes large has revealed the difference in the helical SDW states between fcc Fe and Cr. The difference is considered to arise from the fact that the SDW of Cr is ascribed to the nesting of the Fermi surface but the SDW of fcc Fe is not. Finally, we must add that we have discussed helical SDW states instead of sinusoidal ones for Cr. We expect however that the energy difference between helical and sinusoidal SDW states with the same wave vector is small compared with the energy difference between helical SDW states with different wave vectors. The conclusion for the stable SDW is therefore expected to be unchanged.

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