Spatial modulations of multiple-Q spin density coupled with lattice distortion, and magnetism of γ-Fe precipitated in Cu

1989 J. Phys.: Condens. Matter 1 7971

(http://iopscience.iop.org/0953-8984/1/42/020)

J. Phys.: Condens. Matter **1** (1989) 7971–7975. Printed in the UK

LETTER TO THE EDITOR

Spatial modulations of multiple-Q spin density coupled with lattice distortion, and magnetism of γ-Fe precipitated in Cu

T Jo
Department of Physics, Faculty of Science, Osaka University, Toyonaka 560, Japan

Received 14 August 1989

Abstract. Relations between periods of spatially modulated first-kind antiferromagnetic structure and orthorhombic lattice distortion in an FCC lattice are discussed on the basis of Landau's phenomenological theory. The period of the modulation of the magnetisation is shown to be either the same as or twice that of the lattice distortion. On the basis of the results, the magnetic structure below the Néel point in γ-Fe precipitated in a Cu matrix, which was recently shown to exhibit periodic lattice distortion, is discussed.

γ-Fe precipitated in Cu, which has an FCC structure and dimensions of about a few hundreds or thousands of Å, is well known to exhibit first-kind antiferromagnetism (AF) (see figure 1) [1]. Recently, a periodic lattice distortion with a wavelength of about 100 Å was reported to occur simultaneously with the onset of the magnetic ordering at low temperatures [2, 3]. The spatial modulation of the distortion is restricted to within the c plane and is approximately described by a sinusoidal transverse wave propagating along the (110) direction with an amplitude along the $(1\bar{1}0)$ direction and a local distortion $|a/b - 1| \simeq 0.02$ (see figure 2) [3]. The uniform distortion is very small compared with the local one [3]. This seems to be due to the fact that γ-Fe precipitates are enclosed by a rigid FCC Cu matrix, which prohibits *a free* uniform distortion. The cubic–tetragonal or cubic–orthorhombic distortion, which is considered to be a precursor of the martensitic transformation from FCC to BCC structure, is therefore supposed to emerge as the spatially modulated ones with 'a local orthorhombic structure'. The period of the magnetic modulation, which is supposed to couple with the lattice, is furthermore reported to be the same as that of the lattice distortion [4]. This is in striking contrast to the case of a longitudinal distortion, where in Cr, for example, the wavelength of the magnetic modulation λ_m is usually known to be twice that of the lattice modulation λ_l due to time-reversal symmetry [5]. One of the purposes of the present work is to discuss a relationship between λ_m and λ_l in the case of FCC first-kind AF coupled with the lattice distortion, on the basis of Landau's phenomenological theory. Another purpose is to discuss magnetic structures of γ-Fe based on results from phenomenological theory.

We expand the free-energy density as a function of the coordinate along the direction of wave propagation, s, in terms of magnetic order parameters and symmetry strains. In the case of the FCC first-kind AF structure, we have three equivalent wavevectors to describe it, i.e. $\boldsymbol{Q}_x = (2\pi/a)\,(100)$, $\boldsymbol{Q}_y = (2\pi/a)\,(010)$ and $\boldsymbol{Q}_z = (2\pi/a)\,(001)$ (a being the

0953-8984/89/427971 + 05 $02.50

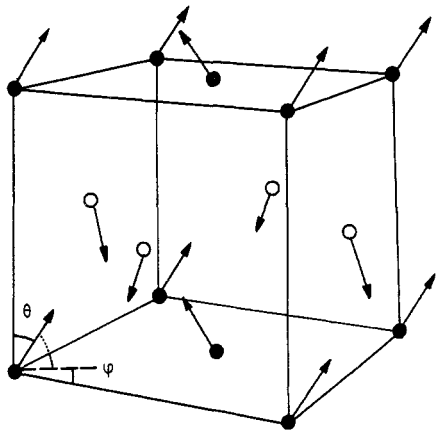

Figure 1. A general first-kind AF structure on an FCC lattice, $\sin\theta\cos\varphi|Q_x\rangle + \sin\theta\sin\varphi|Q_y\rangle + \cos\theta|Q_z\rangle$, with $|Q_i\rangle$ the single-$\boldsymbol{Q}$ state described by the wavevector $\boldsymbol{Q}_i$.

lattice constant) which are not connected by the reciprocal-lattice vectors. A general first-kind structure is therefore described by a superposition of the magnetisations $\boldsymbol{M}_x$, $\boldsymbol{M}_y$ and $\boldsymbol{M}_z$ corresponding to $\boldsymbol{Q}_x$, $\boldsymbol{Q}_y$ and $\boldsymbol{Q}_z$, respectively, i.e. a multiple-spin-density wave (see figure 1), and the relative stability of these magnetic structures has been discussed by many authors [6]. The symmetry strains describing the tetragonal–orthorhombic distortion are $e_2 = (1/\sqrt{2})(e_{xx} - e_{yy})$ and $e_3 = (1/\sqrt{6})(2e_{zz} - e_{xx} - e_{yy})$, where the e_{ii} are strain tensors. Then the free-energy density $f(s)$ is expanded in terms of M_x, M_y, M_z, e_2 and e_3 as

$$\begin{aligned} f(s) = \sum_i \Big(& a_0(\mathrm{d}M_i/\mathrm{d}s)^2 + a_1M_i^2 + a_2M_i^4 + a_3M_i^2 \sum_{j(\neq i)} M_j^2 + a_4M_i^6 \\ & + a_5M_i^4 \sum_{j(\neq i)} M_j^2 + a_6M_i^2 \sum_{j(\neq i)} M_j^2 \sum_{k(\neq i,j)} M_k^2 \Big) \\ & + \sum_n [b_0(\mathrm{d}e_n/\mathrm{d}s)^2 + b_1e_n^2] + b_2(e_3^3 - 3e_2^2e_3) \\ & + c_1[e_2(M_x^2 - M_y^2)/\sqrt{2} + e_3(2M_z^2 - M_x^2 - M_y^2)/\sqrt{6}] \end{aligned} \tag{1}$$

up to the sixth (third) order with respect to the magnetisation (strain) and up to second order with respect to their first derivatives, where the last term denotes the coupling between the magnetisations and the strains. The a_i, the b_i and c_1 are expansion coefficients. When the order parameters are independent of s, the relations between the lattice distortion and the magnetic structure are obtained from symmetry considerations [7]. For $c_1 > 0$, which is expected to apply to AF FCC transition metals and their alloys, we have the following solution. (i) The cubic symmetry for the paramagnetic state with the M_i^z equal to zero or for the triple-$\boldsymbol{Q}$ state with $M_x^2 = M_y^2 = M_z^2$. (ii) The tetragonal symmetry with $c/a < 1$ ($c/a > 1$) for $M_x^2 = M_y^2 < M_z^2$ etc ($M_x^2 = M_y^2 > M_z^2$ etc). (iii) The orthorhombic symmetry for $M_x^2 > M_y^2 > M_z^2$ etc.

By taking into account a recent magnetic measurement [4], we now solve the variational problem of minimising the functional $F = \int \mathrm{d}s\, f(s)$ using the trial functions

$$M_x = M\cos(\theta(s) + \pi/4)) \tag{2a}$$

and

$$M_y = M\sin(\theta(s) + \pi/4) \tag{2b}$$

where M is a constant and, among the order parameters, only e_2 is dependent on s, i.e. M_z and e_3 are independent of s. Then (1) is, apart from constant terms, expressed as

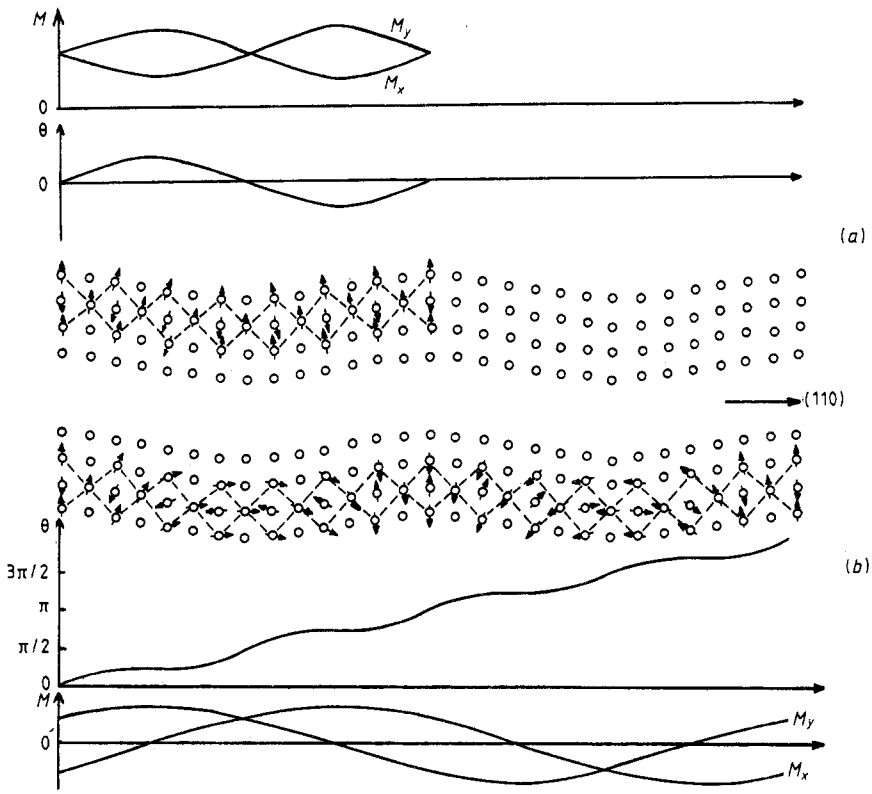

Figure 2. A schematic illustration of elastic and magnetic modulations for the 'oscillatory' (*a*) and 'rotational' (*b*) solutions (see text).

$$f(s) = A/2e_2^2 + (\alpha/2)(\mathrm{d}e_2/\mathrm{d}s)^2 + B\cos 4\theta + (\beta/2)(\mathrm{d}\theta/\mathrm{d}s)^2 + ge_2 \sin 2\theta \tag{3}$$

where A, B, α, β and g are suitable coefficients. We first remove e_2 and $\mathrm{d}e_2/\mathrm{d}s$ from the Euler equation $\partial F/\partial e_2 - (\mathrm{d}/\mathrm{d}s)(\partial F/\partial(\mathrm{d}e_2/\mathrm{d}s)) = 0$, i.e.

$$Ae_2 + g\sin 2\theta - \alpha\,\mathrm{d}^2e_2/\mathrm{d}s^2 = 0. \tag{4}$$

Then (3) reduces to

$$f(s) = (\beta'/2)(\mathrm{d}\theta/\mathrm{d}s)^2 + B'\cos 4\theta + \text{constant}. \tag{5}$$

The coefficients are given as

$$\beta' = \beta[1 + (2\alpha/\beta)(g/A)^2] \tag{6}$$

and

$$B' = B(1 + g^2/4AB) \tag{7}$$

both of which are assumed to be positive. The Euler equation for the functional given by the density (5) is obtained as

$$\beta'\,\mathrm{d}^2\theta/\mathrm{d}s^2 + 4B'\sin 4\theta = 0. \tag{8}$$

This is simply 'the equation of motion for the simple pendulum under a gravitational

field', if we regard 4θ as the angle of the pendulum measured from the potential-minimum position and s as the time. We have two types of solution. (i) If the maximum of $(\beta'/2)(\mathrm{d}\theta/\mathrm{d}s)^2$ is smaller than $2B'$, θ is an oscillatory function with $|\theta(s)| < \pi/4$, where λ_1 is equal to λ_m and we call this the 'oscillatory solution' (see (2) and (4), and figure 2(a)). (ii) If the maximum of $(\beta'/2)(\mathrm{d}\theta/\mathrm{d}s)^2$ is larger than $2B'$, $\theta(s)$ is a function describing 'the rotation of the pendulum exceeding the potential-maximum position', where λ_m is equal to $2\lambda_1$ and we call this the 'rotational solution' (see (2) and (4), and figure 2(b)).

The 'oscillatory' solution is, using Jacobi's elliptic function $\mathrm{sn}(z, k)$ with modulus k, expressed as

$$\theta = \tfrac{1}{2}\sin^{-1}(k\,\mathrm{sn}(4\sqrt{B'/\beta'}s, k)) \tag{9}$$

where $k = \frac{1}{2}\sqrt{\beta'/B'}\,(\mathrm{d}\theta/\mathrm{d}s)_0$ with the subscript 0 denoting the maximum value. The period of modulation of the lattice and magnetisation is expressed as

$$\lambda_1 = \lambda_m = \sqrt{\beta'/B'}K(k) \tag{10}$$

using the complete elliptic integral of the first kind, $K(k)$. The 'rotational' solution is, on the other hand, given by

$$\theta = \tfrac{1}{2}\sin^{-1}(\mathrm{sn}(4\sqrt{B'/\beta'}s, 1/k)) \tag{11}$$

and the period of modulation is expressed as

$$\lambda_m = 2\lambda_1 = (1/2k)\sqrt{\beta'/B'}K(1/k). \tag{12}$$

Since there is more than one magnetic order parameter in the present system, the free energy satisfying the symmetry requirement (see (1)) gives a solution with $\lambda_1 = \lambda_m$ in addition to that with $2\lambda_1 = \lambda_m$ for the coupling between the elastic and magnetic modulations.

Now we discuss magnetism of γ-Fe precipitated in a Cu matrix on the basis of the above result. Experiment [4] shows that the wavelength of the lattice distortion λ_1 is equal to that of the magnetisation λ_m, unlike in the case of longitudinal modulation, such as in Cr. The 'oscillatory' solution discussed above is considered to be realised in γ-Fe precipitated in Cu. λ_1 is furthermore suggested to be nearly proportional to the square root of the diameter of the precipitates [3]. λ_1 is $\simeq$90 Å and $T_N = 50$ K ($\simeq$120 Å and $T_N = 68$ K) for the precipitate with diameter $\simeq$300 Å ($\simeq$1000 Å) [3, 4]. We point out that the larger the maximum of the first term of (5) relative to the second term, the longer λ_1 (see (10)). In γ-Fe with larger dimensions, a nearly single-$\boldsymbol{Q}$ region described by $\boldsymbol{Q}_x$ or $\boldsymbol{Q}_y$ is supposed to be separated by the 'domain wall' or 'soliton lattice' having a double-$\boldsymbol{Q}$ structure with $\theta = 0$ (see (2)). We can furthermore expect that the longer λ_1, the more stabilised the AF state with respect to the paramagnetic state; the density of the higher-energy region reduces with the increase of λ_1. This is consistent with the fact that T_N is higher for larger precipitates. We note that for precipitates with diameters smaller than $\simeq$200 Å, T_N is reported to be $\simeq$50 K and no lattice distortion is observed even below T_N [3, 4]. In this case, the system is considered to be in the double-$\boldsymbol{Q}$ state with $M_x^2 = M_y^2$, avoiding the increase in energy due to modulation.†

† For the undistorted lattice, another magnetic structure other than the first-kind AF has recently been reported [8].

In conclusion, we have shown that the period of magnetic modulation of first-kind AF for an FCC lattice is equal to or twice that of the lattice distortion, by using Landau's phenomenological theory. We discussed, using this, the magnetism of γ-Fe precipitated in a Cu matrix. We expect that a microscopic calculation of elastic and magnetic properties of γ-Fe will confirm the condition $\lambda_1 = \lambda_m$ presented in this work. We furthermore expect that a system with $2\lambda_1 = \lambda_m$ will be found in the future.

The author would like to thank Dr Y Tsunoda for informing him of various experimental data prior to publication and for helpful discussions. Thanks are also due to Professor J Kanamori for enlightening discussions.

References

[1] Abraham S C, Guttman L and Kasper J S 1962 *Phys. Rev.* **127** 2052
[2] Ehrhart P, Schonfeld B, Ettwig H H and Pepperhoff W 1980 *J. Magn. Magn. Mater.* **22** 79
[3] Tsunoda Y and Kunitomi N 1988 *J. Phys. F: Met. Phys.* **18** 1405
[4] Tsunoda Y, Kunitomi N and Nicklow R M 1987 *J. Phys. F: Met. Phys.* **17** 2447
[5] Tsunoda Y, Mori M, Kunitomi N, Teraoka Y and Kanamori J 1974 *Solid State Commun.* **14** 287
[6] Sato H and Maki K 1976 *Prog. Theor. Phys.* **55** 319
Yoshimori A and Inagaki S 1978 *J. Phys. Soc. Japan* **44** 101
Cade N A and Young W 1980 *J. Phys. F: Met. Phys.* **10** 2035
Jo T 1983 *J. Phys. F: Met. Phys.* **13** L211
Hirai K and Jo T 1985 *J. Phys. Soc. Japan* **54** 3567
Long M W and Yeung W 1987 *J. Phys. F: Met. Phys.* **17** 1195
[7] Jo T and Hirai K 1986 *J. Phys. Soc. Japan* **55** 2017
[8] Tsunoda Y 1988 *J. Phys. F: Met. Phys.* **18** L251
Tsunoda Y 1989 *J. Phys.: Condens. Matter* at press