Thermodynamic Analysis for the Magnetic-Field-Induced Precipitation Behaviours in Steels

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Supplementary Note 1: Calculation of Diffraction Patterns

Diffraction patterns are formed by the interference of diffraction waves, which can be decomposed into structural factors ($F_{(hkl)}$) and electron scattering factors $f(s)$. The expression of the atomic scattering factor is as follows:

$$f(s) = \sum_{i=1}^{4} a_i \exp(-b_i s^2) + c \tag{S1}$$

where a_i, b_i (i = 0, 1, 2, 3, 4), and c are nine factors [1]. (Table S1) that can be obtained by consulting literature and $s = \sin\theta/\lambda$.

The structural factors can be expressed as follows:

$$F_{(hkl)} = \sum_{j=1}^{N} f_i(s)\exp[2\pi i(hx_j + ky_j + lz_j)] \tag{S2}$$

where N is the number of atoms in the unit cell, $f_i(s)$ is the atomic scattering factor of the ith atom at (x_i, y_i, z_i) in the unit cell. h, k, l are the indices of the lattice planes.

Table S1. Parameters of C, Cr and Fe in the atomic scattering factor analytical formula.

Atom	a_1	b_1	a_2	b_2	a_3	b_3	a_4	b_4	c
C	0.23238	1.01435	0.81994	5.78949	1.12081	19.2115	0.30422	54.1132	0.03179
Cr	0.88038	1.07250	2.09996	5.53692	2.20830	26.8071	1.65155	98.1169	0.12471
Fe	0.90628	1.01383	1.92631	4.97780	2.41077	24.2683	1.79055	79.4409	0.12842

The positions of atoms in the cell are used as an input file, and the zone axis is entered. The program will eventually obtain a diffraction pattern by reading the atomic coordinates and calculations, which considers the law of extinction.

Supplementary Note 2: Weiss Molecular Field Theory [2]

The magnetization of carbides can be expressed by Equation (S3):

$$M\ (T, B) = Nm(0, 0)\ B_J(\alpha) \tag{S3}$$

where M (T, B) is the magnetization, T is the absolute temperature, B is the external magnetic field, N is the number of atoms per unit volume and m (0, 0) is the magnetic moment at 0 K without the magnetic field (0 T). $B_J(\alpha)$ is the Brillouin function, which is defined as Equations (S4) and (S5),

$$B_J(\alpha) = \frac{2J+1}{2J} cth\left(\frac{2J+1}{2J}\alpha\right) - \frac{1}{2J} cth\frac{\alpha}{2J}) \tag{S4}$$

$$\alpha = \frac{nB\ \ \mu_B B}{k_B T} \tag{S5}$$

where J is the quantum number, n_B is the effective Bohr magneton number, μ_B is the Bohr magneton and k_B is the Boltzmann constant.

Supplementary Note 3: Thermodynamic Properties

The C_m is defined by Equations (S6) and (S7):

$$C_m(T, B) = k_f \frac{T}{T_C(B)} \exp\left[-4\left(1-\frac{T}{T_C(B)}\right)\right] \quad (T<T_C) \tag{S6}$$

$$C_m(T, B) = k_p \frac{T}{T_C(B)} \exp\left[8p\left(1-\frac{T}{T_C(B)}\right)\right] \quad (T>T_C) \tag{S7}$$

where $p = 2$ for all carbides in the present work. The factors k_f and k_p are obtained by Equations (S8) and (S9):

$$k_f = \frac{4(1-f_s)}{1-\exp(-4)} S_{mag} \tag{S8}$$

$$k_p = 8pf_s S_{mag} \tag{S9}$$

$$S_{mag} = Rln(m(T,B)+1) \tag{S10}$$

where f_s is 0.105 and p is two for the alloy carbides studied in this paper. S_{mag} is the magnetic entropy, which can be obtained from Equation (S10). R is the universal gas constant, and m (T, B) is the magnetic moment dependent on temperature T and magnetic field strength B.

Based on the obtained heat capacity formula, the magnetic-field-induced magnetic entropy change (ΔS_m) and magnetic-field-induced magnetic enthalpy change (ΔH_m) can be obtained by a simple mathematical integration of the magnetic capacity, as shown in Equations (S11) and (S12).

$$\Delta S_m(T,B) = \int_0^T \frac{C_{m(T,B)}}{T} dT \tag{S11}$$

$$\Delta H_m(T,B) = \int_0^T C_m(T,B)\, dT \tag{S12}$$

References

1. Jiang, J.S.; Li, F.H. Fitting the atomic scattering factors for electrons to an analytical formula. *Acta Phys. Sin.* **1984**, *33*, 845–849. (In Chinese)
2. Weiss, P. L'hypothèse du champ moléculaire et la propriété ferromagnétique. *J. Phys. Théor. Appl.* **1907**, *6*, 661–690.