

Diffuse scattering intensity near the Bragg reflection in a (para)magnetic bulk face-centred cubic Ni₃Fe-type permalloy

Sergiy M. Bokoch,^{a*} Valentyn A. Tatarenko^b and Iryna V. Vernyhora^{b,c}

^aInstitute for Advanced Materials Science and Innovative Technologies, Department of Materials Design and Technology, 15 Sauletekio Avenue, LT-10224 Vilnius, Lithuania, ^bG. V. Kurdyumov Institute for Metal Physics, N. A. S. of Ukraine, Department of Solid State Theory, 36 Academician Vernadsky Boulevard, UA-03680 Kyiv-142, Ukraine, and ^cInstitute for Applied Physics, N. A. S. of Ukraine, Department of Modeling of Radiation Effects and Microstructure Transformations in Construction Materials, 58 Petropavlivska Street, UA-40030 Sumy, Ukraine. Correspondence e-mail: sergiy.bokoch@gmail.com

Within the scope of the self-consistent-field (SCF) and mean-SCF approximations, the Matsubara–Kanzaki–Krivoglaz lattice-statics method as well as the Krivoglaz–Clapp–Moss approach, the kinematic diffuse scattering intensities near the Bragg reflection caused by the atomic short-range order (taking into account the long-range magnetic order) in a (para)magnetic bulk face-centred cubic Ni–Fe alloy are investigated in detail. The reciprocal-space symmetry analysis of both the ‘direct’ ‘electrochemical’ and short-range ‘exchange’ interactions as well as the long-range ‘indirect’ ‘strain-induced’ contribution to the Fourier components of interatomic ‘mixing’ energies and the diffuse scattering intensity contributions near the ‘fundamental’ $\Gamma(000)$ -point is carried out. In the Γ -point vicinity, the rigorous symmetry regularities for all the energy and diffuse scattering intensity contributions are formulated. As revealed, the short-range order (SRO) diffuse scattering intensity behaves conditionally as $I_{\text{SRO}}(\mathbf{k}) \propto k^2$ for $\mathbf{k} \rightarrow \mathbf{0}$ from all the reciprocal-space directions, which is in contrast to the conventional Huang diffuse scattering intensity conditionally definable as $I_{\text{Huang}}(\mathbf{k}) \propto k^{-2}$ for $\mathbf{k} \rightarrow \mathbf{0}$. Special attention is paid to the *analytic* (i.e. azimuthal) and *nonanalytic* (i.e. first-kind-jump-discontinuous ‘radial’) behaviours of the Fourier components of interatomic ‘mixing’ energies or the SRO intensities near and at the $\Gamma(000)$ -point.

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1. Introduction

Nowadays, the advanced microelectronics components in information (Waser *et al.*, 2009; Siegrist *et al.*, 2011) and energy-storage (Aricò *et al.*, 2005) technologies as well as contemporary physical metallurgy (Cahn & Haasen, 1996) are based on a wide use of imperfect crystals. On the other hand, because of significant miniaturization of working elements, scientific and technological efforts have been directed to the development of ‘condensed matter point defects’ engineering. Usually, point defects are referred to as interacting or non-interacting substitutional and interstitial impurity atoms or their structural vacancies. Thus, depending on the concentration and configurational (ordered or disordered) states of point defects, thermodynamically controlled by ambient conditions such as temperature, pressure and electromagnetic fields, a variety of physical properties can be achieved (Cahn & Haasen, 1996; Aricò *et al.*, 2005; Waser *et al.*, 2009; Siegrist *et al.*, 2011). The circumstances become even more fascinating when the point defects’ magnetic moments’ degrees of

freedom are considered. As a result, by changing both an atomic order and a magnetic one, one can expand the set of desirable properties and new phenomena in condensed matter. Therefore, information on the spatial atomic and magnetic moment configurations in condensed media is critically important for the cutting-edge design of new materials as well as for a deeper understanding of existing materials, and also is of great fundamental interest in researching the basics of interatomic interactions.

To date, one of the powerful experimental probes for investigation of point-defect interactions is the method of diffuse scattering of radiation (X-rays or thermal neutrons) (Krivoglaz, 1996; Billinge & Thorpe, 1998; Barabash *et al.*, 2009) from atomically short-range ordered (SRO) solids. As a result, depending on the interatomic interaction types (‘electrochemical’, magnetic or ‘strain-induced’ ones) and their typical action at a distance, one can experimentally observe the several principal differences in the diffuse scattering patterns. In the event of a pure ‘elastic’ (‘strain-induced’, i.e. owing to the atomic size mismatch) interaction between point

defects, the coherent Bragg reflection [at the $\Gamma(000)$ -point, $\mathbf{k}_\Gamma \equiv \mathbf{0}$] is broadened in accordance with the classical Huang diffuse scattering (Huang, 1947) conditionally definable as $I_{\text{Huang}} \propto k^{-2}$ for any quasi-wavevector $\mathbf{k} \rightarrow \mathbf{0}$. So, by measuring the Huang scattering in materials with different [face-centred cubic (f.c.c.), body-centred cubic (b.c.c.) or hexagonal close-packed (h.c.p.)] host crystal lattices and various (metallic, ionic, covalent *etc.*) host crystal binding, it becomes possible to estimate the static lattice distortions, the critical action radius for randomly distributed and elastically interacting impurities, their clusters *etc.* (Dederichs, 1971, 1973; Trinkaus, 1972; Larson & Schmatz, 1974; Larson, 1975; Peisl, 1975; Charniy *et al.*, 1991; Charniy *et al.*, 1992; Michelič & Wunderlin, 1996; Barabash *et al.*, 1999; Moreno *et al.*, 2003; Campbell, 2010). However, the general picture changes significantly when one considers the strongly ‘electrochemically’ interacting impurities in a host crystal. In this case, the disordered system undergoes atomic ordering or clustering (Krivoglaz, 1996) and hence above the order–disorder phase-transformation temperature, T_K (Kurnakov point), a variety of maxima of the diffuse scattering intensity, $I_{\text{SRO}}(\mathbf{k})$, caused by the atomic SRO are observed (Schönfeld, 1999; Ice & Sparks, 1999). Note that, in the case of an atomic ordering tendency, the SRO intensity maxima are usually located at the high-symmetry points of the first Brillouin zone (1st BZ) with the superstructural wavevectors $\mathbf{k}_s \neq \mathbf{0}$ (Schönfeld, 1999). Often, but not always, these points are the superstructural reflection positions on the diffraction patterns in the atomically long-range ordered (LRO) state. While the diffuse intensity distribution, $I_{\text{SRO}}(\mathbf{k}_s)$, is a precursor of the disorder–order reaction, the intensity at the Bragg reflection position, $I_{\text{SRO}}(\mathbf{0})$, is controlled by the microscopic atomic diffusion processes during the atomic SRO relaxation and determined

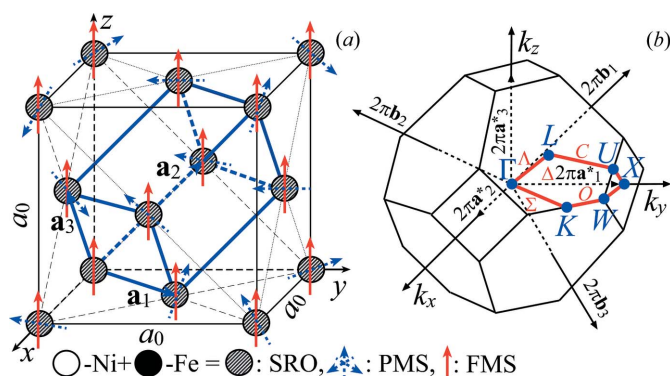


Figure 1
(a) An f.c.c. lattice and its primitive unit cell (blue solid lines) defined by the primitive fundamental translation vectors $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}$; (b) the 1st BZ of f.c.c. lattice reciprocal space; here, $\{\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3\}$ are the reciprocal-lattice translation vectors, and the triple of $\{2\pi\mathbf{a}_1^*, 2\pi\mathbf{a}_2^*, 2\pi\mathbf{a}_3^*\}$ composes the quasi-wavevector ‘star’ corresponding to the central $X(001)$ point of the 1st BZ square lateral faces and generates an atomic ordering. In (a), PMS and FMS denote the paramagnetic and ferromagnetic states of f.c.c. Ni–Fe alloys with atomic SRO only, respectively. In (b), $\Gamma, X, W, L, K(U)$ and $\Delta, Z, Q, \Lambda, \Sigma, C, O, B'$ are the high-symmetry points and the high-symmetry directions, respectively, within the irreducible part (delineated with red solid lines) of the 1st BZ.

by the ground-state energy of the *nonideal* solid solution itself (Krivoglaz, 1996). A systematic analysis of $I_{\text{SRO}}(\mathbf{k})$ near and at the \mathbf{k}_Γ -point, which takes into account the atomic and magnetic spatial orders, including the atomic size mismatch effects, is still absent in the condensed matter physics literature.

In this work, we report the classical-models-based investigation of the diffuse scattering intensities distributed near the Bragg reflection in a complex system governed by both ‘direct’ short-range and ‘indirect’ long-range interactions between point defects. We consider a (para)magnetic f.c.c. Ni_3Fe -type permalloy with atomic SRO only. This classical alloy is chosen because the concentration-dependent Curie temperatures of its magnetic phase transition, T_C , are higher than the Kurnakov points, T_K (Béranger *et al.*, 1996). Thus, while at absolute temperatures $T > T_C$ an alloy is paramagnetic with atomic SRO only, in the temperature interval (T_K, T_C) it is already macroscopically ferromagnetic with atomic SRO too.

2. Theory

The interrelation between the SRO diffuse scattering intensities and the total ‘mixing’ energy Fourier components has been proposed by Krivoglaz independently of Clapp and Moss within the scope of the self-consistent-field (SCF) fluctuation wave method (Krivoglaz, 1957; Clapp & Moss, 1966, 1968; Moss & Clapp, 1968). Nowadays, this expression is widely known as the KCM formula. For a binary substitutional alloy, e.g. f.c.c. $\text{Ni}_{1-c}\text{Fe}_c$, it is

$$I_{\text{SRO}}(\mathbf{k}) \propto \tilde{\alpha}(\mathbf{k}) \cong \frac{D}{1 + c(1 - c)\tilde{w}_{\text{tot}}(\mathbf{k})/(k_B T)}, \quad (1)$$

where $\tilde{\alpha}(\mathbf{k})$ is the equilibrium SRO parameter Fourier component [evaluated from the diffuse scattering intensity, $I_{\text{SRO}}(\mathbf{k})$, in dimensionless Laue units (L. u.) (Schönfeld, 1999)]; c is the relative concentration of an alloying component (Fe); k_B is the Boltzmann constant; T is the temperature; D is the normalization factor defined as (Krivoglaz, 1957; Khachatryan, 1974)

$$\begin{aligned} D &\cong \left[\frac{1}{\Omega} \int_{\mathbf{k} \in 1\text{st BZ}} d\mathbf{k} \tilde{\alpha}(\mathbf{k}) \right] \left[\frac{1}{N_{\text{u.c.}}} \sum_{\mathbf{k} \in 1\text{st BZ}} \frac{1}{1 + c(1 - c)\tilde{w}_{\text{tot}}(\mathbf{k})/(k_B T)} \right]^{-1} \\ &= \left[\frac{1}{N_{\text{u.c.}}} \sum_{\mathbf{k} \in 1\text{st BZ}} \frac{1}{1 + c(1 - c)\tilde{w}_{\text{tot}}(\mathbf{k})/(k_B T)} \right]^{-1} \\ &= \Omega \left[\int_{\mathbf{k} \in 1\text{st BZ}} \frac{d\mathbf{k}}{1 + c(1 - c)\tilde{w}_{\text{tot}}(\mathbf{k})/(k_B T)} \right]^{-1} \cong 1. \end{aligned} \quad (2)$$

In equation (2), the integration is made over the 1st BZ volume Ω (containing $N_{\text{u.c.}}$ \mathbf{k} -points, where $N_{\text{u.c.}}$ is the total number of unit cells). [Fig. 1 illustrates the direct-lattice conditional cubic and primitive unit cells (as well as the reciprocal-space 1st BZ) for f.c.c. Ni–Fe alloys with atomic SRO only.] Note that equation (2) is valid with a high accuracy for many close-packed alloys (Khachatryan, 1974).

As shown within the scope of the mean self-consistent-field (MSCF) approximation (Tatarenko & Radchenko, 2003; Bokoch & Tatarenko, 2008, 2010; Tatarenko *et al.*, 2008), the total ‘mixing’ energy Fourier component, $\tilde{w}_{\text{tot}}(\mathbf{k})$, with any quasi-wavevector \mathbf{k} for f.c.c. Ni–Fe-type alloys can be presented as

$$\begin{aligned}\tilde{w}_{\text{tot}}(\mathbf{k}) &= \tilde{w}_{\text{prm}}(\mathbf{k}) + \tilde{w}_{\text{mag}}(\mathbf{k}) \\ &\simeq \tilde{\varphi}_{\text{chem}}(\mathbf{k}) + \tilde{V}_{\text{si}}^{\beta\beta}(\mathbf{k}) + \tilde{w}_{\text{mag}}(\mathbf{k}) \\ &\cong \tilde{\varphi}_{\text{chem}}(\mathbf{k}) + \tilde{V}_{\text{si}}^{\beta\beta}(\mathbf{k}) + \tilde{J}_{\text{NiNi}}(\mathbf{k})s_{\text{Ni}}^2\sigma_{\text{Ni}}^2 \\ &\quad + \tilde{J}_{\text{FeFe}}(\mathbf{k})s_{\text{Fe}}^2\sigma_{\text{Fe}}^2 - 2\tilde{J}_{\text{NiFe}}(k)s_{\text{Ni}}s_{\text{Fe}}\sigma_{\text{Ni}}\sigma_{\text{Fe}}.\end{aligned}\quad (3)$$

In equation (3), $\tilde{\varphi}_{\text{chem}}(\mathbf{k})$, $\tilde{V}_{\text{si}}^{\beta\beta}(\mathbf{k})$, $\tilde{w}_{\text{prm}}(\mathbf{k})$ and $\tilde{w}_{\text{mag}}(\mathbf{k})$ are the ‘electrochemical’, ‘strain-induced’, ‘paramagnetic’ [in fact, $\tilde{\varphi}_{\text{chem}}(\mathbf{k}) + \tilde{V}_{\text{si}}^{\beta\beta}(\mathbf{k})$] and magnetic ‘mixing’ energy Fourier component contributions, respectively (Tatarenko & Radchenko, 2003; Bokoch & Tatarenko, 2008, 2010; Tatarenko *et al.*, 2008); $\tilde{J}_{\beta\beta'}(\mathbf{k})$ is an ‘exchange integral’ Fourier component as a parameter of the magnetic β – β' interaction ($\beta, \beta' = \text{Ni, Fe}$). To determine the relative spontaneous magnetizations, σ_{Ni} and σ_{Fe} , of both Ni and Fe subsystems with any allowable atomic spin numbers, s_{Ni} and s_{Fe} , let us consider the statistical thermodynamics model of a (para)magnetic f.c.c. permalloy with atomic SRO only. Thus, we are looking for the total configuration-dependent part of free energy in the form $F_{\text{conf}}^{\text{tot}} = U_{\text{conf}}^{\text{at}} + U_{\text{conf}}^{\text{mag}} - T[S_{\text{conf}}^{\text{at}} + \sum_{\beta} S_{\text{conf}}^{\text{mag}(\beta)}]$, where U_{conf} and S_{conf} are the configurational parts of the internal energies and entropies of both atomic (at) and magnetic (mag) interacting subsystems (*i.e.* $\beta = \text{Ni, Fe}$), respectively. Within the scope of both the atomic subsystem SCF and magnetic subsystem MSCF approximations according to Tatarenko & Radchenko (2003), Bokoch & Tatarenko (2008, 2010) and Tatarenko *et al.* (2008), one can obtain these configurational terms for a (para)magnetic f.c.c. Ni–Fe alloy with atomic SRO only in the simplest form as

$$U_{\text{conf}}^{\text{at}} \simeq \Delta U_{0\text{prm}}(c) + \frac{N_{\text{u.c.}}}{2} \tilde{w}_{\text{prm}}(\mathbf{0})c^2, \quad (4)$$

$$\begin{aligned}U_{\text{conf}}^{\text{mag}} &\cong \frac{N_{\text{u.c.}}}{2} \left[\tilde{J}_{\text{NiNi}}(\mathbf{0})(1-c)^2\sigma_{\text{Ni}}^2s_{\text{Ni}}^2 + \tilde{J}_{\text{FeFe}}(\mathbf{0})c^2\sigma_{\text{Fe}}^2s_{\text{Fe}}^2 \right. \\ &\quad \left. + 2\tilde{J}_{\text{FeNi}}(\mathbf{0})c(1-c)\sigma_{\text{Fe}}\sigma_{\text{Ni}}s_{\text{Fe}}s_{\text{Ni}} \right],\end{aligned}\quad (5)$$

$$S_{\text{conf}}^{\text{at}} \cong -N_{\text{u.c.}}k_{\text{B}}[c \ln c + (1-c) \ln(1-c)], \quad (6)$$

$$\begin{aligned}S_{\text{conf}}^{\text{mag}(\beta)} &\cong N_{\text{u.c.}}k_{\text{B}}c_{\beta} \left\{ \ln \sinh \left[\left(1 + \frac{1}{2s_{\beta}} \right) \xi_{\beta} \right] \right. \\ &\quad \left. - \ln \sinh \left(\frac{1}{2s_{\beta}} \xi_{\beta} \right) - \xi_{\beta} \mathcal{B}_{s_{\beta}}(\xi_{\beta}) \right\}.\end{aligned}\quad (7)$$

In equation (7), $c_{\text{Ni}} = 1 - c$, $c_{\text{Fe}} = c$ and $\mathcal{B}_{s_{\beta}}(\xi_{\beta})$ is the classical Brillouin function (Aharoni, 2000) defined as

$$\begin{aligned}\mathcal{B}_{s_{\beta}}(\xi_{\beta}) &= \left(1 + \frac{1}{2s_{\beta}} \right) \coth \left[\left(1 + \frac{1}{2s_{\beta}} \right) \xi_{\beta} \right] \\ &\quad - \frac{1}{2s_{\beta}} \coth \left(\frac{1}{2s_{\beta}} \xi_{\beta} \right);\end{aligned}\quad (8)$$

here $\xi_{\beta} \equiv s_{\beta}H_{\text{mol}}^{\beta}/(k_{\text{B}}T)$ is a characteristic magnetic-interaction-to-thermal-fluctuation energy ratio and $H_{\text{mol}}^{\beta} \cong -g_{\beta}\mu_{\text{B}}\sum_{\beta'}\Gamma_{\beta\beta'}\sigma_{\beta'}$ is the Weiss’s intracrystalline ‘molecular’-field (*i.e.* MSCF) value with coefficients $\{\Gamma_{\beta\beta'}\}$; g_{β} is the Landé factor (as assumed for transition metals, $g_{\text{Fe}} \cong g_{\text{Ni}} \cong g = 2$); μ_{B} is the Bohr magneton; $\Delta U_{0\text{prm}}$ is a configuration-independent part of an internal energy, which is a linear function of c ; $N_{\text{u.c.}}$ is the total number of f.c.c. lattice sites or primitive unit cells. Equation (7) can be obtained by the steepest-descent method (see references in Tatarenko & Radchenko, 2003; Bokoch & Tatarenko, 2008, 2010; Tatarenko *et al.*, 2008) and is valid for non-interacting magnetic moments with any non-negative integer or half-integer local spin numbers, s_{β} .

By combining equations (4)–(7), one can obtain the total configuration-dependent part of free energy for a magnetic f.c.c. Ni–Fe alloy with atomic SRO only in the form

$$\begin{aligned}\frac{F_{\text{conf}}^{\text{tot}}}{N_{\text{u.c.}}} &\cong \frac{\Delta U_{0\text{prm}}(c)}{N_{\text{u.c.}}} + \frac{1}{2} \left[\tilde{w}_{\text{prm}}(\mathbf{0})c^2 + \tilde{J}_{\text{NiNi}}(\mathbf{0})s_{\text{Ni}}^2(1-c)^2\sigma_{\text{Ni}}^2 \right. \\ &\quad \left. + 2\tilde{J}_{\text{NiFe}}(\mathbf{0})s_{\text{Ni}}s_{\text{Fe}}(1-c)c\sigma_{\text{Ni}}\sigma_{\text{Fe}} + \tilde{J}_{\text{FeFe}}(\mathbf{0})s_{\text{Fe}}^2c^2\sigma_{\text{Fe}}^2 \right] \\ &\quad + k_{\text{B}}T[c \ln c + (1-c) \ln(1-c)] \\ &\quad - k_{\text{B}}T(1-c) \left\{ \ln \sinh \left[\left(1 + \frac{1}{2s_{\text{Ni}}} \right) \xi_{\text{Ni}}(\sigma_{\text{Ni}}, \sigma_{\text{Fe}}) \right] \right. \\ &\quad \left. - \ln \sinh \left[\frac{1}{2s_{\text{Ni}}} \xi_{\text{Ni}}(\sigma_{\text{Ni}}, \sigma_{\text{Fe}}) \right] \right. \\ &\quad \left. - \xi_{\text{Ni}}(\sigma_{\text{Ni}}, \sigma_{\text{Fe}}) \mathcal{B}_{s_{\text{Ni}}}[\xi_{\text{Ni}}(\sigma_{\text{Ni}}, \sigma_{\text{Fe}})] \right\} \\ &\quad - k_{\text{B}}Tc \left\{ \ln \sinh \left[\left(1 + \frac{1}{2s_{\text{Fe}}} \right) \xi_{\text{Fe}}(\sigma_{\text{Fe}}, \sigma_{\text{Ni}}) \right] \right. \\ &\quad \left. - \ln \sinh \left[\frac{1}{2s_{\text{Fe}}} \xi_{\text{Fe}}(\sigma_{\text{Fe}}, \sigma_{\text{Ni}}) \right] \right. \\ &\quad \left. - \xi_{\text{Fe}}(\sigma_{\text{Fe}}, \sigma_{\text{Ni}}) \mathcal{B}_{s_{\text{Fe}}}[\xi_{\text{Fe}}(\sigma_{\text{Fe}}, \sigma_{\text{Ni}})] \right\}.\end{aligned}\quad (9)$$

For the paramagnetic state (PMS) domain, equation (9) transforms obviously into its conventional SCF-approximation form (Khachatryan, 1974; Krivoglaz, 1996):

$$\begin{aligned}\frac{F_{\text{conf}}^{\text{tot}}}{N_{\text{u.c.}}} &\cong \Delta U_{0\text{prm}}(c)/N_{\text{u.c.}} + \tilde{w}_{\text{prm}}(\mathbf{0})c^2/2 \\ &\quad + k_{\text{B}}T[c \ln c + (1-c) \ln(1-c)].\end{aligned}$$

Using equation (9) and the minima conditions, $\partial F_{\text{conf}}^{\text{tot}}/\partial \sigma_{\text{Ni}} \equiv 0$ and $F_{\text{conf}}^{\text{tot}}/\partial \sigma_{\text{Fe}} \equiv 0$, we can find the equilibrium values of $\sigma_{\text{Ni}}(T)$ and $\sigma_{\text{Fe}}(T)$ as solutions of the following equations:

$$\sigma_{\text{Ni}} \cong \mathcal{B}_{s_{\text{Ni}}} \left\{ -\frac{1}{(1-c)k_{\text{B}}T} \left[\tilde{J}_{\text{NiNi}}(\mathbf{0})s_{\text{Ni}}^2(1-c)^2\sigma_{\text{Ni}} + \tilde{J}_{\text{NiFe}}(\mathbf{0})s_{\text{Ni}}s_{\text{Fe}}(1-c)c\sigma_{\text{Fe}} \right] \right\}, \quad (10a)$$

$$\sigma_{\text{Fe}} \cong \mathcal{B}_{s_{\text{Fe}}} \left\{ -\frac{1}{ck_{\text{B}}T} \left[\tilde{J}_{\text{FeFe}}(\mathbf{0})s_{\text{Fe}}^2c^2\sigma_{\text{Fe}} + \tilde{J}_{\text{NiFe}}(\mathbf{0})s_{\text{Ni}}s_{\text{Fe}}(1-c)c\sigma_{\text{Ni}} \right] \right\}. \quad (10b)$$

3. Results and discussion

To estimate all the ‘mixing’ energy Fourier component contributions entering into equation (3), let us first evaluate the ‘exchange integrals’ of magnetic interactions, namely, $\{\tilde{J}_{\beta\beta'}(\mathbf{0})\}$. For this goal, we use the MSCF approximation (Tatarenko & Radchenko, 2003; Bokoch & Tatarenko, 2008, 2010; Tatarenko *et al.*, 2008) for the Curie temperature–concentration dependence in the form

$$T_{\text{C}}(c) \cong -\left((1+s_{\text{Ni}})s_{\text{Ni}}\tilde{J}_{\text{NiNi}}(\mathbf{0})(1-c) + (1+s_{\text{Fe}})s_{\text{Fe}} \times \tilde{J}_{\text{FeFe}}(\mathbf{0})c - \{[(1+s_{\text{Ni}})s_{\text{Ni}}\tilde{J}_{\text{NiNi}}(\mathbf{0})(1-c) - (1+s_{\text{Fe}})s_{\text{Fe}}\tilde{J}_{\text{FeFe}}(\mathbf{0})c]^2 + 4(1+s_{\text{Ni}})s_{\text{Ni}} \times (1+s_{\text{Fe}})s_{\text{Fe}}\tilde{J}_{\text{NiFe}}^2(\mathbf{0})(1-c)c\}^{1/2} \right) / (6k_{\text{B}}). \quad (11)$$

Fitting the experimental data on $T_{\text{C}}(c)$ by equation (11) (Bokoch & Tatarenko, 2008) with $s_{\text{Ni}} = 1/2$ and $s_{\text{Fe}} = 3/2$, we get $\tilde{J}_{\text{NiNi}}(\mathbf{0}) \cong -215.9$ meV, $\tilde{J}_{\text{NiFe}}(\mathbf{0}) \cong -231.5$ meV and $\tilde{J}_{\text{FeFe}}(\mathbf{0}) \cong +54.9$ meV. Taking into account $\tilde{J}_{\beta\beta'}(\mathbf{0}) \cong 12J_{\beta\beta'}(r_1)$, we estimate respective ‘exchange integrals’ for the first nearest-neighbour coordination shell with a radius $r_1 = a_0/2^{1/2}$ (Fig. 1a) as follows: $J_{\text{NiNi}}(r_1) \cong -17.99$ meV, $J_{\text{NiFe}}(r_1) \cong -19.29$ meV and $J_{\text{FeFe}}(r_1) \cong +4.58$ meV. Such ‘exchange integrals’ for Ni–Ni and Ni–Fe atomic pairs correspond to the ferromagnetic interactions, and for Fe–Fe pairs to the antiferromagnetic interaction. This result is in overall agreement with many experimental and theoretical data for f.c.c. $\text{Ni}_{1-c}\text{Fe}_c$ alloys obtained over years¹ as well as with the conception of γ -Fe itself. So, using the values of $\tilde{J}_{\beta\beta'}(\mathbf{0})$ and equations (10a), (10b), and (3), we can calculate the magnetic ‘mixing’ energy Fourier components, $\tilde{w}_{\text{mag}}(\mathbf{k})$, for all quasi-wavevectors \mathbf{k} near and at the \mathbf{k}_{Γ} -point. In spite of ‘exchange’ interaction differences for various atomic pairs, the resulting ‘mixing’ energy parameter, $\tilde{w}_{\text{mag}}(\mathbf{k})$, at each $T \in (T_{\text{K}}, T_{\text{C}})$ corresponds to the macroscopically ferromagnetic state. It is also evident that, due to the significant T -dependence of $\sigma_{\text{Ni}}(T)$ and $\sigma_{\text{Fe}}(T)$ [equations (10a), (10b)] at a certain concentration c , the magnetic ‘mixing’ energy Fourier components will also be strong T -dependent functions, $\tilde{w}_{\text{mag}}(\mathbf{k}, T)$, which leads to pronounced dependences of

$\tilde{w}_{\text{tot}}(\mathbf{k}, T)$ [equation (3)] (Bokoch & Tatarenko, 2010). Moreover, in view of the short-range and almost isotropic character of spin-orientation-averaged magnetic interactions, one can assume the following magnetic ‘mixing’ energy properties for f.c.c. $\text{Ni}_{1-c}\text{Fe}_c$ in a reciprocal-space representation: $\tilde{w}_{\text{mag}}(\mathbf{k})|_{\mathbf{k} \rightarrow \mathbf{0}} \equiv \tilde{w}_{\text{mag}}(\mathbf{0}) > 0$.

Let us now briefly consider the ‘strain-induced’ ‘mixing’ energy contribution, $\tilde{V}_{\text{si}}^{\beta\beta}(\mathbf{k})$, in equation (3). The relevant semi-phenomenological theory (Khachatryan, 1974; Bugaev & Tatarenko, 1989) is based on the Matsubara–Kanzaki–Krivoglaz lattice-statics method (Matsubara, 1952; Kanzaki, 1957; Krivoglaz, 1958). Within the scope of the superposition (Khachatryan, 1974) and quasi-harmonic (Khachatryan, 1974; Bugaev & Tatarenko, 1989) approximations, the gauged ‘strain-induced’ interaction energy Fourier components for each $\mathbf{k} \neq \mathbf{0}$ and $\mathbf{k} = \mathbf{0}$ are defined as

$$\tilde{V}_{\text{si}}^{\beta\beta}(\mathbf{k}) \simeq - \sum_{i,j=x,y,z} \tilde{F}^{i*}(\mathbf{k}) \tilde{G}^{ij}(\mathbf{k}) \tilde{F}^j(\mathbf{k}) + N_{\text{u.c.}}^{-1} \sum_{\mathbf{k}' \neq \mathbf{0}} \sum_{i,j=x,y,z} \tilde{F}^{i*}(\mathbf{k}') \tilde{G}^{ij}(\mathbf{k}') \tilde{F}^j(\mathbf{k}'), \quad (12)$$

$$\tilde{V}_{\text{si}}^{\beta\beta}(\mathbf{0}) \simeq -3\nu(C_{11} + 2C_{12})(L^{\beta})^2 + N_{\text{u.c.}}^{-1} \sum_{\mathbf{k}' \neq \mathbf{0}} \sum_{i,j=x,y,z} \tilde{F}^{i*}(\mathbf{k}') \tilde{G}^{ij}(\mathbf{k}') \tilde{F}^j(\mathbf{k}'). \quad (13)$$

In equations (12) and (13), $\tilde{\mathbf{F}}(\mathbf{k})$ is the Fourier-transform vector of the so-called Kanzaki fictive ‘coupling’ forces acting from dissolved β atoms onto the host crystal atoms; $\tilde{\mathbf{G}}(\mathbf{k}) = [\tilde{\mathbf{A}}(\mathbf{k})]^{-1}$ ($\mathbf{k} \neq \mathbf{0}$), where $\tilde{\mathbf{A}}(\mathbf{k})$ is the Fourier transform of the dynamic matrix of a host crystal;¹ $i, j = x, y, z$ are the Cartesian indices; $\nu = a_0^3/4$ is the volume of a primitive unit cell with a lattice parameter a_0 (Fig. 1a); C_{11} , C_{12} and C_{44} are moduli of elasticity for cubic crystals; $L^{\beta} = \{\partial \ln a_0 / \partial c_{\beta}\}|_{c_{\beta}=0}$ is the concentration coefficient of a host crystal lattice dilation (for f.c.c. α -Ni alloyed with Fe or f.c.c. γ -Fe alloyed with Ni).¹

As shown (Bokoch & Tatarenko, 2010; Oliinyk *et al.*, 2011), the long-range ‘strain-induced’ interaction energy Fourier components, $\tilde{V}_{\text{si}}^{\beta\beta}(\mathbf{k})$, along various high-symmetry directions in the 1st BZ from its surface high-symmetry points to the central $\Gamma(000)$ -point (Fig. 1b) behave in different ways [and the discontinuities of the first kind of the $\tilde{V}_{\text{si}}^{\beta\beta}(\mathbf{k})$ function take place at the \mathbf{k}_{Γ} -point: $\lim_{\mathbf{k} \rightarrow \mathbf{0}} \tilde{V}_{\text{si}}^{\beta\beta}(\mathbf{k}) \neq \tilde{V}_{\text{si}}^{\beta\beta}(\mathbf{0})$]. Namely, the gauged ‘strain-induced’ ‘mixing’ energy symmetry regularities are satisfied (Bokoch & Tatarenko, 2010; Oliinyk *et al.*, 2011) in a reciprocal-space representation as

$$\tilde{V}_{\text{si}}^{\beta\beta}(\mathbf{0}) < \tilde{V}_{\text{si}}^{\beta\beta}(\mathbf{k}_{\downarrow\uparrow\mathbf{k}_X} \rightarrow \mathbf{0}) < \tilde{V}_{\text{si}}^{\beta\beta}(\mathbf{k}_{\downarrow\uparrow\mathbf{k}_W} \rightarrow \mathbf{0}) < \tilde{V}_{\text{si}}^{\beta\beta}(\mathbf{k}_{\downarrow\uparrow\mathbf{k}_{X(U)}} \rightarrow \mathbf{0}) < \tilde{V}_{\text{si}}^{\beta\beta}(\mathbf{k}_{\downarrow\uparrow\mathbf{k}_L} \rightarrow \mathbf{0}) < 0, \quad (14)$$

as far as $C_{11} - C_{12} - 2C_{44} < 0$ and $C_{12} < C_{11}$.

Based on the analysis of diffuse scattering data obtained for disordered (para)magnetic f.c.c. Ni–Fe alloys (Bokoch & Tatarenko, 2008, 2010), we showed that the concentration dependence of ‘paramagnetic’ ‘mixing’ energy Fourier components for a few related quasi-wavevectors in the 1st BZ can be fitted as $\tilde{w}_{\text{prm}}(\mathbf{k}) \cong K_0(\mathbf{k}) + K_1(\mathbf{k})c + K_2(\mathbf{k})c^2$, where $K_m(\mathbf{k})$ ($m = 0, 1, 2$) are adjustable coefficients.¹ Using these

¹ Supplementary material for this article is available from the IUCr electronic archives (Reference: IB5019). Services for accessing this material are described at the back of the journal.

data for the f.c.c. Ni₃Fe permalloy composition, we calculate $\tilde{w}_{\text{prm}}(\mathbf{0}) \cong +0.405$ eV and $\tilde{w}_{\text{prm}}(\mathbf{k}_X) \cong -0.302$ eV. [By applying the conventional Fourier transform, we can roughly estimate ‘mixing’ energies within the two nearest-neighbour coordination shells with radii r_1 and $r_2 = a_0$ as follows: $w_{\text{prm}}(r_1) \cong +44.14$ meV and $w_{\text{prm}}(r_2) \cong -20.83$ meV, respectively.] Taking into account both the definition $\tilde{\varphi}_{\text{chem}}(\mathbf{k}) \simeq \tilde{w}_{\text{prm}}(\mathbf{k}) - \tilde{V}_{\text{si}}^{\beta\beta}(\mathbf{k})$ [equation (3)] and the short-range and isotropic character of ‘electrochemical’ ‘mixing’ energies resulting in relations $\tilde{\varphi}_{\text{chem}}(\mathbf{k})|_{\mathbf{k} \rightarrow \mathbf{0}} \equiv \tilde{\varphi}_{\text{chem}}(\mathbf{0}) > 0$ in a reciprocal-space representation, we reveal the following reciprocal-space symmetry regularities for total ‘paramagnetic’ mixing energies in the form

$$\begin{aligned} \tilde{w}_{\text{prm}}(\mathbf{0}) &< \tilde{w}_{\text{prm}}(\mathbf{k}_{\downarrow\uparrow\mathbf{k}_X} \rightarrow \mathbf{0}) < \tilde{w}_{\text{prm}}(\mathbf{k}_{\downarrow\uparrow\mathbf{k}_W} \rightarrow \mathbf{0}) \\ &< \tilde{w}_{\text{prm}}(\mathbf{k}_{\downarrow\uparrow\mathbf{k}_{K(U)}} \rightarrow \mathbf{0}) < \tilde{w}_{\text{prm}}(\mathbf{k}_{\downarrow\uparrow\mathbf{k}_L} \rightarrow \mathbf{0}) > 0. \end{aligned} \quad (15)$$

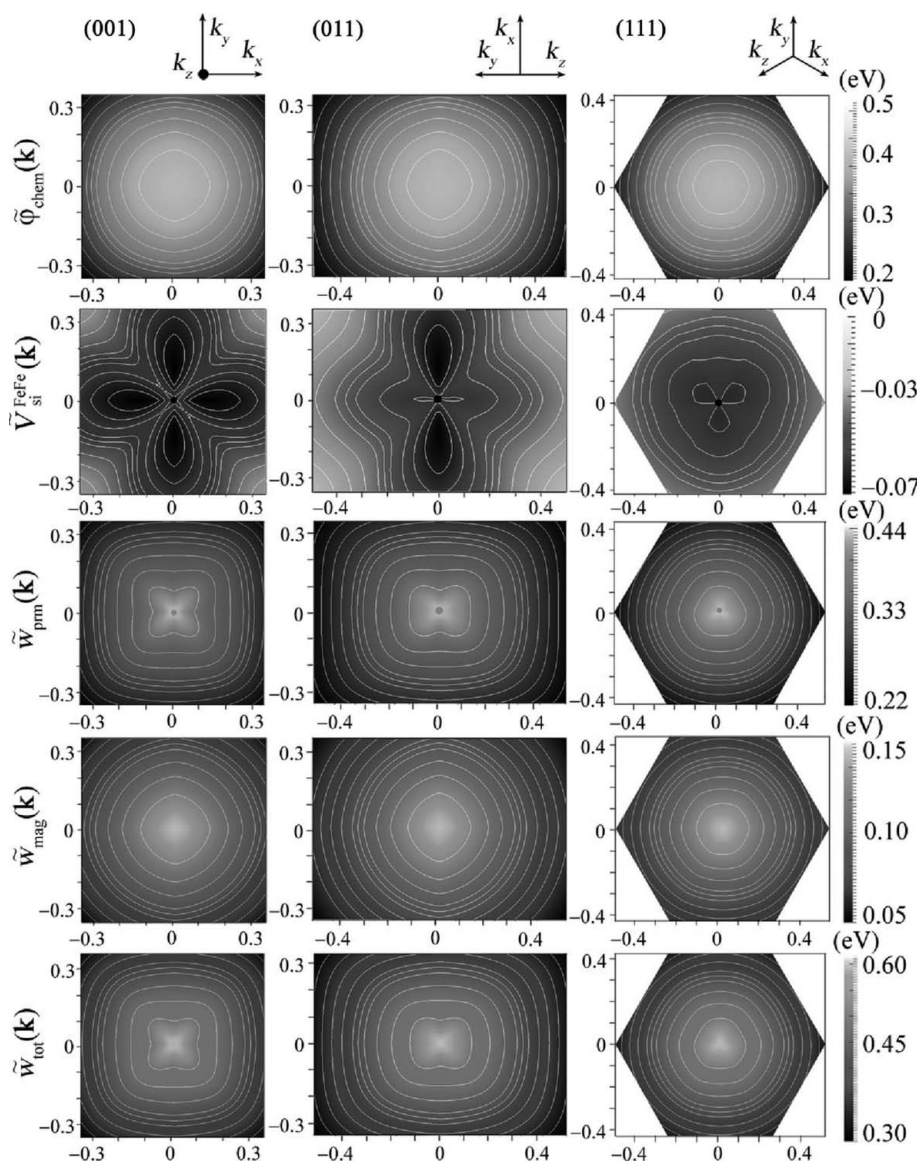


Figure 2

The various ‘mixing’ energy Fourier component contributions near the ‘fundamental’ $\Gamma(000)$ -point in the three \mathbf{k} -space high-symmetry planes: (001), (011) and (111), calculated for the FMS f.c.c. Ni₃Fe permalloy domain at 800 K (reciprocal-space level-hypersurfaces map).

The ‘mixing’ energy Fourier components [equation (3)] near and at the \mathbf{k}_Γ -point calculated for the ferromagnetic state (FMS) f.c.c. Ni₃Fe permalloy domain at 800 K are illustrated in Fig. 2. In Fig. 2, one can see an agreement of the estimated and predicted [equations (14) and (15)] ‘mixing’ energy symmetry regularities.

Using the ‘mixing’ energies represented within the reciprocal space in Fig. 2 and applying the KCM formula [equation (1)], we can calculate the equilibrium SRO diffuse scattering intensity distribution near and at the \mathbf{k}_Γ -point. As shown in Fig. 3, in the case of a pure ‘electrochemical’ interaction of atoms in an alloy, the resulting SRO intensity level hypersurface, $I_{\text{chem}}(\mathbf{k})$, is an *analytic* (and isotropic) function of (small) \mathbf{k} , *i.e.* $I_{\text{chem}}(\mathbf{k})|_{\mathbf{k} \rightarrow \mathbf{0}} \equiv I_{\text{chem}}(\mathbf{0}) > 0$. However, for (para)magnetic permalloys with the ‘strain-induced’ or ‘strain-induced’ + magnetic interactions of substitutional atoms, the

SRO intensities $I_{\text{prm}}(\mathbf{k})$ and $I_{\text{tot}}(\mathbf{k})$ demonstrate both the *analytic* (*i.e.* azimuthal) and *nonanalytic* (*i.e.* first-kind-jump-discontinuous ‘radial’) parts. So, we write the $I_{\text{SRO}}(\mathbf{k})$ regularities as

$$\begin{aligned} I_{\text{SRO}}(\mathbf{0}) &> I_{\text{SRO}}(\mathbf{k}_{\downarrow\uparrow\mathbf{k}_X} \rightarrow \mathbf{0}) \\ &> I_{\text{SRO}}(\mathbf{k}_{\downarrow\uparrow\mathbf{k}_W} \rightarrow \mathbf{0}) > I_{\text{SRO}}(\mathbf{k}_{\downarrow\uparrow\mathbf{k}_{K(U)}} \rightarrow \mathbf{0}) \\ &> I_{\text{SRO}}(\mathbf{k}_{\downarrow\uparrow\mathbf{k}_L} \rightarrow \mathbf{0}) > 0, \end{aligned} \quad (16)$$

which are valid for both cases of $I_{\text{SRO}}(\mathbf{k})$: $I_{\text{prm}}(\mathbf{k})$ and $I_{\text{tot}}(\mathbf{k})$, but only with the distinction that $|I_{\text{prm}}(\mathbf{k})| > |I_{\text{tot}}(\mathbf{k})|$ for small $\mathbf{k} \rightarrow \mathbf{0}$ and \mathbf{k}_Γ . This means that, in experiments done for the PMS domain, the azimuthal dependence of $I_{\text{SRO}}(\mathbf{k})$ will be more pronounced as compared with that for the FMS domain (see Fig. 3). In addition, our results on an *analytic* part of the SRO intensity, *i.e.* azimuthal dependence [for both $I_{\text{prm}}(\mathbf{k})$ and $I_{\text{tot}}(\mathbf{k})$ in Fig. 3], are in good qualitative agreement with the experimental diffuse scattering data reported for f.c.c. Ni–Fe Invar compositions (Ono *et al.*, 1995; Tsunoda *et al.*, 2008).

In conclusion, we have recalculated the total ‘mixing’ energies and the SRO intensities in a reciprocal-space representation shown in Figs. 2 and 3 as functions of both the quasi-wavevector magnitude $|\mathbf{k}| = k$ along the high-symmetry directions within the 1st BZ and the temperature for the PMS and FMS domains (Fig. 4). From Figs. 4(a) and 4(b), one can see the rigorous compliances of the symmetry regularities [inequalities [equations (15) and (16)]]. Both functions, $\tilde{w}_{\text{tot}}(\mathbf{k})$ and $I_{\text{tot}}(\mathbf{k})$, are *analytic* for each $\mathbf{k} \rightarrow \mathbf{0}$ and *nonanalytic* at the \mathbf{k}_Γ -point precisely

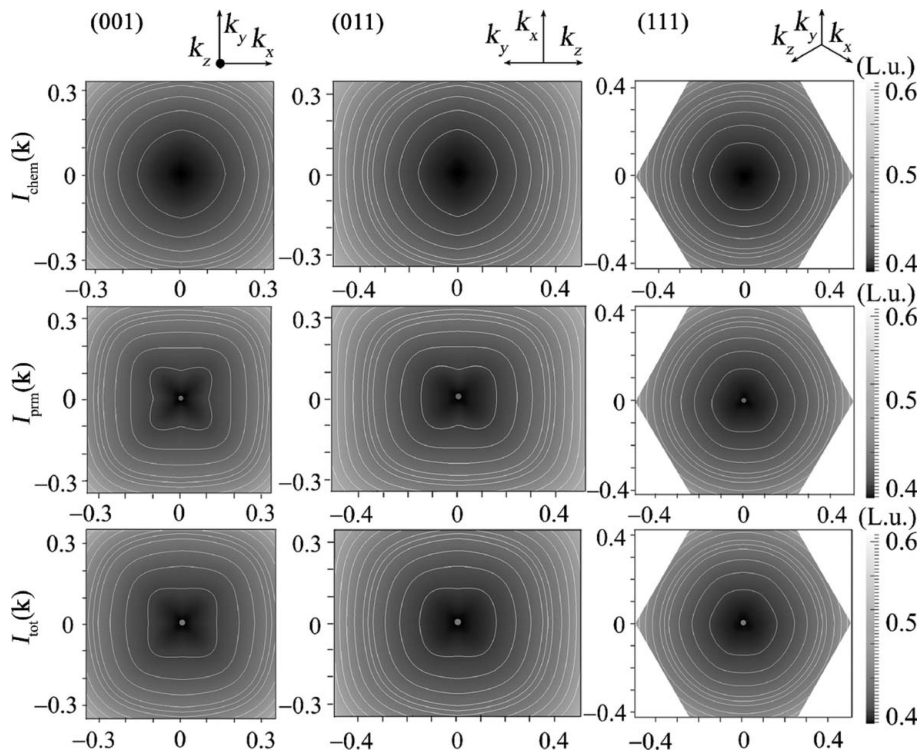


Figure 3 The various SRO intensity contributions near the ‘fundamental’ $\Gamma(000)$ -point in the three reciprocal-space high-symmetry planes: (001), (011) and (111), calculated for the FMS f.c.c. Ni_3Fe permalloy domain at 800 K with use of equation (2) and data shown in Fig. 2 (level-hypersurfaces map).

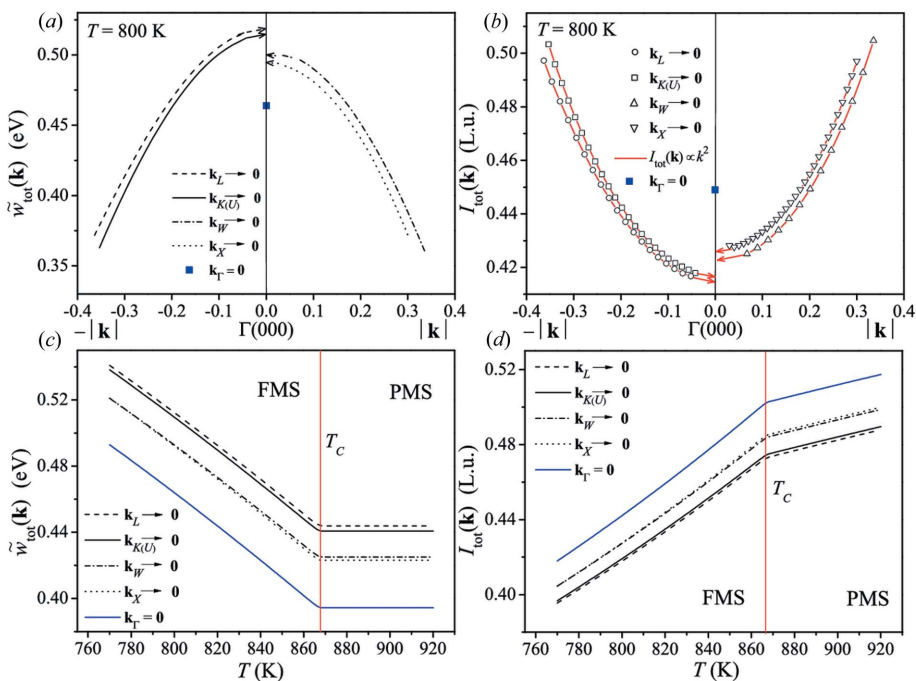


Figure 4 $\tilde{w}_{\text{tot}}(\mathbf{k})$ (a) and $I_{\text{tot}}(\mathbf{k})$ (b) for some $\mathbf{k} \rightarrow \mathbf{0}$ and \mathbf{k}_r (Fig. 1b) as calculated for the FMS f.c.c. Ni_3Fe permalloy domain at 800 K. T -dependences of $\tilde{w}_{\text{tot}}(\mathbf{k}, T)$ (c) and $I_{\text{tot}}(\mathbf{k}, T)$ (d) for the PMS and FMS domains [according to equation (11), $T_C(c = 0.25) \cong 868$ K; $T_C^{\text{exp}} \cong 870$ K].

$[\lim_{\mathbf{k} \rightarrow \mathbf{0}} \tilde{w}_{\text{tot}}(\mathbf{k}) \neq \tilde{w}_{\text{tot}}(\mathbf{0}), \lim_{\mathbf{k} \rightarrow \mathbf{0}} I_{\text{tot}}(\mathbf{k}) \neq I_{\text{tot}}(\mathbf{0})]$. Moreover, it is worth noting that, in contrast to the conventional Huang diffuse scattering (Huang, 1947) with intensities $I_{\text{Huang}}(\mathbf{k}) \propto k^{-2}$ for small $\mathbf{k} \rightarrow \mathbf{0}$, the equilibrium SRO intensities for PMS and FMS domains behave as $I_{\text{SRO}}(\mathbf{k}) \propto k^2$ (Fig. 4b). This means that, in diffraction experiments for concentrated solid solutions of strongly interacting impurities (inclined to order), $I_{\text{SRO}}(\mathbf{k})$ is dominant, while for dilute solutions of ‘elastically’ interacting point defects, only $I_{\text{Huang}}(\mathbf{k})$ still plays a crucial role. As revealed in addition, $\tilde{w}_{\text{tot}}(\mathbf{k}, T)$ and $I_{\text{tot}}(\mathbf{k}, T)$ as functions of T change their slopes at the PMS-to-FMS transition (Figs. 4c and 4d). This temperature-controlled effect is caused by initiation of the magnetic LRO state of both Ni and Fe subsystems, $0 \leq |\sigma_{\text{Ni,Fe}}(T)| \leq 1$ at $T \leq T_C$ [equations (10a), (10b)], that leads immediately to the pronounced T -dependence of the total ‘mixing’ energies [see equation (3) and Fig. 4c]. At $T > T_C$ (*i.e.* for the PMS domain) $\tilde{w}_{\text{prn}}(\mathbf{k}, T) \cong \text{const}$ (see Fig. 4c) and $I_{\text{prn}}(\mathbf{k}, T)$ behaves in accordance with the classical KCM theory.

4. Summary

In this work, the diffuse scattering intensities caused by the short-range atomic order (taking into account the long-range magnetic order) near the Bragg reflection in a (para)magnetic bulk f.c.c. Ni_3Fe -type permalloy are investigated in detail. The *analytic* (*i.e.* azimuthal) and *nonanalytic* behaviours (symmetry regularities) of the SRO intensities and the different ‘mixing’ energy Fourier component contributions are revealed and analysed. Here, we have not considered explicitly an interplay between the long-range ‘strain-induced’ effects and the magnetic ordering (*i.e.* local magneto-volume phenomena); however, we argue that the reported results are sufficient for providing additional basics on the kinematic diffuse scattering of radiations near the Bragg reflection in equilibrium (para)magnetic bulk alloys. Moreover, it is worth noting that the above-presented results are based

solely on the local magnetic moments model, which is valid within the lattice-gas approximation only and cannot be applied to the accounting of the 'itinerant' magnetism of quasi-free electrons. Nonetheless, a reader can find both approaches and their comparative analysis based on a reciprocal-space symmetry consideration in critical reviews (Tatarenko *et al.*, 2008; Bokoch & Tatarenko, 2010); the comprehensive list of references to the most salient literature on this matter can be found elsewhere (Aharoni, 2000; Tatarenko *et al.*, 2008; Bokoch & Tatarenko, 2010; Vernyhora *et al.*, 2010).

5. Related literature

The magnetic 'mixing' energy in f.c.c. Ni-Fe alloys is discussed in Tatarenko & Radchenko (2003), Bokoch & Tatarenko (2008, 2010), Tatarenko *et al.* (2008), Men'shikov & Yurchikov (1972), Lawrence & Rossiter (1986), Hatherly *et al.* (1964), Maeda *et al.* (1973), Dubé *et al.* (1995), Dang *et al.* (1995), Taylor & Gyorffy (1992) and Taylor *et al.* (1991). 'Strain-induced' interatomic interaction energies of dissolved atoms in solid solutions are discussed in Tatarenko & Nadutov (2004), Bugaev & Tatarenko (1989), Beiden & Vaks (1992), Birgeneau *et al.* (1964), Bokoch & Tatarenko (2010) and Tatarenko & Tsinman (1992). The 'paramagnetic' 'mixing' energy in f.c.c. Ni-Fe alloys is discussed in Bokoch & Tatarenko (2010); Lefebvre *et al.* (1980, 1981); Bley *et al.* (1988); Ice *et al.* (1992, 1998); Jiang *et al.* (1995, 1996), Ice, Sparks *et al.* (1996); Ice, Painter *et al.* (1996); Ice & Sparks (1999); Robertson *et al.* (1999) and Cenedese *et al.* (1984). For a phase diagram for f.c.c. Ni-Fe alloys, see Swartzendruber *et al.* (1991), for the lattice dynamics of f.c.c. lattices in general see Kushwaha & Kushwaha (1978), and for the lattice spacing of f.c.c. Ni as a function of Fe concentration, see Pearson (1958, 1968).

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