Errata - Structural study of the charge density wave phase transition of the blue bronze : K0.3MoO 3

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I. The X-ray diffuse scattering intensity reported in section 3.2 (see for example that shown in figure 5) has been measured as the extra scattering above the background. Thus it cannot be accounted for by the equation :

$$S(\mathbf{q}, t = 0) \equiv I(q) = kTX(\mathbf{q}) \propto kT/\hbar^2 \Omega_q^2 \qquad \text{(2) in section 3.2}$$

which gives an absolute value of the diffuse intensity, without reference to the background. With a background contribution of $kT/\hbar^2 \omega_0^2$, corresponding to the response of the unstable lattice mode in the absence of its coupling with the electron gas, the measured diffuse intensity is actually given by :

$$\tilde{I}(q) = kT\tilde{X}(q) \propto kT\left[\frac{1}{\hbar^2 \Omega_q^2} - \frac{1}{\hbar^2 \omega_0^2}\right], \qquad (2')$$

where $\tilde{X}(q)$ is proportional to the CDW response function :

$$\tilde{X}(q) = -\frac{g^2}{\hbar^2 \omega_0^2} \frac{\chi_0(q)}{1 + \left(\frac{g^2}{\hbar\omega_0} - V\right)\chi_0(q)}. \qquad (5')$$

As a consequence the peak intensity of the diffuse scattering and the inverse correlation length in chain direction (defined now by the H.W.H.M. of $\tilde{X}(q)$) are given respectively by :

$$\tilde{I}(q_c) = kT\tilde{X}(q_c) \propto kT \frac{\text{Log}\,(1.14\,E_F/kT)}{\text{Log}\,(T/T_c)}, \tag{7'}$$

$$\xi_{\|}^{-1} = 4.34 \frac{kT}{V_F} \sqrt{\frac{\text{Log}\,(1.14\,E_F/kT)\,\text{Log}\,(T/T_c)}{\text{Log}\left(\frac{1.14\,E_F}{kT_c}\right)}}. \tag{12'}$$

These expressions replace respectively the equations (7) and (12) of the section 4.2, for the analysis of the data.

The replacement of $X(q)$ by $\tilde{X}(q)$ does not change, as expected, the conclusion of section 4.2 concerning the critical behaviour of $\tilde{I}(q_c)$ and $\xi_{\|}$ in the vicinity of T_c. However it modifies the temperature dependence of these quantities at higher temperatures. In particular equation (7') cannot account for the temperature dependence of the peak intensity of the diffuse scattering near room temperature when adjusted to the data in the vicinity of T_c. Because of its prefactor kT, equation (12') can still describe the temperature dependence of $\xi_{\|}^{-1}$ within its uncertainties, on all the temperature range.

Finally the temperature T_1, defined by equation (8), does not appear in the expression of $\tilde{X}(q)$. Thus the set of parameters, previously given in (14), cannot be determined.

Further theoretical and experimental works are in progress to improve this analysis.

II. The last paragraph of the discussion (p. 1740) contains two errors :

a) Due to the high temperature C 2/m space group symmetry of the blue bronzes, the Landau free energy expansion cannot contain Umklapp term of the 4th order, because 4 $\mathbf{q}_{com}$ = (0, 1, 2) has its components which do not fulfil the condition of the C centring symmetry, $h + k$ = even, required to preserve the translational invariance. Thus as only the Umklapp term in the 8th power of the order parameter is allowed at the lowest order, the order of commensurability is $n = 8$ in the blue bronzes. In consequence a weaker commensurability potential is expected, and a separation of $8(\mathbf{q}_{inc} - \mathbf{q}_{com})$ between the main satellite reflections and the multisoliton satellite reflections, instead of $4(\mathbf{q}_{inc} - \mathbf{q}_{com})$, will be realized if a discommensuration lattice is formed. These multisoliton satellites have not been observed in the low temperature part of our study, when the commensurability potential is the strongest.

b) Contrary to our assertion, the NMR study of reference [18] does not show evidence of a discommensuration lattice in $Rb_{0.3}MoO_3$.