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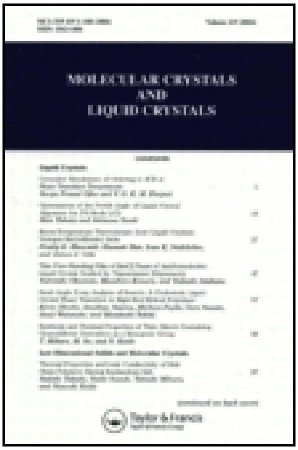

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DEFECT DENSITY WAVES IN MODULATED SYSTEMS

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Abstract - Experiments and theory show that in modulated structures, impurities may have a periodic concentration modulation if allowed to interact for a sufficient time with a standing modulation. A quadratic impurity order parameter coupling, relevant to the case of thiourea, was discussed previously. The case of a linear impurity-order parameter coupling, relevant to impurities in Charged Density Wave systems, is significantly different. The order-disorder transition temperature may exhibit large positive shifts. Different relaxation times occur at short and long times, with large temperature dependence around the unperturbed transition temperature and the shifted one.

There is evidence that, in modulated structures, mobile impurities order periodically in the modulation field if allowed to interact for a sufficient time with the latter.[1-5] The notion of a Defect Density Wave (DDW) is at variance with the standard treatments of impurities as a random field.[6] In this paper, we describe the condensation of a DDW when the latter is a slow process, i.e. when the modulation order parameter thermalises in times short compared with impurity diffusion times. We neglect impurity-impurity interactions. The modulation is assumed to be purely sinusoïdal.

A procedure to study DDW kinetics might be to start with frozen random impurities and allow the phase to distort in that field.[6] Then one would allow impurities to diffuse and let the distortion relax to zero. If all impurities are mobile, the equilibrium state has a DDW and long range order. What probably happens in reality is that after mobile impurities have relaxed, some phase distortion continues to exist because of other frozen defects. This is more difficult to describe, so that we resorted to the simplest approach : impurities relax in the rigid undistorted potential of the pure system ; phase dynamics is absent, all time dependence

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stems from impurity diffusion. This is a crude approximation for short times and strong pinning.

DDW have been discussed until now in systems where the impurity-order parameter interaction is quadratic in the order parameter.[1,2] However in Charge Density Wave (CDW) systems, the coupling of impurities to the CDW is linear ; this leads to interesting differences with the former case. In both cases, our approach is to set the free energy as $F = F_m + F_i + V_{m-i}$ where F_m is the pure system free energy, F_i is the impurities free energy and V_{m-i} the interaction term. Minimizing F with respect to the order parameter and to the DDW amplitude yields the equilibrium state of the system (after an infinite time). The interaction is turned on at time $t = 0$ and the impurity concentration $c(\vec{r},t)$ obeysthe diffusion equation :[2]

$$\frac{\partial c}{\partial t} = D\Delta c + \frac{D}{k_BT} \vec{\nabla}(c \vec{\nabla} V_{m-i}) \qquad (1)$$

where D is the diffusion constant, t the time, k_B Boltzmann's constant and T the temperature. Since the order parameter is in thermal equilibrium with the instantaneous value of the DDW amplitude, this yields a differential equation for the time variation of the order parameter. First we recall results for the quadratic coupling.[1,2] The impurity concentration becomes $c(r,t) = c_o\,[1 + b(t) \cos 2qr]$ and $b(t) = \frac{2V_oP_q^2}{k_BT}(1 - \exp - 4Dq^2t)$.

P_q is the order parameter amplitude, V_o the coupling strength and q the modulation wave vector at the arbitrary temperature T where the system has been stabilized during a time t. We also have (k_B=1 in the following) :

$$P_q^2(t) = P_q^2(o)[1 - \frac{4V_oc_o}{T_i - T}(1 - \frac{b}{2}(t)] \simeq P_q^2(o)\ [1 - \frac{4V_oc_o}{T_i - T}] \qquad (2)$$

where T_i is the modulation-disorder transition temperature of the pure system. The shift of T_i due to the DDW is negligible.

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In the linear coupling case, we chose $F_m = \frac{T-T_i}{2}\rho_q^2 + \frac{T_i}{4}\rho_q^4$ where ρ_q is the CDW amplitude and $F_i = T\int dr[c\,\ell nc + (1-c)\,\ell n(1-c)]$ with $c = c_o - c_q \cos qr$. Finally, $V_{m-i} = -V_o\, c_q\, \rho_q$. V_o can always be chosen positive. As a result, at equilibrium, $c_q = 2c_oV_o\rho_q/T$ and $\rho_q^2 = (T_i - T)/T_i + 2c_oV_o^2/T_iT$. The order-disorder temperature is shifted to <u>higher</u> temperatures and depends on the DDW amplitude. One has $T_i' \simeq T_i + 2c_oV_o^2/T_i$. Typically, for $V_o = 0{,}2$ eV, $T_i = 200$ K, $c_o = 10^{-3}$, $T_i' - T_i \simeq 50$ K. The DDW time evolution obeys the coupled equations :

$$(T - T_i)\rho_q + T_i\rho_q^3 - V_oc_q = 0$$

$$\frac{dc_q}{dt} = -\frac{c_q}{\tau} + \frac{2}{\tau}\,\frac{c_oV_o}{T}\,\rho_q \quad \text{with } \tau^{-1} = Dq^2$$

whence
$$\frac{T-T_i}{T_i}\,\frac{d\rho_q}{dt} + \frac{d\rho_q^3}{dt} = \frac{T_i-T}{T_i}\,\frac{\rho_q}{\tau}\,(1+y) - \frac{\rho_q^3}{\tau} \qquad (3)$$

with $y = 2c_oV_o^2/T(T_i-T)$. Although $c_q \ll c_o$, i.e. $2V_o\rho_q \ll T$, one may have $y \gg 1$. Various cases arise. a) $T < T_i$ and short times, then $\rho_q(t) = \rho_q(0)(1 + t/\tau_1)$ with $\tau_1 = 2\tau/y$. This linear regime vanishes near $T = T_i$. At $T < T_i$ and $t \gg \tau_1$,
$\rho_q(t) = \rho_q(o)\sqrt{1+y}\,(1 - \exp.-t/\tau_2)$ with $\tau_2 = \frac{\tau}{2}\,\frac{2+3y}{1+y}$.

When $T \to T_i$, $\tau_2 = 3\tau/2$. b) At $T = T_i$ and $t < \tau$,
$\rho_q = 2(c_oV_o^2/3T_iT)^{1/2}\,(t/\tau)^{1/2}$.
For $t \gg \tau$, $\rho_q = (2c_oV_o^2/T_iT)^{1/2}(1 - \exp - t/\tau_3)$ with $\tau_3 = 3\tau/2$.

c) For $T_i < T < T'_i$ and short times : there is an exponential growth of the order parameter and DDW, with relaxation time $\tau_4 = \tau(T - T_i)/(T'_i - T)$. When $t \gg \tau_4$, saturation occurs with relaxation time $\tau_5 = \frac{\tau}{2}\,\frac{3T'_i - T_i - 2T}{T'_i - T}$ which varies from $3\tau/2$ to infinity when T varies from T_i to T_i'.

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Thus, contrary to the quadratic coupling case, the solutions of the non linear differential equation cannot be described with a single relaxation time. The behaviour of DDW in BSN, an insulating compound [4] is qualitatively accounted for by this theory. Critical behaviour, described here within molecular field, is expected at $T = T_i$ and T_i'.

After the DDW has condensed at a given temperature T^*, it behaves as an external staggered field of wave vector $q^* = q(T^*)$ and intensity $- V_o c(q^*,T^*)$, conjugate to the CDW order parameter, if the system is brought to another temperature and measured in times short with DDW relaxation time. One of the consequences is a memory effect [1,2]. Another consequence would be the appearance of non-linearities in electrical transport properties of various CDW systems [5,7]. We expect DDW to be responsible in some cases for the observed anomalies.

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