Possible existence of thermodynamic-equilibrium heterogeneous states in metallic systems

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We discuss the indirect large-radius interaction that arises when the superstructure reciprocal-lattice vector $\mathbf{K}$ is close to the distance $2\mathbf{k}_F$ between almost plane sections of the Fermi surface (PSFS). It can lead to formation of an inhomogeneous structure consisting of ordered regions (OR) and disordered regions (DOR).

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1. Long-range forces can lead to the appearance of equilibrium heterogeneous structures. In semiconductors they are connected with the screened Coulomb interaction (see, e.g., [1]). In metallic systems, the large-radius interactions can occur, for example, if $\mathbf{K} \approx 2\mathbf{k}_F$. Then the Friedel oscillations $r^{-1}\cos(2\mathbf{k}_F r + \phi)$ lead to an interaction between the changes of the order parameter η of the type $r^{-1}\cos(Qr + \phi)$, where $\mathbf{r} \parallel \mathbf{k}_F$, $Q = 2k_F - K$ and $Q \ll K$.

This interaction is connected with the logarithmic singularity in the dependence of the polarization operator $P(\mathbf{k})$ and the specific electron energy E_e on the wave vector $\mathbf{k} - \mathbf{K}$ of the static order wave. [2] In the case of a one-dimensional distribution of $\eta(x)$ in crystals with one pair of PSFS, we have in second-order approximation in the interaction $V(k)\eta(k-K)$ between the electrons and the inhomogeneities of the order parameter

$$E_e = -\sum_k A(k)\,|\eta(k-K)|^2; \quad A(k) = \frac{1}{2}|V(k)|^2 \frac{P(\mathbf{k})}{\epsilon(\mathbf{k})} \approx A \ln \frac{\kappa^2}{(k-2k_F)^2 + k_0^2}. \qquad (1)$$

Here $k \equiv k_x$, $\hbar = 1$, $A \sim (2\pi)^{-3} S/v_x$, $\kappa \sim \epsilon_F/v_x$, S is the PSFS area, ϵ_F and v_x are

the energy and velocity of electrons on this section, and k_0 is of the order of the largest of the quantities kT/v_x, $|V(k)\eta(k-K)|/v_x$, the reciprocal electron mean free path, or the PSFS "corrugation amplitude." The first formula for $A(k)$ is valid in the pseudopotential approximation at $|k-2k_F| \gg k_0$, while the second is valid when the dielectric constant is $\epsilon(\mathbf{k}) \approx 1$.

2. At low temperatures, the singularity of $A(k)$ leads to the appearance of structures with wave-like variation of $\eta(x) = \eta_0(x) \sim \cos(qx+\psi)$ (see, e.g., [3]). At increased temperatures, however, if the non-singular (local) part of the thermodynamic potential $\phi(\eta)$ is lower in the disordered phase and is not an even function of η, then an inhomogeneous structure, containing alternating OR and DOR of large dimensions $\sim \pi/Q$, may be more convenient. In this structure the OR is preserved only near the maxima of the order-parameter modulation wave at $\eta > 0 (\phi(\eta>0) < \phi(\eta<0))$; near the minima, on the other hand, DOR with much smaller $\phi(\eta)$ are produced in place of OR with $\eta < 0$. The somewhat smaller decrease of the singular part of the electron energy in comparison with the case $\eta_0(x)$ is offset in this case by the gain in the average value of $\phi(\eta)$.

Let us examine, for example, the simplest model of a one-dimensional structure with a period $2L = 2\pi/q$, containing OR of thickness $2L = p2L_0$ with $\eta(x) = \eta$ = const and DOR with $\eta(x) = 0$, when $\eta(nq) = \eta(nqL_0)^{-1} \sin(nqL)$. To simplify the analogies we confine ourselves to the case $Q \gg k_0$ and neglect the terms $\sim \zeta = (\ln Q/k_0)^{-1}$. Then, taking (1) into account, the difference between the specific thermodynamic potentials of the heterogeneous system and the fully disordered phase at $\epsilon(\mathbf{k}) \approx 1$ can be expressed in the form

$$\Delta\Phi = p\phi(\eta) + \frac{\sigma}{L_0} - A\eta^2 p^2 \frac{\sin^2 qL}{(qL)^2} \ln \frac{Q^2}{k_0^2 + (q-Q)^2}; \quad qL = \pi p. \tag{2}$$

We have taken here into account the fact that the sum (over n) of the terms in E_e without a singularity of the type $1/\zeta$ is proportional to p. It is included in $p\phi(\eta)$ and it is assumed that $\phi(0) = 0$. On the other hand, the singular part of the term with $n = 1$, which is connected with the long-range action and is proportional to $1/\zeta$ (at $q \approx Q$), is contained in a separate term. It is important that this term depend nonlinearly on p (this important effect of nonlocality of $\Delta\Phi$ was not taken into account in the interesting phenomenological model wherein the OR were regarded as fluctuation formations[4]). If the surface energy σ is sufficiently low ($\sigma Q \ll \phi(\eta)$), then the values of $2L_0$, p and η corresponding to the minimum of $\Delta\Phi$ are determined by the formulas

$$\pi/L_0 = q \approx Q; \quad \sin 2\pi p = B(\eta) = \frac{\pi\phi(\eta)}{2\eta^2 A \ln Q/k_0} < 0.72 \quad \text{at} \quad \frac{1}{2} > p > 0.37;$$

$$\eta\left(\frac{\phi'(\eta)}{\phi(\eta)}\right) = \frac{\operatorname{tg}\pi p}{\pi p}. \tag{3}$$

Thus, if the parameter $B(\eta)$ is small (and $\phi(\eta) > 0$), then a first-order phase transition into an inhomogeneous state, with an appreciable fraction p of the OR located at the maxima of the modulation wave, takes place at $T < T_c$, where $B < B_c < 0.72$. In order for the OR not to occur near the minima of the modulation wave and to prevent formation of the ordinary wave $\eta_0(x)$, the function $\phi(\eta)$ must not be even and the condition $B(-\eta) > \alpha \sim 1$ must be satisfied in addition. Allow-

ance for the dependence of η on x in the OR, for the redistribution of the concentration in the solutions, and for the elastic energy should lower $\Delta\Phi$ and stabilize the inhomogeneous state.

3. In quasi-one-dimensional crystals one can neglect the interaction between the chains of molecules, and the aforementioned structure should arise in each chain independently. Random phase shifts in the chains will lower not only the fluctuating part of $\Delta\Phi$, but also E_e. The reason is that the smearing of the reciprocal-lattice sites into disks parallel to the PSFS decreases $\epsilon(\mathbf{k}) = 1 + 4\pi e^2 k^{-2} P(\mathbf{k})$ (increasing k^2 on the average) without changing $P(\mathbf{k})$. Allowance for the Coulomb interaction can lead to the onset of a three-dimensional structure, where OR and DOR are neighbors in the transverse direction (cf. [3]). The formation of such a structure may also be facilitated by the elastic energy. Such a structure with alternating needle-like sections perpendicular to the PSFS can be produced not only in transverse systems, if the gain of E_e and of the elastic energy exceed the growth of the surface energy of the lateral boundaries.

4. If several vectors $\mathbf{K}$ are located in the cubic ordered phases near the PSFS, then in order for all such sections to contribute to E_e a three-dimensional heterogeneous structure must arise. Let us consider, for example, crystals with a primitive cubic lattice, and let the PSFS be located in the crystals near sites of the type $(h00)$. Assume that the resultant structure consists of cubic OR of thickness $2L$, which are periodically arranged in the disordered matrix $2L_0 = 2\pi/q$ apart. Then at $\sqrt{S} \gg Q$ and $\ln Q/k_0 \gg 1$ we have

$$\Delta\Phi = p\phi(\eta) + \frac{3}{L_0} p^{2/3}\sigma - \frac{3}{\pi^2} p^{2/3}\eta^2 A \ln \frac{Q^2}{k_0^2 + (q-Q)^2} \sin^2 \pi \frac{L}{L_0}; \qquad p = \left(\frac{L}{L_0}\right)^3. \tag{4}$$

The function (4) has a minimum that lies lower than the minimum of (2). The fraction p of the OR increases monotonically with decreasing B and σ, reaching a value $p \approx 0.27$ in the limit $B \ll 1$ and $\sigma \ll \phi(\eta)/Q$.

5. Although the foregoing results were obtained, for simplicity, in a model using a periodic heterogeneous structure, the establishment of correlation at infinity is not necessary, for even a short-range order in the disposition of the OR at not very large $\ln Q/k_0$ produces not much less gain in E_e. The reason is that the short-range order causes a sufficiently sharp peak of the structure factor in k-space (even for a stack of three layers, the square of the structure factor decreases by one-half when the distance from the maximum is $\approx q/7$). Therefore a phase transition into a heterogeneous state that has apparently a short-range order in the arrangement of the OR should take place with decreasing temperature. Only with further decrease of temperature can a correlation be established between them at large distances. These can be followed by a phase transition to a state with constant or wave-like order.

We note that the considered heterogeneous state may be connected not only with the PSFS, but with any other sufficiently sharp minima of the function $A(k)$. Analogous effects can arise also in the case of magnetic ordering.

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