THE CRYSTAL SIZE INFLUENCE ON THE FOURIER SPECTRUM OF THE AMPLITUDE FUNCTION OF THE INCOMMENSURATE SUPERSTRUCTURE

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The linear size reducing of the samples of crystals $(N(CH_3)_4)_2MeCl_4$ causes the effect of the phase slip, the temperatures of phase transitions lowering and the temperature range narrowing of the incommensurate (IC) phase. This behavior of the properties of the IC of the superstructure is due to the influence of surface energy increasing on the energy of the incommensurate superstructure. Numerical calculations show that the surface effect cannot be replaced by the effect of electric field strength on the incommensurate superstructure. Therefore, the influence of the size limitation on evolution of the existence of a wave of the incommensurate modulation in the work considered.

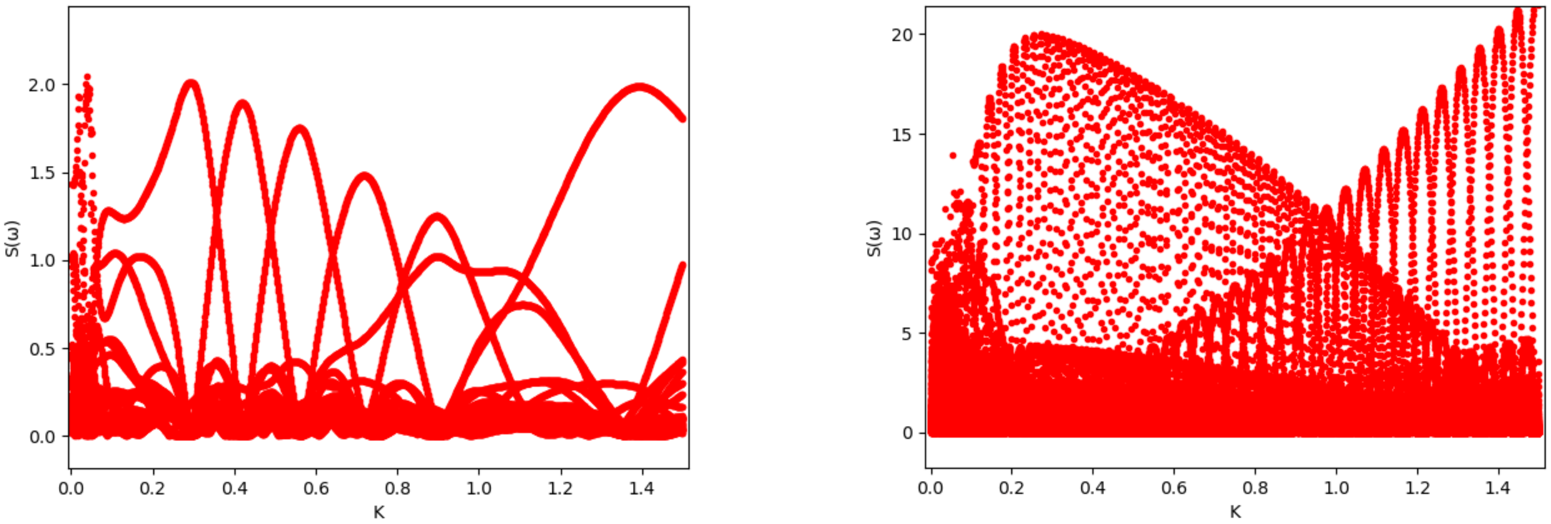
Calculations of spatial changes in the amplitude of the order parameter were performed for systems described by two second-order differential equations with the symmetry of the thermodynamic potential $n = 3$ and the value of the longinfluence interaction $T = 1$.

$$R'' - R^3 + \left(1 - \varphi'^2 + T\varphi'\right)R - R^{n-1}K\left(\cos n\varphi + 1\right) = 0\,, \qquad (1)$$

$$\varphi'' + 2\frac{R'}{R}(\varphi' - \frac{T}{2}) + R^{n-2}K\sin n\varphi = 0\,. \qquad (2)$$

where $T = \frac{\sigma}{(\gamma r)^{\frac{1}{2}}}$, $K = 2^{-\frac{n}{2}} r^{\frac{n}{2}-2} n\omega u^{1-\frac{n}{2}}$ — dimensionless parameters, n — is an integer that characterizes the symmetry of the potential, and dimensionless variables $\eta = \left(\frac{r}{2u}\right)^{1/2} R$, $z = \left(\frac{\gamma}{r}\right)^{1/2} \xi$.

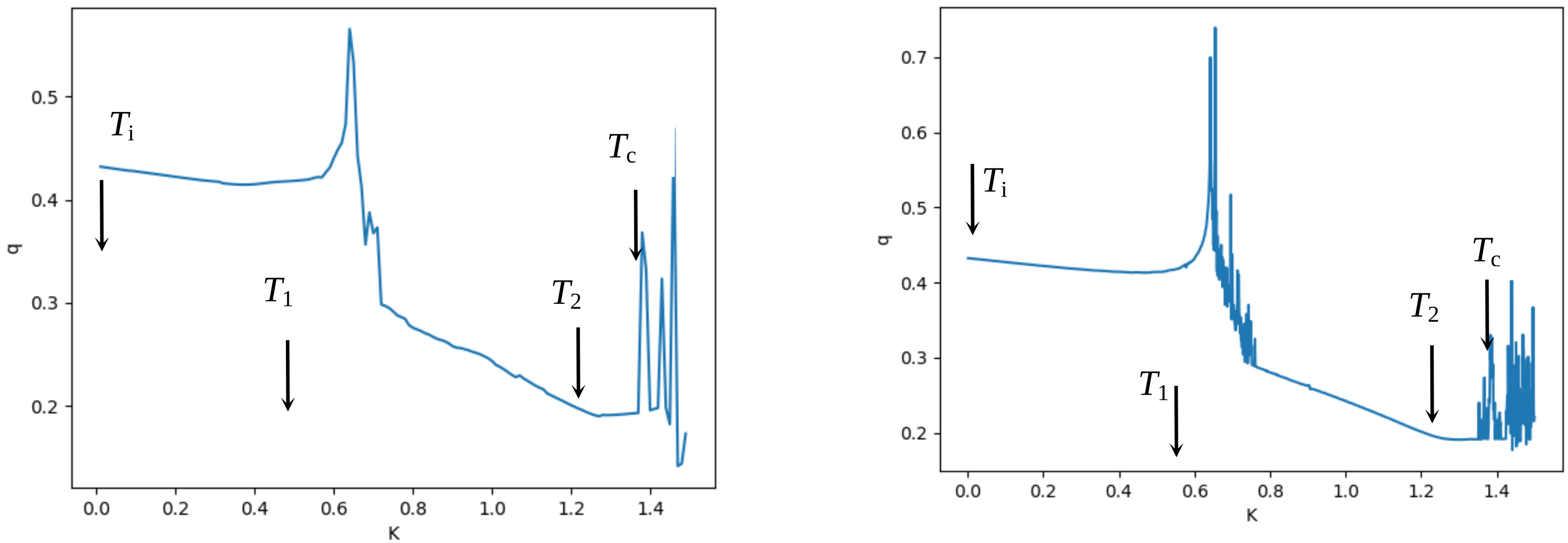
This system (1,2) was solved by the numerical BDF method. The calculation of the spatial changes in the amplitude and phase of the order parameter was performed in the Python environment using the Skipy and JiTCODE libraries.



a **b**

Fig.1. The Fourier spectrum of oscillations of the amplitude function of the superstructure

Figure 1 shows the Fourier spectrum of oscillations of the amplitude function of the superstructure dependence to the parameter K at different values of the linear dimensions of the crystal sample (sample size is equal to 10 modulation wavelengths (Fig. 1 a) and 100 modulation wavelengths (Fig. 1 b). According to the obtained dependences, this structure is characterized by an increase in the period of spatial oscillations with the number of existing spatial modulation waves decrease. The transition to soliton mode is accompanied by the appearance of new oscillations (K = 0.6). The modulation harmonics behavior from the parameter K indicates complex transformations that occur during the transition from one mode to another, regardless of the sample size.



a b

Fig.2. Evolution of the wave vector of the incommensurate superstructure dependence to the value of the anisotropic interaction (described by parameter *K*) and to the linear dimensions of the crystal sample (the linear sample size is 10 modulation wavelengths a) and 100 modulation wavelengths b)). Where T_i is the temperature of transition to the incommensurate phase; T_1 - transition to the soliton mode of the superstructure; T_2 - transition to the stochastic mode of the superstructure; T_c -phase transition to the commensurate phase.

The behavior of the wave vector of the incommensurate modulation q from the value of the anisotropic interaction indicates that the decrease in the linear crystal size attend by a decrease in the number of existing harmonics of modulation in the transition from sinusoidal to soliton mode of the superstructure (Fig. 2)

The monotonic decrease of the q value at a constant T and the increase of K , indicates the modulation IC wavelength increase with temperature decreasing. As is known the magnitude of the wave vector of the IC superstructure decreases with temperature decreasing (and hence the value of the anisotropic interaction K is increase), which indicates a good correlation between experimental and theoretical results.

So, based on the studies of the Fourier spectra of oscillations of the amplitude function of the incommensurate modulation, it can be argued that the linear size of the crystal decrease cause a change in the spectrum of frequencies of the incommensurate modulation.