Properties of Anisotropic Interaction of the Incommensurate Superstructure as Described by Dzialoshinsky’s Invariant

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Abstract—BDF method was applied for calculation of phase portrait of incommensurate superstructure with the Dzialoshinsky’s invariant. The Python language was used to create the corresponding application. The value of the parameter of the anisotropic interaction is determined by the number of existing harmonics of the IC of the modulation wave. The contribution of anisotropic interaction in the dynamics of the IC superstructure grows if numbers of harmonics of the IC modulation are growing. According to the received attractors, this system is less stable at lower values of n.

Index Terms—anisotropic interaction; BDF method; Python language; incommensurate superstructure; Dzialoshinsky’s invariant; phase system portrait.

One of the peculiarities of the existence of incommensurate superstructures is the localization of the wave vector of incommensurability at comparable values of higher order. The nature of this phenomenon is pinning (fixing) the wave of incommensurate in defects and impurities [1]. Under these conditions, the magnitude of the incommensurate vector is a rational number, which can be written as a ratio of two integer m/n, where m and n are integer positive numbers. It should be noted that the number n characterizes the symmetry of the thermodynamic potential, and determines the magnitude of the anisotropic interaction, which is described by the Dzialoshinsky invariant [2] (1). In dimensionless variables η = (r / (2n))^{1/2} R, z = (r / R)^{3/2} ξ, the free energy functional for a two-component order parameter in polar coordinates has the form:

\[ \Phi = \frac{\sigma}{2} \left[ -R^2 + \frac{R^4}{2} + \frac{w R^4}{2} \right] R^2 \left( 1 + \cos n \phi \right) - \frac{\sigma}{2 R^2} R^2 \left( 1 - \phi^2 \right) - \frac{\sigma}{2 R^2} R^2 \left( 1 + \phi^2 \right) - \frac{\sigma}{2 R^2} R^2 \left( 1 - \phi^2 \right) \]

(1)

The variation of the free energy functional (1) gives a system of two equations for phase and amplitude functions:

\[ R^* - R^3 + \left( 1 - \phi^2 + T \phi \right) R - R^{-1} K \cos n \phi + 1 = 0 \]

(2)

\[ T = \frac{\pi}{\sqrt{\sigma}} \]

here: \( nKRRR = 2 \pi \), \( K = 2 \pi^n \frac{n \omega}{\pi} - \frac{n \omega}{\pi} \) — dimensionless parameters, n is an integer characterizing the potential symmetry.

Thus, according to expression (2), the parameter K, which characterizes the anisotropic interaction, depends on the value of n. Assume that the coefficient of expansion of the thermodynamic potential is less than one, then with increasing n the parameter K will nonlinearly decrease. This finds a good correlation with the experimental studies of the metastable states of the incommensurate superstructure. Namely, the higher the value of n causes the lower temperature interval of the existence of metastable states.

Consequently, the study of the influence of the symmetry of the thermodynamic potential on anisotropic interaction, described by the Dzialoshinsky’s invariant was carried out. Namely, the study of phase portraits of this system was obtained. The phase portrait is a complete set of different phase trajectories. He clearly illustrates the behavior of the system and its basic properties, such as equilibrium points. With the help of phase portraits you can analyze the state of stability and the nature of the movements of the system.

The construction of phase portraits of a nonlinear dynamical system is carried out in the Python software environment using the scipy library. In this library, the class scipy.integrate.ode (f, jac = None) is the common interface class to numeric integrators. This class solves the system of equations \((\dot{y}(t) = f(t, y))\) with \( \text{jac} = \text{d}f/\text{dy} \). Using the set_integrator method, the integrator "vode", which is the usual solver of the differential equation, with the introduction of a fixed-leading coefficient. The leading factor is the integer in the set_integrator class of the ode class, which takes the following parameters [3]:

\[ \phi^* + 2R^*(\phi^2 - T/2) + R^{-2} K \sin n \phi = 0 \]
from scipy.integrate import ode
import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D

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def f(t, y):
c0=1.0
c1=0.7
c2=4
y0, y1, y2, y3, = y
return [y1,y0**3-(1+c0*y3-y3**2)*y0+c1*(y0**(c2-1))*(1+np.cos(c2*y2)),y3,-(y1/y0)*(2*y3-c0)-c1*(y0**(c2-2))*np.sin(c2*y2)]

# from scipy.integrate import ode
r = ode(f).set_integrator("vode", method="BDF", order=10, rtol=0, atol=1e-6, with_jacobian=False)
y0 = [0.3,0.0,0.0,0.75]
r.set_initial_value(y0, 0)
T =200
dt = 0.0004
y = []; t = []
while r.successful() and r.t <= T:
r.integrate(r.t + dt)
y.append(r.y); t.append(r.t)
y=np.array(y)
fig, ax = plt.subplots()
fig.set_facecolor('white')
ax=Axes3D(fig)
plt.xlabel('R')
plt.ylabel('dR/dx')
plt.title("Фазовий портрет")
plt.plot(y[:,0],y[:,1],y[:,3],linewidth=1)
plt.grid(True)
plt.show()
It is known [5] that an incommensurate superstructure is characterized by a sinusoidal and a soliton modulation regime. In a soliton regime, the superstructure is characterized by pinning on defects and impurities, resulting in the localization of the wave vector of incommensurability at commensurate of higher order values \( q = m / n \). This testifies to the appearance of anisotropic interaction of inequality, which is described by the Dzyaloshinsky invariant. With the subsequent increase in the number of harmonics there is a process of increasing anisotropic interaction leading to the emergence of a stochastic regimen of IC modulation with the onset of a chaotic phase [5].

With the help of mathematical simulation, consider the effect of the symmetry of the potential \( n \) on the value of \( K \), in which the system passes into a chaotic state. Fig. 3 shows the attractor's appearance at the boundary of transition to a chaotic state provided: \( n = 2, T = 1, K = 0.465 \). This attractor is characterized by a complex trajectory, and consists of two boundary cycles that are located at a small angle to each other. With an increase in the value of \( n \) the character of the attractor changes on the verge of transition to a chaotic state. So, the value of the parameter \( K = 214.5 \) (Fig. 4). In other words,
taking into account the results of work [6], the transition to chaos at large values of \( n \) \((n > 5)\) occurs as a result of bifurcation, and at lower values \( n \) the transition to chaos is carried out through the intermediate chaotic phase.

Thus, the anisotropic interaction described by the Dzyaloshinsky’s invariant depends on the symmetry of the thermodynamic potential. As the magnitude \( n \) increases, the parameter \( T \) is nonlinear (according to the power law) decreases.

Proceeding from the results shown in Fig. 3 and Fig. 4, the value of the parameter of the anisotropic interaction is determined by the number of existing harmonics of the IC of the modulation wave. The contribution of anisotropic interaction in the dynamics of the IC superstructure grows if numbers of harmonics of the IC modulation are growing. According to the received attractors, this system is less stable at lower values \( n \).

Hence, a richer picture of the dynamics of the IC superstructure should be expected at lower values of \( n \). Under this condition, the parameter of anisotropic interaction becomes proportional (we may say identically) of the stability of the IC superstructure (parameter \( T \)).

Regarding the nature of the modulation of the secondary order parameter (ferroelectric or ferroelastic), it does not affect the character of the anisotropic interaction of the IC modulation.

REFERENCES