Small amplitude approximation and stabilities for dislocation motion in a superlattice*

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Starting from the traveling wave solution, in small amplitude approximation, the Sine–Gordon equation can be reduced to a generalized Duffing equation to describe the dislocation motion in a superlattice, and the phase plane properties of the system phase plane are described in the absence of an applied field. The stabilities are also discussed in the presence of an applied field. It is pointed out that the separatrix orbit describing the dislocation motion as the kink wave may transfer the energy along the dislocation line, keep its form unchanged, and reveal the soliton wave properties of the dislocation motion. It is stressed that the dislocation motion process is the energy transfer and release process, and the system is stable when its energy is minimum.

Keywords: superlattice, Sine–Gordon equation, Duffing equation, stabilities, dislocation dynamics

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1. Introduction

Strained superlattice is of multilayer structure alternately generated using two materials with different lattice parameters. For instance, the multilayer structure generated alternately by using GaAs and $Ga_{1-x}Al_xAs$ is of classical strained superlattice. The special geometry structure of a superlattice, arousing much interest, may open up a new field of seeking new material and a new light source. In fact, based on this concept, photoelectric properties of semiconductor material become much better, and people find photon crystal and phonon crystal in turn. Based on this concept, interaction of charged particles with material has a completely new research area–channeling effect and channeling radiation of a superlattice.[1–11] As the two material lattice parameters mismatch in the growing direction or are not ideal in the extension condition, the strain and stress are generated in the region of the superlattice interface. The stress will cause dislocation, dislocation motion, accumulation, and pinning, which will make the superlattice segregated or broken. Research in dislocation dynamics near the superlattice interface, can adjust the actual physical requirements for superlattice preparation, also improve the superlattice material property further (for example photoelectric properties, mechanical behavior, etc.).

Based on the general Seeger equation,[12] the motion behavior of superlattice dislocation in the small amplitude approximation is discussed in this paper. Based on the traveling wave solution, the Seeger equation describing dislocation motion is reduced to a generalized Sine–Gordon equation, the phase plane properties of the system in the small amplitude approximation is discussed in the absence of an applied field, separatrix orbit (heterolytic orbit) and period orbit are also analyzed. Chaotic behavior of the heterolytic orbit in the manner of a horseshoe is analyzed by the Melnikov method. The result shows that the separatrix orbit describing dislocation moves along the dislocation line due to the kink wave, and energy transfers from one side to another along the dislocation line; the period orbit motion is also in the kink wave form, but the wave can move only in the neighboring field of equilibrium position, and cannot finish energy transferring to a great extent. The result shows that the stability of the orbit is related to system parameters only by selecting relevant parameters, and that the processes of energy transfer and release are stable.

2. Motion equation

2.1. General Seeger equation

Suppose that the dislocation is a segment edge dislocation and the dislocation line is parallel to the x axis (intersecting the line of the superlattice neighboring lattice plane). In the slip plane, the transverse displacement of dislocation in the direction vertical to the x axis is denoted as $\psi(x,t)$, so $\psi(x,t)$ satisfies the general Seeger equation[12]

$$E(\psi)\frac{\partial^2\psi}{\partial x^2} = \frac{\partial E(\psi)}{\partial \psi} - b\sigma(x,t) + m\frac{\partial^2\psi}{\partial t^2}, \tag{1}$$

where b is the Burgers vector, m is the effective mass of unit dislocation length, $\sigma(x,t)$ is the stress of unit dislocation length, and $E(\psi)$ is the elastic potential energy relating to the strain.

2.2. Elastic potential energy

Note the periodicity of the superlattice system. For the thin layer of equivalent thickness, elastic potential energy of the system can be described as follows:[12]

$$E(\psi) = \frac{a_0}{2} + \sum a_n \cos\frac{2n\pi\psi}{d}, \quad n = 1,2,3\ldots, \tag{2}$$

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where $a_0 = E_0/2$, with E_0 being the potential barrier height, and

$$a_n = \frac{2}{d}\int_{-d/2}^{d/2} E(\psi)\cos\frac{2n\pi\psi}{d}\,\mathrm{d}\psi = \frac{4kd}{(n\pi)^2}, \quad n = 1,2,3,\ldots. \tag{3}$$

Note that a_n is inversely proportional to n^2. In general, letting n equal one in Eq. (2), one can obtain

$$E(\psi) = \frac{a_0}{2} + a_1\cos\frac{2\pi\psi}{d}; \quad a_1 = \frac{4kd}{\pi^2}. \tag{4}$$

The stress of the unit dislocation line can be described as

$$F(\psi) = -\frac{\partial E(\psi)}{\partial\psi} = \frac{2\pi a_1}{d}\sin\frac{2\pi\psi}{d}. \tag{5}$$

Note that both sides of Eq. (1) have $E(\psi)$'s, as their positions are different, their roles are different. On the right-hand side, the determining role is variation speed; on the left-hand side, the determining role is the magnitude of $E(\psi)$. Approximately, it can be maximum, average or the first term of the expanded form. In this paper the first term of expanded form $E(\psi) = a_0/2$ is used to substitute it.

2.3. Motion equation

Substituting Eq. (5) into Eq. (1), noting that the left term $E(\psi) = a_0/2$, and the motion damping $2\gamma\mathrm{d}\psi/\mathrm{d}t$ (γ is the damping coefficient), equation (1) can be turned into a general Sine–Gordon equation as follows:

$$\frac{\partial^2\psi}{\partial t^2} - c_0^2\frac{\partial^2\psi}{\partial x^2} + 2\gamma_1\frac{\partial\psi}{\partial t} + \delta_1^2\sin\frac{2\pi\psi}{d} = f_1\sigma(x,t), \tag{6}$$

where

$$c_0^2 = \frac{a_0}{2m}, \quad \gamma_1 = \frac{\gamma}{m}, \quad f_1 = \frac{b}{m}, \quad \delta_1^2 = \frac{2\pi a_1}{m\,d}. \tag{7}$$

Supposing that equation (6) has the traveling wave solution in the following form

$$\psi = \psi(\xi); \quad \xi = x + vt. \tag{8}$$

Substituting Eq. (8) into Eq. (6) can lead to

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}\xi^2} + 2\gamma_2\frac{\mathrm{d}\psi}{\mathrm{d}\xi} + \delta^2\sin\frac{2\pi\psi}{d} = f_2\sigma(\xi), \tag{9}$$

where

$$\delta^2 = \frac{\delta_1^2}{v^2 - c_0^2}, \quad \gamma_2 = \frac{\gamma_1 v}{2(v^2 - c_0^2)}, \quad f_2 = \frac{f_1}{v^2 - c_0^2}. \tag{10}$$

Let

$$u = \frac{2\pi\psi}{d}, \quad \mu = \frac{\gamma_2}{\delta}\sqrt{\frac{2\pi}{d}}, \quad \tau = \sqrt{\frac{2\pi}{d}}\delta\,\xi \quad f_3 = \frac{f_2}{\delta^2}. \tag{11}$$

Equation (9) can be reduced to

$$\frac{\mathrm{d}^2u}{\mathrm{d}\tau^2} + 2\mu\frac{\mathrm{d}u}{\mathrm{d}\tau} + \sin u = f_3\sigma(\tau). \tag{12}$$

Noting that stress field σ is a complicated function of

$$\tau = \sqrt{\frac{2\pi}{d}}\delta\,\xi = \sqrt{\frac{2\pi}{d}}\delta(x+vt),$$

and it can be transferred into Fourier series as the following form

$$\sigma(\tau) = \frac{p_0}{2} + \sum(p_n\cos n\tau + q_n\sin n\tau), \quad n = 1, 2, \ldots, \tag{13}$$

where $p_0 = 2p(0) = 2\sigma_0$, with σ_0 being the amplitude of stressed field,

$$p_n = \frac{1}{d}\int_{-d/2}^{d/2}\sigma(\tau)\cos n\tau\,\mathrm{d}\tau \quad \text{and} \quad q_n = \frac{1}{d}\int_{-d/2}^{d/2}\sigma(\tau)\sin n\tau\,\mathrm{d}\tau.$$

Considering the influence of n-order harmonic wave, equation (12) can be reduced to

$$\frac{\mathrm{d}^2u}{\mathrm{d}\tau^2} + 2\mu\frac{\mathrm{d}u}{\mathrm{d}\tau} + \sin u = f\cos\omega\tau, \tag{14}$$

where

$$f^2 = f_3(p_n^2 + q_n^2). \tag{15}$$

Equation (14) is the generalized pendulum equation containing damping term and forced term, $\omega = n$ is the ratio of the applied field frequency to the natural frequency of the system. Expanding trigonometric function $\sin u$ as $\sin u = 1 - u^3/6 + \cdots$, in small amplitude approximation, equation (14) can be turned into the following form

$$\begin{aligned} u' &= \varsigma, \\ \varsigma' &= -u + u^3/6 + \varepsilon\left(-2\mu\frac{\mathrm{d}u}{\mathrm{d}t} + f\cos\omega\tau\right), \end{aligned} \tag{16}$$

where ε is a small parameter that is introduced to show the accompanying term, and it is a small quantity (only need to set $\varepsilon = 1$ in result). System (14) or (16) is a typical dynamics system with complicated global bifurcating property and chaotic behavior. Two cases will be discussed in the cases of $\varepsilon = 0$ and $\varepsilon \neq 0$ below.

3. The phase plane properties of the system in the case $\varepsilon = 0$

The system with $\varepsilon = 0$ is an unperturbated system. For the unperturbated system, equation (12) can be written as

$$\frac{\mathrm{d}u}{\mathrm{d}\tau} = \varsigma, \quad \frac{\mathrm{d}\varsigma}{\mathrm{d}\tau} = -u + u^3. \tag{17}$$

Equation (17) describes a Hamilton system without time variable, and integrating it once we can obtain the system Hamiltonian,

$$H = \frac{\varsigma^2}{2} + \frac{u^2}{2} - \frac{u^4}{4} = h. \tag{18}$$

From Eq. (17), we can see that in phase plane (u, ς), there are three fixed points, one is middle point (0, 0), the other two are saddle points (1, 0) and (−1, 0). Figure 1 shows the effective potential and phase plane properties of unperturbated system (17). There are two separatrix orbits (heterolytic orbits) when $h = 1/4$

$$u(\tau)_{\pm} = \pm \operatorname{th}(\sqrt{2}\tau/2),$$
$$\varsigma(\tau)_{\pm} = \pm\frac{\sqrt{2}}{2}\operatorname{sech}^2(\sqrt{2}\tau/2). \tag{19}$$

There is a family-period orbit around center (0, 0) when $0 < h < 1/4$

$$u = \frac{\sqrt{2}\kappa}{\sqrt{1+\kappa^2}}\operatorname{sn}\left(\frac{\tau}{\sqrt{1+\kappa^2}}, \kappa\right),$$
$$\varsigma = \frac{\sqrt{2}\kappa}{\sqrt{1+\kappa^2}}\operatorname{cn}\left(\frac{\tau}{\sqrt{1+\kappa^2}}, \kappa\right)\operatorname{dn}\left(\frac{\tau}{\sqrt{1+\kappa^2}}, \kappa\right), \tag{20}$$

where $\operatorname{sn}(u)$, $\operatorname{cn}(u)$, $\operatorname{dn}(u)$ are the Jacobi elliptic functions, κ is the modulus of elliptic function and $0 < \kappa < 1$. Also, $h^2(k) = k/(1+k^2)$, corresponding orbital period is

$$T = 4\sqrt{1+\kappa^2}\,\mathrm{K}(\kappa), \tag{21}$$

where $\mathrm{K}(\kappa)$ is the first kind of the elliptic integral. Note that the orbit when $h = 1/4$ is a separatrix orbit. In Fig. 1, separatrix orbit ($h = 1/4$) divides the phase plane into two parts: internal and external. For external separatrix orbit ($h > 1/4$), phase orbit is open; when time approaches to infinity, coordinate ξ (hence ψ) also approaches to infinity, and this orbit determines whether the dislocation can realize energy transfer and release to a great extent. For internal separatrix orbit ($0 < h < 1/4$), phase orbit is closed, corresponding to periodic motion of dislocation surrounding equilibrium position. This motion can realize the energy transferring in a small field. It is noted that the motion behavior of the system in separatrix orbit can be described using the kink solution. When time approaches to infinity, the dislocation moves from one side to another along the x direction in the form of a kink wave and the form is kept unchanged, which is one of the soliton wave properties.

Figure 2 shows the soliton solutions of the Sine–Gordon equation in the approximation of small amplitude. The upper figures show how the dislocation transfers and releases energy in the forms of a kink wave and anti-kink wave. The bottom figures shows how the velocity wave transfers and releases energy in clockwise and counterclockwise form. It is also worth noting that the dislocation with periodic motion can obtain energy to make energy constant $h > 1/4$ by fluctuation, so closed periodic orbit can be turned into open orbit, and hence it has all properties of open orbit. That is, the dislocation can transfer and release energy by fluctuating. By fluctuating dislocation, the system can obtain proper energy, which can make open orbit or periodic orbit neighboring separatrix orbit ($h = 1/4$), and the dislocation motion can be described by separatrix orbit (19), and the system can show soliton behavior further.

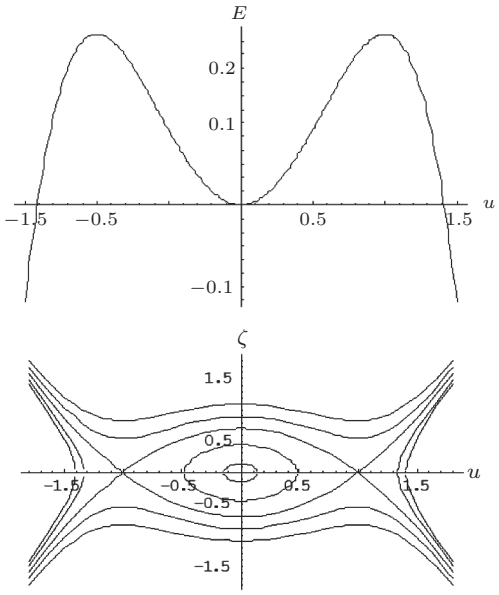


Fig. 1. Effective potential (upper) of the system and its phase plane characteristic (bottom), where the values of parameter h are 0.01, 0.10, 0.25, 0.40, 0.60 (from inside to outside).

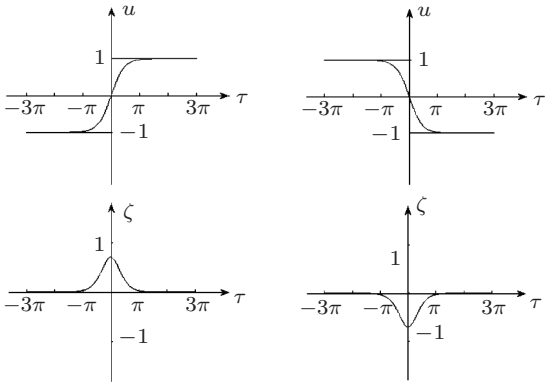


Fig. 2. Kink solutions (left) and anti-kink solutions (right) of the superlattice system.

4. Stability of the system when $\varepsilon \neq 0$

4.1. Melnikov function of heterolytic orbit and physical significance of Smale horseshoe chaos

For heterolytic orbit (19) of the system, the following form of the Melnikov function can be constructed:

$$M_{\pm}(\tau_0) = \int_{-\infty}^{+\infty} \varsigma_{\pm}(\tau)\left[-2\mu\varsigma_{\pm}(\tau) + f\cos\omega(\tau+\tau_0)\right]\mathrm{d}\tau$$
$$= -2\mu I_1(m,n) + fI_2(m,n)\cos\omega\tau_0, \tag{22}$$

where $\varsigma_{\pm}$ can be given by the second expression of Eq. (19), and

$$I_1 = \frac{2\sqrt{2}}{3}, \quad I_2 = \sqrt{2}\pi\omega\operatorname{csch}(\sqrt{2}\pi\omega/2). \tag{23}$$

If parameters f and 2μ can satisfy the following inequality:

$$\frac{f}{2\mu} > \frac{3}{3\pi\omega}\operatorname{sh}(\sqrt{2}\pi\omega/2) = R_{\infty}^{(1)}(\omega), \tag{24}$$

then Poincare mapping of system (16) has a 2-transverse loop, the system has chaos in the sense of the Smale horseshoe, and $R_{\infty}^{(1)}(\omega)$ is the threshold appearing in the Smale horseshoe transform. When condition (24) is satisfied, the right-hand side of Eq. (22) can be negative automatically.

Substituting Eqs. (10), (11), and (15) into Eq. (24), the inequality can be shown by the system?s original parameters

$$\left|\frac{2\gamma}{b\sigma_n}\right| < \frac{2\omega v d}{3\sqrt{m/a_1}}\sqrt{v^2-c_0^2}\,\mathrm{csch}(\sqrt{2}\pi\omega/2), \tag{25}$$

where $\sigma_n = \sqrt{p_n^2+q_n^2}$ is the amplitude of n times the harmonic component of stress field. When condition (25) is satisfied, there will be Smale horseshoe chaos. The chaos means instability. Just by adjusting the system parameters, such a circumstance can be avoided. From inequality (25), the following conclusions can be drawn.

(i) The smaller the stress, the more difficult it is for the condition to be satisfied. When the following condition is satisfied:

$$|b\sigma_n|_{\mathrm{c}} = \frac{3\gamma\sqrt{m/a_1}}{\omega v d\sqrt{v^2-c_0^2}}\mathrm{sh}(\sqrt{2}\pi\omega/2), \tag{26}$$

the system is in the critical condition. When $b\sigma_n < |b\sigma_n|_{\mathrm{c}}$, the system is stable, otherwise, there appears Smale horseshoe chaos in the system.

(ii) The smaller the system damping coefficient 2γ, the more easily the condition is met, in other words, only when damping is strong enough, can it inhibit chaos, and its critical value can be shown as follows:

$$|2\gamma|_{\mathrm{c}} = \frac{2\omega v d b\sigma_n}{3\sqrt{m/a_1}}\sqrt{v^2-c_0^2}\,\mathrm{csch}(\sqrt{2}\pi\omega/2), \tag{27}$$

that is, when damping coefficient satisfies $2\gamma > |2\gamma|_{\mathrm{c}}$, the system is stable.

4.2. Subharmonic bifurcation of periodic orbital

For random relatively prime positive integers m and n, there is a single $k_{m/n} \in (0,1)$, which meets

$$T(k_{m/n}) = 4K(k_{m/n}) = \frac{m}{n}T = \frac{2\pi m}{n\omega},$$

and constructs the Melnikov function of this periodic orbital, so we can obtain

$$\begin{aligned} M_{\pm}^{m/n}(\tau_0) &= \int_{-\infty}^{+\infty} \varsigma_{\pm}(\tau)\left[-2\mu\varsigma_{\pm}(\tau) + f\cos\Omega(\tau+\tau_0)\right]\mathrm{d}\tau \\ &\quad -2\mu J_1 + FJ_2\cos\Omega\tau_0, \end{aligned} \tag{28}$$

where $\varsigma_{\pm}$ can be given by the second expression of Eq. (20), and

$$J_1 = \frac{8n}{3(1+\kappa^2)^{3/2}}[(1-\kappa^2)\mathrm{K}(\kappa) - (1+\kappa^2)\mathrm{E}(\kappa)],$$

$$J_2 = \begin{cases} 0, & n \neq 1 \text{ or } m \text{ is even}, \\ 2\sqrt{2}\pi\omega\,\mathrm{cosech}(2mK'/2K), & \\ n = 1 \text{ and } m \text{ is odd}. \end{cases} \tag{29}$$

From Eqs. (28) and (29), it should be seen when $n = 1$ and m is odd number, in parameter (f,u) plane, if the following condition is satisfied

$$\left|\frac{2\mu}{f}\right| < \frac{3\sqrt{2}(1+\kappa^2)^{3/2}\pi\omega\cos\omega\tau_0}{4[(1-\kappa^2)\mathrm{K}(\kappa) - (1+\kappa^2)\mathrm{E}(\kappa)]}\,\mathrm{csch}\left(\frac{\pi m K'}{2K}\right), \tag{30}$$

then, for sufficiently small ε, there is an odd subharmonic bifurcation in the system (8), and it will be turned into chaos after infinite subharmonic bifurcation. In Eq. (30), $\mathrm{K}'(\kappa) = \mathrm{K}(\kappa), \kappa' = (1-\kappa^2)^{1/2}$ is the complementary module of elliptic function, $\mathrm{E}(\kappa)$ is the second category of elliptic integrals.

Substituting Eqs. (10), (11), and (15) into Eq. (30), the inequality (30) can be shown by the system?s original parameters, i.e.,

$$\begin{aligned} \left|\frac{2\gamma}{b\sigma_n}\right| &< \frac{\sqrt{2}\omega v d(1+\kappa^2)^{3/2}}{2\sqrt{m/a_1}[(1-\kappa^2)K - (1+\kappa^2)E]} \\ &\quad \times\sqrt{v^2-c_0^2}\,\mathrm{csch}(\sqrt{2}\pi\omega/2). \end{aligned} \tag{31}$$

When condition (31) is satisfied, there will be subharmonic bifurcation in the system, and bifurcation means being unstable. Just by adjusting system parameters, such a circumstance may be avoided. From condition (31), we can draw the conclusions as follows.

i) The smaller the stress, the more difficult it is for the condition to be met. When it meets

$$\begin{aligned} |b\sigma_n|_{\mathrm{c}} &= \frac{4\gamma\sqrt{m/a_1}\left[\left(1-\kappa^2\right)K - (1+\kappa^2)E\right]}{\sqrt{2}\omega v d(1+\kappa^2)^{3/2}} \\ &\quad \times\mathrm{sh}(\sqrt{2\pi}\omega/2), \end{aligned} \tag{32}$$

the system is in the critical state. When $|b\sigma_n| < |b\sigma_n|_{\mathrm{c}}$, the system is stable. Otherwise, when $b\sigma_0 > (b\sigma_0)_{\mathrm{c}}$, it meets condition (31), the system is instable.

ii) The smaller the system damping coefficient $(2\mu_0)$, the more easily the condition is met. In other words, only when damping is strong enough, can the bifurcation be inhibited. The critical value can be shown as

$$\begin{aligned} |2\gamma|_{\mathrm{c}} &< \frac{\sqrt{2}b\sigma_n\omega v d(1+\kappa^2)^{3/2}}{2\sqrt{m/a_1}\left[(1-\kappa^2)K - (1+\kappa^2)E\right]} \\ &\quad \times\sqrt{v^2-c_0^2}\,\mathrm{csch}(\sqrt{2}\pi\omega/2), \end{aligned} \tag{33}$$

that is, when damping coefficient $|2\gamma| > |2\gamma|_{\mathrm{c}}$, the system is stable. Oscillation mode periodic orbit describes the situation of system periodic motion around a stable point. Its coordinate ξ (thus ψ) and momentum ς are always in periodic motion around a stable point, which has Liyapunov significance and engineering stability.

Noting that in the growing process of superlattice, with the increase of periodicity, the strain and strain energy of epitaxial layer are also increased continuously, once the thickness of the superlattice exceeds the critical thickness strain

that can be allowed, a dislocation will appear. How the dislocation moves in the slip plane is related to the original state of the system (or the size parameter of system h). It can make the influence of the dislocation decrease to a minimum by introducing a cushion layer. As there is a cushion, the moving direction of the dislocation will be changed, and will be bent in the growing plane under the stress field, and will be annihilated by the interaction with other dislocations in the moving process, or be finished on the two sides of the superlattice. Secondly, it will make the dislocation density decrease in the presence of the cushion, and make the pinning possibility decrease by new dislocation. It will be bent in the growth plane by the stress field, and will pass through the superlattice side, thus the energy of the growth plane will be transferred and released.

5. Conclusions

It is noted that a superlattice is stratified and broken because there is a mismatch of the lattice constant or it is not ideal in the growing process for superlattice material. Research on the dislocation motion behavior near the superlattice interface can propose not only more actual physics requirements for superlattice preparation, but also a new idea for improving superlattice material property further. System stability and dislocation motion behavior are discussed by the Melnikov method, and the result shows that the heterolytic orbit divides the phase plane into two regions: internal and external, and the stability of heterolytic orbit is determined by the relative size of stress field and motion damp. When the motion damp is larger, the system is stable.

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