Kinks in a system of adatomic chains

1990 J. Phys.: Condens. Matter 2 5961

(http://iopscience.iop.org/0953-8984/2/27/003)

J. Phys.: Condens. Matter 2 (1990) 5961–5970. Printed in the UK

Kinks in a system of adatomic chains

O M Braun† and Yu S Kivshar‡

† Institute of Physics, UkrSSR Academy of Sciences, 46 Science Avenue, 252028 Kiev, USSR

‡ Institute for Low Temperature Physics and Engineering, UkrSSR Academy of Sciences, 47 Lenin Avenue, 310164 Kharkov, USSR

Received 5 June 1989, in final form 26 February 1990

Abstract. The quasi-two-dimensional system of coupled Frenkel–Kontorova chains (so-called x-chains, which are classical harmonic chains of atoms in a periodic substrate potential) is considered. We study the case when each x-chain has a kink (x-kink) that corresponds to the x-chain state with an excess atom with respect to the commensurate atomic structure. The model parameters for which x-kinks in the neighbouring atomic chains attract one another and form a stable chain of x-kinks (a y-chain of x-kinks) are determined. We derive an effective Hamiltonian describing the behaviour of the y-chain and calculate the parameters of a y-kink (secondary kink). The applicability of the model to describe the dynamics of quasi-two-dimensional atomic layers adsorbed on metal surfaces is discussed.

1. Introduction

Investigations of non-linear phenomena in two-dimensional systems are very important from theoretical and experimental viewpoints (see e.g. [1]). In particular, the study of the mobility of atoms in two-dimensional atomic layers adsorbed on crystal surfaces has a special practical interest (e.g. [2, 3]). But the examination of an isotropic two-dimensional layer of adatoms is a rather difficult problem (e.g. [4]). However, in a number of cases the adlayer is highly anisotropic, and it can be considered as a quasi-one-dimensional system of interacting chains [5]. First, this is the case of adsorption on 'furrowed' crystal surfaces, such as the (1 1 2) face of a BCC crystal or the (1 1 0) face of a FCC crystal, when the surface potential along the 'furrow' is much lower than that in another direction. Secondly, this situation takes place for adsorption on stepped (vicinal) surfaces when substrate atoms on the step have additional unsaturated chemical bonds and, therefore, the adatoms are predominantly adsorbed on the step, where their coupling with the substrate is stronger. In both cases we can assume that adatom motion is possible in one direction only, i.e. along the furrows or the steps. As a result, we can consider a quasi-two-dimensional model corresponding to a system of parallel Frenkel–Kontorova (FK) chains [6]. Similar models including a harmonic local interaction between neighbouring chains were used in a number of theoretical papers (see e.g. [2] and [7]).

In the present paper we propose and study a quasi-two-dimensional model describing a system of FK chains with local inter-chain interactions of a general type. The paper is organised as follows. The model is described in section 2. Section 3 is devoted to the investigation of the interaction between kinks in the neighbouring FK chains and

0953-8984/90/275961 + 10 $03.50

determination of the conditions when the kinks form a bound inter-chain state that is perpendicular to the x-chain direction. In section 4 we obtain an effective Hamiltonian for the chain of x-kinks (y-chain) and study excitations of this system. Finally, in section 5 we discuss the applicability of the proposed model to describe the dynamic characteristics of atomic layers adsorbed on metal surfaces.

2. Model

The dynamics of an isolated atomic chain adsorbed on a surface can be considered in the framework of the FK model [6], which describes a chain of atoms of mass m_a subjected to a periodic substrate potential with period a and amplitude ε_a. The nearest-neighbour atoms of the chain interact by a harmonic potential with constant g, so that the Hamiltonian of the system takes the form

$$H = \sum_k \left\{ \tfrac{1}{2} m_a \left(\frac{\mathrm{d}u_k}{\mathrm{d}t} \right)^2 + \tfrac{1}{2}\varepsilon_a \left[1 - \cos\left(\frac{2\pi u_k}{a} \right) \right] + \tfrac{1}{2} g (u_k - u_{k-1})^2 \right\}. \tag{2.1}$$

Here the functions u_k are the displacements of adatoms from the bottoms of the periodic substrate potential. Below, we will use dimensionless units in which $a = 2\pi$, $m_a = 1$ and $\varepsilon_a = 2$.

It is important to note that the Hamiltonian (2.1) also describes a number of physical phenomena such as dislocations in one-dimensional solids, planar domain walls in magnetic systems, charge-density waves in quasi-one-dimensional conductors, and so on (see e.g. [1] and [8]). Besides, there are various generalisations of the usual FK model that take into account a non-sinusoidal substrate potential [9–11], an anharmonic [11, 12] and non-local [11] inter-particle interactions, and the case of arbitrary concentration of adatoms [11].

It is well known that in the FK model a mass transfer is carried out by topological solitons or so-called kinks (or antikinks), which describe the behaviour of excess atoms (vacancies) in the commensurate adatomic structure. These 'primary' kinks we will call x-kinks. The x-kink is a quasi-particle with coordinate X, size (or width) d_0 and effective mass m_0; the creation of a kink–antikink pair in the commensurate structure needs some energy $2\varepsilon_0$.

In this paper we will consider the case of the so-called rigid chain ($g \gg 1$), when the inter-particle interaction along the chain is much greater than the interaction with the substrate potential. In this case we may use the continuum approximation ($i \to x = ka$, $u_k \to u(x)$); the Hamiltonian (2.1) transfers to that of the well known sine–Gordon system:

$$H[u] = a^{-1} \int \mathrm{d}x \left[\tfrac{1}{2} \left(\frac{\partial u}{\partial t} \right)^2 + \tfrac{1}{2} d_0^2 \left(\frac{\partial u}{\partial x} \right)^2 + (1 - \cos u) \right] \tag{2.2}$$

and a kink (antikink) with the topological charge $\sigma = +1$ ($\sigma = -1$) has the simple analytical form

$$u(x) = u_{SG}(x; X, d_0) = 4 \tan^{-1}\{\exp[-\sigma(x - X)/d_0]\} \tag{2.3}$$

so that

$$d_0 = a g^{1/2} \tag{2.4}$$

$$m_0 = 4/\pi d_0 \tag{2.5}$$

and

$$\varepsilon_0 = 4d_0/\pi. \tag{2.6}$$

If $X = Vt$, V being a constant, then the expression (2.3) describes the kink motion in the non-relativistic case ($V^2 \ll 1$). However, it should be taken into account that, in a real discrete chain, kinks move in a periodic Peierls potential with period a and amplitude ε_P. The latter is related to the kink width d_0 by the approximate relation (e.g. [13])

$$\varepsilon_P \simeq \tfrac{4}{3}\pi^2 d_0^3 \exp(-\pi d_0/2). \tag{2.7}$$

In the general case, adatomic chains are not isolated; there is an interaction between chains due to the interaction between adatoms in different chains. It should be pointed out that the energy $v(x)$ of the interaction between two neighbouring atoms chemisorbed in nearest wells of different chains and relatively shifted by some distance x can be measured experimentally as well as estimated theoretically (see the survey [14]). In [5] we have proposed the following local form for the addendum to the system Hamiltonian due to the interaction of two nearest adatomic chains,

$$H_{\text{int}}[u_1, u_2] = a^{-1} \int \mathrm{d}x \left(-\alpha[1 - \cos(u_1 - u_2)] + \gamma \frac{\partial u_1}{\partial x} \frac{\partial u_2}{\partial x} \right) \tag{2.8}$$

where $u_1(x)$ and $u_2(x)$ are the atomic displacements in the chains. The first term in (2.8) is a generalisation of the usual expression of elasticity theory. Indeed, in the case of small relative shifts ($|u_1 - u_2| \ll 2\pi$) it takes the form

$$H_{\text{int}}[u_1, u_2] \simeq a^{-1} \tfrac{1}{2}(-\alpha) \int \mathrm{d}x\, (u_1 - u_2)^2 \tag{2.9}$$

and the parameter

$$\alpha = -\mathrm{d}^2 v/\mathrm{d}^2 x \tag{2.10}$$

is the elastic constant; usually $|\alpha| \lesssim g$. The expression (2.9) was used in a number of papers [2, 7]. However, the expression (2.8) takes into account that the energy should be unchanged if the positions of all atoms of one chain are shifted by the value $2\pi k$, k being an integer. The second term ($\sim\gamma$) in (2.8) takes into account the interaction of non-uniform states of chains. Using the method of our paper [11] it can be shown that this interaction should have the form

$$H_{\text{int}}[u_1, u_2] \simeq a^{-2} \iint \mathrm{d}x_1\, \mathrm{d}x_2 \frac{\partial u_1(x_1)}{\partial x_1} v(x_1 - x_2) \frac{\partial u_2(x_2)}{\partial x_2} \tag{2.11}$$

where it is assumed that $v(\infty) = 0$. The physical sense of the expression is rather simple: it describes the interaction of excess atoms in the chains, the density of excess atoms being proportional to $\partial u(x)/\partial x$. If the interaction range l of the potential $v(x)$ is much less than the kink width d, then a local approximation can be used in which the expression $v(x) = a\gamma\delta(x)$ is postulated. Then the expression (2.11) reduces to the second term of (2.8), and the parameter γ can be estimated as

$$\gamma = a^{-1} \int \mathrm{d}x\, v(x). \tag{2.12}$$

From equations (2.10) and (2.12) it can be seen that, in the case of a monotonic attraction of adatoms, we must take $\alpha, \gamma < 0$, and in the opposite case, e.g. for the dipole–dipole repulsion of adatoms [14], the inequality $\alpha, \gamma > 0$ is valid.

The interaction between chains leads to interaction between x-kinks belonging to different x-chains of adatoms. In the case of weak coupling ($|\alpha|, |\gamma|/d_0^2 \ll 1$) this inter-

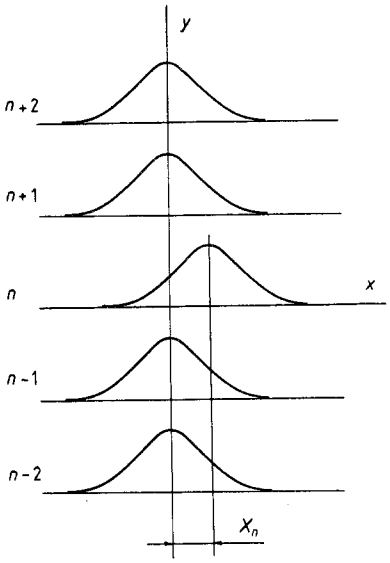

Figure 1. The system of x-chains containing kinks of equal polarities. For simplicity, we present functions $\partial u_n(x)/\partial x$ on the figure.

action was investigated in the framework of the soliton perturbation theory [5]. In the present paper we will consider the planar (quasi-two-dimensional) system of coupled adatomic chains with the Hamiltonian

$$\mathcal{H} = \sum_n \{H[u_n] + H_{\text{int}}[u_n, u_{n-1}]\} \tag{2.13}$$

where n stands for the number of the chain. It is important to note that the simplified version of the model, when $\gamma = 0$, $-1 \ll \alpha < 0$ (i.e. $|u_n - u_{n-1}| \ll 2\pi$) was used in [2, 7].

3. Stability of the y-chain of x-kinks

Let us consider an adsorbed layer with a constant concentration of adatoms when each x-chain contains only one x-kink, all x-kinks being of the same polarity, $\sigma_n = 1$. As was shown in [5], x-kinks belonging to different interacting chains can repel as well as attract one another depending on the parameters of the model. It is obvious that, in the case of attraction, two x-kinks belonging to different chains will form a bound state. Therefore, in this case the quasi-two-dimensional chain-like system has a stable linear chain of kinks, which we will call the y-chain of x-kinks (see figure 1). To describe the ground state in the case of kink attraction, we put $u_n(x) \equiv u(x)$ for all n, so that the Hamiltonian (2.13) takes the form

$$\mathcal{H}_0 = N\left\{a^{-1}\int \mathrm{d}x\left[\tfrac{1}{2}\left(\frac{\partial u}{\partial t}\right)^2 + \tfrac{1}{2}d^2\left(\frac{\partial u}{\partial x}\right)^2 + (1-\cos u)\right]\right\} \tag{3.1}$$

where N is the number of the x-chains ($N \gg 1$), and

$$d^2 \equiv d_0^2 + 2\gamma. \tag{3.2}$$

Thus, the shape of x-kinks in the y-chain is described by the same function (2.3) but with d_0 replaced by d, i.e.

$$u(x) = u_{\text{SG}}(x; X, d). \tag{3.3}$$

As we may see from (3.2) and (3.3), repulsion of adatoms ($\gamma > 0$) leads to increasing of

the kink width ($d > d_0$), and their attraction ($\gamma < 0$) leads to kink contraction ($d < d_0$). However, our local approximation (2.8) is valid only for $d \gg l, a$; otherwise the non-local model (2.11) has to be used.

To investigate the stability of the y-chain of x-kinks we substitute the expression

$$u_n(x) = u(x) + \psi_n(x) \exp(i\lambda^{1/2}t) \qquad |\psi_n| \ll 2\pi \tag{3.4}$$

into equations (2.13), (2.2) and (2.8), and linearise the Hamiltonian and equations of motion in small displacements $\psi_n(x)$. As a result, we obtain the linear equation

$$\hat{L}\Psi(x) = \lambda\Psi(x) \tag{3.5}$$

where $\Psi(x)$ is the column vector with elements $\psi_n(x)$, and $\hat{L}$ is the three-diagonal symmetric matrix

$$\hat{L} = \begin{pmatrix} \cdots & & & & & & & \cdots \\ \cdots & 0 & L_1 & L_0 & L_1 & 0 & 0 & \cdots \\ \cdots & 0 & 0 & L_1 & L_0 & L_1 & 0 & \cdots \\ \cdots & 0 & 0 & 0 & L_1 & L_0 & L_1 & \cdots \\ \cdots & & & & & & & \cdots \end{pmatrix}$$

where

$$L_0 \equiv \cos u(x) - 2\alpha - d_0^2\,\partial^2/\partial x^2 \tag{3.6}$$

$$L_1 \equiv \alpha - \gamma\,\partial^2/\partial x^2. \tag{3.7}$$

It is easy to show that oscillations of the y-chain with wavenumber κ, presented as

$$\psi_n(x) = e^{i\kappa n}\,\psi(x) \qquad |\kappa| < \pi \tag{3.8}$$

have smallest energy. Therefore, the function $\psi(x)$ must be an eigenfunction of the operator $L \equiv L_0 + (e^{i\kappa} + e^{-i\kappa})L_1$. Thus, we come to the eigenvalue equation

$$L(\kappa)\psi(x) = \lambda(\kappa)\psi(x) \tag{3.9}$$

with the operator

$$L(\kappa) \equiv \cos u(x) - 2\alpha(1 - \cos\kappa) - [d^2 - 2\gamma(1 - \cos\kappa)]\,\partial^2/\partial x^2. \tag{3.10}$$

Substituting the expression (3.3) for the function $u(x)$ into (3.10), we obtain that the operator $L(\kappa)$ is a Pöschl–Teller type operator (see e.g. [15]). Its minimum eigenvalue $\lambda_{\min}(\kappa)$ is

$$\lambda_{\min}(\kappa) = 1 - 2\alpha(1 - \cos\kappa) - \mu^2[1 - 2\beta(1 - \cos\kappa)] \tag{3.11}$$

where $\beta \equiv \gamma/d^2$, and the parameter μ is determined by the equation

$$\mu(\mu + 1) = 2[1 - 2\beta(1 - \cos\kappa)]^{-1}. \tag{3.12}$$

The y-chain will be stable if $\lambda_{\min}(\kappa) > 0$. It can be seen that the oscillations with maximum wavenumber are mostly unstable. Substituting $\kappa = \pi$ into equations (3.11) and (3.12), solving (3.12) and substituting the value of μ into (3.11), we obtain that the inequality $\lambda_{\min} > 0$ reduces to

$$\beta(1 - 4\alpha) + \alpha(3 + 4\alpha) < 0. \tag{3.13}$$

Inequality (3.13) is the condition for stability of the y-chain. For small coupling between chains, i.e. $|\alpha|, |\beta| \ll 1$, this condition is transferred to the weaker condition

$$\beta + 3\alpha < 0. \tag{3.14}$$

The latter result was obtained in our paper [5] in the framework of soliton perturbation theory.

4. Parameters of *y*-kinks

Let us again consider an adsorbed layer with a single x-kink in each x-chain, and denote by X_n the coordinate of the kink in the nth chain (in the previous section it was assumed that all X_n are the same). It is important that an x-kink can move along the chain, the motion being carried out in a periodic Peierls potential

$$V_P(X_n) \simeq \tfrac{1}{2}\varepsilon_P(1 - \cos X_n).$$

Of course, x-kinks are deformable quasi-particles, i.e. the shape and parameters of the kink in the nth x-chain depend on the coordinates of kinks in the nearest chains, $X_{n\pm1}$. However, for small relative distances between kinks $|X_n - X_{n\pm1}| \ll 2\pi$, these effects may be neglected, and the shape of the x-kink in the nth chain can be described by the expression

$$u_n(x, t) = u_{SG}(x; X_n(t), d). \tag{4.1}$$

Let us substitute this expression into the Hamiltonian (2.13) with (2.2) and (2.8), and artificially take into account the fact that the motion of the x-kink is carried out in the potential $V_P(X_n)$. As a result, we obtain an effective Hamiltonian

$$\mathcal{H}_{ad} = \sum_n \left[\varepsilon + \tfrac{1}{2}m\left(\frac{dX_n}{dt}\right)^2 + V(X_n - X_{n-1}) + \tfrac{1}{2}\varepsilon_P(1 - \cos X_n) \right] \tag{4.2}$$

which describes the system of quasi-particles (x-kinks) placed in the periodic potential (the Peierls potential for x-kinks) and interacting by the next-nearest potential $V(X_n - X_{n-1})$. The Hamiltonian (4.2) describes the system in the so-called adiabatic approximation when radiative effects may be neglected (see [5]). In equation (4.2), according to (2.5) and (2.6),

$$\varepsilon \equiv 4d/\pi \qquad \text{and} \qquad m \equiv 4/\pi d. \tag{4.3}$$

Straightforward calculations lead to the pairwise potential for the kink interactions between the nearest x-chains:

$$V(X) = -\varepsilon[\alpha W_1(X/d) + \beta W_2(X/d)] \tag{4.4}$$

with

$$W_1(z) = (1 + z/\sinh z)\tanh^2(z/2) \tag{4.5}$$

$$W_2(z) = 1 - z/\sinh z. \tag{4.6}$$

The same result was obtained in [5] by means of soliton perturbation theory. In the case of small $|X| \ll d$, we obtain

$$V(X) \simeq \tfrac{1}{2}GX^2 \tag{4.7}$$

with

$$G = -m(\alpha + \beta/3) \tag{4.8}$$

as well as at $X \to \infty$ it follows that

$$V(\infty) \equiv E_{dis} = -\varepsilon(\alpha + \beta). \tag{4.9}$$

If $G > 0$, x-kinks will form a y-chain that is perpendicular to the initial x-chains of adatoms. The condition $G > 0$ coincides with the above inequality (3.14). Thus, for

small displacements $|X| \ll d$ the Hamiltonian (4.2) with (4.7) is again that of the FK model. The topologically stable soliton (or the y-kink) is the one-soliton solution of the sine–Gordon equation reduced from (4.2) and (4.7). This solution describes a state of the y-chain with a kink, when one half of the y-chain is shifted to a nearest-neighbour minimum of the Peierls potential of x-kinks.

In the case $G \gg \varepsilon_P$, y-kinks are characterised by a width along the y-chain

$$D \simeq b(2G/\varepsilon_P)^{1/2} \tag{4.10}$$

where b is the distance between the x-chains. The effective mass is

$$M \simeq \frac{2m}{\pi^2(2G/\varepsilon_P)^{1/2}} \simeq \frac{4}{\pi}\left(-\frac{2d}{\pi(3\alpha+\beta)}\right)^{1/2} \exp\left(-\frac{\pi d}{4}\right) \tag{4.11}$$

and the energy of kink–antikink pair creation is $2E$, where

$$E \simeq 4(2\varepsilon_P G)^{1/2} \simeq \tfrac{16}{3}\,[-2\pi d(3\alpha+\beta)]^{1/2} \exp(-\pi d/4). \tag{4.12}$$

The motion of the y-kink along the y axis is carried out in a periodic Peierls potential with amplitude

$$E_P \simeq \tfrac{16}{3}\,\pi^4 G \exp[-\pi^2(2G/\varepsilon_P)^{1/2}]. \tag{4.13}$$

In the opposite case of weakly coupled x-kinks, $G \ll \varepsilon_P$, we have $D \simeq b$, $M \simeq 1$,

$$E \simeq 2\pi^2 G \tag{4.14}$$

and

$$E_P \simeq \varepsilon_P - \pi^2 G. \tag{4.15}$$

It is important to note that an infinite y-chain of coupled x-kinks can be torn apart to form two semi-infinite y-chains. This process needs the energy $\simeq E_{dis}$; see (4.9). Similarly, to remove an x-kink from the y-chain one needs the energy $\simeq 2E_{dis}$.

It is interesting to note that if the two inequalities

$$\alpha > 0 \qquad \text{and} \qquad -3\alpha < \beta < -\alpha, \tag{4.16}$$

or the same ones,

$$G < 0 \qquad \text{and} \qquad E_{dis} > 0 \tag{4.17}$$

hold simultaneously, then the potential $V(X)$ of (4.4) has a minimum at a value $X_* \neq 0$ (see also [5]). In this case x-kinks should form an 'oblique' y-chain that makes an acute angle with the initial x-chains of adatoms. In the general case the value of X_* is incommensurate with the period of the Peierls potential along the x-direction, $a = 2\pi$.

5. Discussion

In this section we discuss the applicability of the model to describe quasi-two-dimensional chemisorbed layers. As is well known, adatoms practically always have some dipole moment p, which can be experimentally measured because it changes the substrate work function [16]. As a result, there is the so-called dipole–dipole interaction between adatoms with the potential [14]

$$U_{dip}(r) \simeq 2p^2/r^3 \tag{5.1}$$

where r is the distance between adatoms in the layer. We suppose that this repulsion is the main interaction between atoms along x-chains, so that

$$g \equiv U''_{dip}(a) = 12U_{dip}(a)/a^2 \tag{5.2}$$

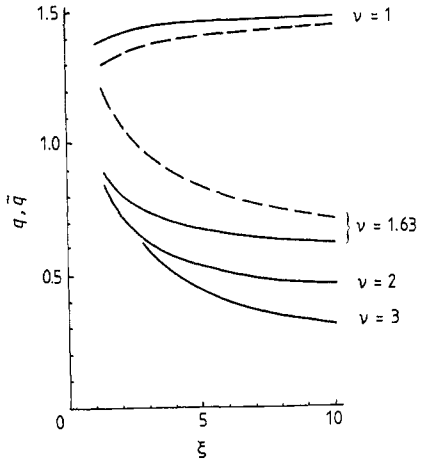

Figure 2. Dependence of q and $\tilde{q}$ introduced by the equations (5.9) and (4.9) on the parameter $\xi \equiv U_{\rm dip}(a)/\varepsilon_a$ at different values of $\nu \equiv b/a$.

and

$$d_0 = [12U_{\rm dip}(a)]^{1/2}. \tag{5.3}$$

The specific properties of the interaction (5.1) caused by its long-range nature are studied in our paper [11] in detail.

If the interaction (5.1) is the only interaction of adatoms, then x-kinks in neighbouring adatomic x-chains will repel each other. However, in a number of adsystems the anisotropic 'indirect' interaction of adatoms caused by electron exchange through the substrate also plays an important role [14]. If two adatoms occupy nearest states in the neighbouring 'furrows' of the (112) face of a BCC crystal, then electron exchange is carried out through the nearest 'bulging' substrate atom, and we can suppose that the energy of the indirect interaction is described by the law $U_{\rm ind} \sim \exp(-x^2/a^2)$. Then the potential $v(x)$ takes the form

$$v(x) = U_{\rm dip}[(b^2 + x^2)^{1/2}] - U_{\rm ind}(b)\exp(-x^2/a^2) \tag{5.4}$$

and from equations (2.10), (2.12), (3.2) and (5.3) we may calculate the following parameters:

$$\alpha = 3U_{\rm dip}(b)/b^2 - 2U_{\rm ind}(b)/a^2 \tag{5.5}$$

$$\gamma = 2\nu U_{\rm dip}(b) - \pi^{1/2}U_{\rm ind}(b) \tag{5.6}$$

$$d^2 = 2\{2[3U_{\rm dip}(a) + \nu U_{\rm dip}(b)] - \pi^{1/2}U_{\rm ind}(b)\} \tag{5.7}$$

where $\nu \equiv b/a$. From the inequality (3.14) it follows that x-kinks belonging to different x-chains attract one another if the condition

$$U_{\rm ind}(b) > qU_{\rm dip}(b) \tag{5.8}$$

is valid, where the value of q is determined by the solution of the equation

$$6\xi(3 - 2\nu^2 q)(6\nu^3 + 2\nu - q\pi^{1/2}) + 4\pi^2\nu^5(\nu - q\pi^{1/2}/2) = 0 \tag{5.9}$$

and the parameter ξ stands for $U_{\rm dip}(a)/\varepsilon_a$. Similarly, we can introduce the parameter $\tilde{q}$ corresponding to the condition $E_{\rm dis} = 0$; see (4.9). The dependence of q and $\tilde{q}$ on the parameter ξ at $\nu = 1$, 2 and 3 as well as at $\nu = 1.63$ (the latter value corresponds to the (112) face of the BCC crystal) is shown in figure 2 (q is shown by full curves and $\tilde{q}$ by broken curves).

Thus, the following situations are possible depending on the adsystem parameters.

(i) If $U_{ind}(b) > U_{dip}(b)$, y-chains of adatoms should be formed. A similar situation was observed in a number of adsystems (see the survey [14]).

(ii) If $U_{ind}(b) > qU_{dip}(b)$, y-chains of x-kinks should be formed. This situation is experimentally observed for the adsorption of Li on the (112) face of W or Mo at the coverage (relative concentration of adatoms) $\theta \leqslant 1$ (see [14]). It is interesting that usually we have $q < 1$ at $\nu > 1$ (see figure 2). Therefore, in some cases y-chains of x-kinks can be formed, while the formation of y-chains of adatoms is not possible.

(iii) For

$$qU_{dip}(b) < U_{int}(b) < \tilde{q}U_{dip}(b) \tag{5.10}$$

'oblique' chains of x-kinks should be formed. Maybe, this situation takes place for the adsorption of Li or Na on the (112) face of W or Mo near the coverage $\theta \geqslant 0.5$ (see [14]).

(iv) Finally, in the case $U_{ind}(b) < \max(q, \tilde{q})U_{dip}(b)$ x-kinks repel each other so that x-kinks should form the $c(2 \times 2)$ structure with smoothly changing period along the x axis when the concentrations of adatoms is increased. Such structures were observed for the adsorption of Cs or K on the 'furrowed' faces of W, Mo and Re (see details in the review [14]).

The statistical properties of different kink-like structures of adatoms are considered in the book [2]. Here we briefly discuss the effect of formation of y-chains on the diffusion characteristics of adlayers. First of all, we note that for non-interacting x-chains of adatoms the activation energy of surface diffusion ε_B is equal to the amplitude of the Peierls potential $\varepsilon_P(d_0)$. It is also known (see e.g. [3]) that the repulsion of x-kinks (case (iv)) decreases the activation energy, $\varepsilon_B < \varepsilon_P$. In the case of attraction of x-kinks (case (ii)) the value of ε_B should usually increase. For example, the motion of a finite y-chain is carried out by the creation of a y-kink at an edge of the chain, so that $\varepsilon_B \simeq E + E_P$ [12]. For an infinite y-chain the motion starts from the creation of a kink–antikink pair, and the kink and antikink move in opposite directions. This process needs activation energy $\varepsilon_B \simeq 2E + E_P$. If the infinite y-chain has various defects ('stopors'), then motion of the y-chain as a whole will be possible only after its breaking, so that the energy E_{dis} would be needed [2]. Finally, for an 'oblique' y-chain of coupled x-kinks (case (iii)) the activation energy may exceed the value of ε_P at $X_* \simeq na$, n being an integer, as well as being lower than ε_P in an incommensurate case, at $X_* \simeq (n + \frac{1}{2})a$.

Thus, in quasi-two-dimensional adatomic layers, there may be various structures of x-kinks: direct or oblique y-chains, $c(2 \times 2)$ structures, as well as different mechanisms of surface diffusion depending on adsystem parameters. These structures and adsystem dynamics may be described in the framework of the above model.

Acknowledgments

We would like to thank Professors A G Fedorus, V K Medvedev and A G Naumovets for useful discussions, and Professor A M Kosevich for attention to the work. We would like also to thank a referee for useful comments.

References

[1] Kosevich A M 1982 *Foundation of Crystal Lattice Mechanics* (Moscow: Nauka) p 238

[2] Lyuksyutov I F, Naumovets A G and Pokrovsky V L 1988 *Two-Dimensional Crystals* (Kiev: Naukova Dumka) p 219

[3] Naumovets A G and Vedula Yu S 1984 *Surf. Sci. Rep.* **4** 365
[4] Srolovitz D J and Londahl P S 1986 *Physica* **23D** 402
[5] Braun O M, Kivshar Yu S and Kosevich A M 1988 *J. Phys. C: Solid State Phys.* **21** 3881
[6] Frenkel J and Kontorova T 1938 *Phys. Z. Sowjetun.* **13** 1
[7] Kato H, Okwamoto Y and Nakayama T 1983 *J. Phys. Soc. Japan* **52** 3334
[8] Dodd R K, Eilbeck J C, Gibbon J D and Morris H C 1984 *Solitons and Nonlinear Wave Equations* (London: Academic)
[9] Peyrard M and Remoissenet M 1982 *Phys. Rev.* B **26** 2886
[10] Ishibashi Y and Suzuki I 1984 *J. Phys. Soc. Japan* **53** 4250
[11] Braun O M, Kivshar Yu S and Zelenskaya I I 1989 *Phys. Rev.* B
[12] Markov I and Milchev A 1985 *Thin Solid Films* **126** 83
[13] Willis C, El-Batanouny M and Stancioff P 1986 *Phys. Rev.* B **33** 1904
[14] Braun O M and Medvedev V K 1989 *Usp. Fiz. Nauk* (*Sov. Phys.–Usp.*) **157** 631
[15] Flügge S 1971 *Practical Quantum Mechanics I* (Berlin: Springer)
[16] Bolshov L A, Napartovich A P, Naumovets A G and Fedorus A G 1977 *Usp. Fiz. Nauk* (*Sov. Phys.–Usp.*) **122** 125