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LETTER TO THE EDITOR

Double-sine–Gordon solitons in two-dimensional crystals

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Abstract. We consider a model of a crystal monolayer, which consists of a monatomic step on an anisotropic substrate of a periodic substrate interaction potential. The formation of the surface mono-atomic step is described by a surface misfit phenomenon involving large-amplitude displacements of atoms on the crystal surface. These large-amplitude displacements are misfit dislocations whose dynamics are governed by a two-dimensional double-sine–Gordon equation. Some solutions of this equation, namely the bi-kink soliton solutions, are found with emphasis on effects of the surface boundaries. It is shown that the soliton density, which measures the bi-kink fraction in a multi-soliton configuration, can be conserved in two dimensions.

Since the pioneering work of Frank and van der Merwe [1], the surface misfit phenomenon and that of adsorption of atoms on a crystal surface have gained interest these last two decades due to their applications in a large variety of physical situations. These phenomena can be summarized as follows: the substrate atoms located on the crystal step have unsaturated chemical bonds, and therefore these atoms are predominantly adsorbed close to the step where their coupling with the substrate atoms is stronger.

A model of surface misfit is that of a crystal monolayer, which consists of a mono-atomic step on an anisotropic substrate. The question concerning the epitaxy and misfit accommodation in this model is about the nature and features of the substrate interaction potential. To this point, the behaviour of a monolayer adsorbate (adatoms) on a crystalline substrate surface as well as the principles governing its formation and stability involve the account of adsorbate–adsorbate and adsorbate–substrate interactions [2–8]. The adsorbate–substrate interaction has the periodicity and symmetry of the crystalline substrate surface (for a single adatom as well as for a completed monolayer or multilayer). For surface phenomena, the surface geometry is predominated by a two-dimensional (2D) map. In BCC crystals [2–8], the interaction potential displays the twofold symmetry of the rhombic unit cell of the {110} atomic plane.

In this letter, following van der Merwe *et al* [2–8], we use a doubly periodic adatom–substrate interaction potential to construct the static theory of surface adatom migration in the large-amplitude regime. In this regime, the equation that governs the adatom displacements in two dimensions can be written

$$\mathrm{d}^2u/\mathrm{d}l^2 + b^2\,\mathrm{d}^2u/\mathrm{d}k^2 = \left(1/2p^2\right)\left[C_1\sin(\pi u) + C_2\sin(2\pi u)\right] \tag{1}$$

where b^2 depends on the vertex angle of the 2D map and on surface strain coefficients along the x and y axes, p^2 is proportional to the adatom–substrate inverse scale, and C_1 and C_2 are constant [5a]. Actually, equation (1) which is a 2D double-sine–Gordon (DSG) equation, describes adatomic displacements in a privileged direction (along the x axis) but with influence of the y direction. A complete description had led to a set of two coupled, 2D DSG equations. However, when the misfit is subcritical we need to consider only single-dislocation solutions [5a].

When the vertex angle equals zero, equation (1) turns into a one-dimensional (1D) DSG equation. van der Merwe *et al* [5a] have already used a 1D DSG equation to estimate the characteristic parameters associated with the formation and growth of a misfit in crystal surfaces. Nevertheless, they restricted their analysis to cases in which the misfit has small sizes, so small that also the monolayer atomic displacements are everywhere small enough for their theory to be valid only in the linear approximation.

As our goal is to go beyond the linear approximation, we shall solve equation (1) in the large-adatomic-displacement limit and using appropriate surface boundary conditions, i.e. $0 \leqslant 1 \leqslant L$ and $0 \leqslant k \leqslant Q$, where L and Q are the total numbers of adatoms along the x and y axes respectively. For mathematical simplicity, we introduce the scaled variables

$$n = 1/p(2)^{1/2}\pi \qquad m = k/bp(2)^{1/2}\pi \qquad \varphi = \pi u. \tag{2}$$

Then (1) becomes

$$\varphi_{nn} - \varphi_{mm} = \left[C_1 \sin(\varphi) + C_2 \sin(2\varphi)\right]. \tag{3}$$

Solving (3), we assume a misfit dislocation described by a soliton *ansatz* of the form [13–15]

$$\varphi(n, m) = 2\tan^{-1}[f(n)/g(m)] \tag{4}$$

where $f(n)$ and $g(m)$ are the generating functions of the misfit dislocation soliton waveform along the x and y axes, respectively. When (4) is substituted into (3), we arrive at the following two polynomial equations in f and g

$$(f_n)^2 = (a/2)f^4 + b_1 f^2 + d_1 \tag{5a}$$

$$(g_m)^2 = (a/2)g^4 + b_2 g^2 + d_2 \tag{5b}$$

subject to constraints

$$d_1 = d_2 = d \tag{6a}$$

$$b_1 + b_2 = 2C_2 - C_1\left(1 + \alpha^2\right)/\left(1 - \alpha^2\right). \tag{6b}$$

The constraint relation (6b) is imposed from the assumption ($z(n, m) = f(n)/g(m)$)

$$z(n, m) = z(n = 0,\ m = 0) = z\left(n = L/p(2)^{1/2}\pi,\ \ m = Q/bp(2)^{1/2}\pi\right) = \pm\alpha. \tag{7}$$

In this last relation, α must be a constant parameter, else the *ansatz* (4) will not be valid.

The polynomial equation (5) can be solved in terms of Jacobi elliptic functions. Indeed, this method seems more appropriate for finite-length systems [13–16]. In the present case there may exist several such solutions depending on the relations between the parameters in (5). In what follows we derive some such solutions.

(i) Cnoidal solutions

The first class of solutions is obtained from the set of relations

$$-2d/a = \alpha_1^2\alpha_2^2 = \beta_1^2\beta_2^2 \qquad 2b_1/a = \alpha_1^2 - \alpha_2^2 \qquad 2b_2/a = \beta_1^2 - \beta_2^2 \tag{8a}$$

$$k_1^2 = \alpha_2^2/\left(\alpha_1^2 + \alpha_2^2\right) \qquad k_2^2 = \beta_2^2/\left(\beta_1^2 + \beta_2^2\right) \qquad 0 \leqslant k_i^2 \leqslant 1 \qquad i = 1,\ 2. \tag{8b}$$

These conditions lead to the following expressions for f and g

$$f(n) = \alpha_2 \,\mathrm{cn}\left[(n - n_0)/D_x\right] \tag{9a}$$

$$g(m) = \beta_2 \,\mathrm{cn}\left[(m - m_0)/D_y\right] \tag{9b}$$

where the sizes of the misfit dislocation along the x and y directions are respectively defined as

$$D_x = (2)^{1/2}/\left(\alpha_1^2 + \alpha_2^2\right)^{1/2}(-a)^{1/2} \qquad D_y = (2)^{1/2}/\left(\beta_1^2 + \beta_2^2\right)^{1/2}(-a)^{1/2}. \tag{10}$$

These relations instruct us that the parameter a must be negative for the misfit accommodation to be possible on the monolayer surface.

(ii) Snoidal solutions

For this second class of solutions, the relations between parameters are

$$2d/a = \alpha_1^2 - \alpha_2^2 = \beta_1^2\beta_2^2 \qquad -2b_1/a = \alpha_1^2 + \alpha_2^2 \qquad -2b_2/a = \beta_1^2 + \beta_2^2 \tag{11a}$$

$$k_1^2 = \left(\alpha_1^2 - \alpha_2^2\right)/\alpha_1^2 \qquad k_2^2 = \left(\beta_1^2 - \beta_2^2\right)/\beta_1^2 \qquad 0 \leqslant k_i^2 \leqslant 1 \qquad i = 1,\ 2. \tag{11b}$$

These relations lead to the following expressions for f and g

$$f(n) = \pm\alpha_2 \,\mathrm{sn}\left[(n - n_0)/D_x\right] \tag{12a}$$

$$g(m) = \pm\beta_2 \,\mathrm{sn}\left[(m - m_0)/D_y\right]. \tag{12b}$$

where the sizes of the misfit dislocation along the x and y directions are now respectively

$$D_x = (2)^{1/2}/\alpha_1(a)^{1/2} \qquad D_y = (2)^{1/2}/\beta_1(a)^{1/2}. \tag{13}$$

So that a must be positive, but b_i negative.

(iii) Dnoidal solutions

In this third case the relations between parameters are

$$2d/a = \alpha_1^2\alpha_2^2 = \beta_1^2\beta_2^2 \qquad -2b_1/a = \alpha_1^2 + \alpha_2^2 \qquad -2b_2/a = \beta_1^2 + \beta_2^2 \tag{14a}$$

$$k_1^2 = \left(\alpha_1^2 - \alpha_2^2\right)/\alpha_1^2 \qquad k_2^2 = \left(\beta_1^2 - \beta_2^2\right)/\beta_1^2 \qquad 0 \leqslant k_i^2 \leqslant 1 \qquad i = 1,\ 2 \tag{14b}$$

and the corresponding solutions are

$$f(n) = \alpha_1 \,\mathrm{dn}\left[(n - n_0)/D_x\right] \tag{15a}$$

$$g(m) = \beta_1 \,\mathrm{dn}\left[(m - m_0)/D_y\right] \tag{15b}$$

where the sizes of the misfit dislocation along the x and y directions are respectively

$$D_x = (2)^{1/2}/\alpha_1(-a)^{1/2} \qquad D_y = (2)^{1/2}/\beta_1(-a)^{1/2}. \tag{16}$$

Hence a must be negative and b_i positive.

(iv) Dsoidal solutions

For the fourth class of solutions we set

$$2d/a = \alpha_1^2\alpha_2^2 = \beta_1^2\beta_2^2 \qquad -2b_1/a = \alpha_1^2 - \alpha_2^2 \qquad -2b_2/a = \beta_1^2 - \beta_2^2 \tag{17a}$$

$$k_1^2 = \alpha_2^2/\left(\alpha_1^2 + \alpha_2^2\right) \qquad k_2^2 = \beta_2^2/\left(\beta_1^2 + \beta_2^2\right) \qquad 0 \leqslant k_i^2 \leqslant 1 \qquad i = 1,\ 2. \tag{17b}$$

These conditions lead to the following expressions for f and g

$$f(n) = \left(\alpha_1^2 + \alpha_2^2\right)^{1/2} \mathrm{ds}\left[(n - n_0)/D_x\right] \tag{18a}$$

$$g(m) = \left(\beta_1^2 + \beta_2^2\right)^{1/2} \mathrm{ds}\left[(m - m_0)/D_y\right] \tag{18b}$$

where the sizes of the misfit dislocation along the x and y directions are respectively defined as

$$D_x = (2)^{1/2}/\left(\alpha_1^2 + \alpha_2^2\right)^{1/2}(a)^{1/2} \qquad D_y = (2)^{1/2}/\left(\beta_1^2 + \beta_2^2\right)^{1/2}(a)^{1/2} \tag{19}$$

and as a consequence, a is positive and b_i positive.

(v) Inverse snoidal solutions

This is the last class of solutions. The relations are

$$2d/a = \alpha_1^2\alpha_2^2 = \beta_1^2\beta_2^2 \qquad 2b_1/a = \alpha_1^2 + \alpha_2^2 \qquad 2b_2/a = \beta_1^2 + \beta_2^2 \tag{20a}$$

$$k_1^2 = \left(\alpha_1^2 - \alpha_2^2\right)/\alpha_1^2 \qquad k_2^2 = \left(\beta_1^2 - \beta_2^2\right)/\beta_1^2 \qquad 0 \leqslant k_i^2 \leqslant 1 \qquad i = 1,\ 2 \tag{20b}$$

and the corresponding solutions are

$$f(n) = \pm\alpha_1\, \mathrm{ns}\left[(n - n_0)/D_x\right] \tag{21a}$$

$$g(m) = \pm\beta_1\, \mathrm{ns}\left[(m - m_0)/D_y\right] \tag{21b}$$

where the sizes of the misfit dislocation along the x and y directions are respectively

$$D_x = (2)^{1/2}/\alpha_1(a)^{1/2} \qquad D_y = (2)^{1/2}/\beta_1(a)^{1/2} \tag{22}$$

with a and b_i positive.

The set of solutions listed in (i)–(v) are all periodic, owing to the periodicity of Jacobi elliptic functions. The periodicity conditions which allow for the accommodation of misfit dislocations with the waveforms obtained above, and on the finite support $0 \leqslant l \leqslant L$, $0 \leqslant k \leqslant Q$ are given by

$$L = \pi p(2)^{1/2} D_x K\left(k_1^2\right) \qquad Q = \pi p(2)^{1/2} D_y K\left(k_2^2\right) \tag{23}$$

where $K(k_i^2)$ is the complete elliptic integral of the first kind and k_i the associated modulus. It is worth remarking that the large-amplitude solutions of the infinite-surface counterpart of the 2D DSG equation (3) are derived from the asymptotic expansions of the Jacobi elliptic functions in (i)–(v) when $k_i^2 \to 1$. In this limit, sn $\to$ tanh, cn $\to$ sech, dn $\to$ sech, ds $\to$ cosech and ns $\to$ cotanh. Therefore, we recover the soliton-generating functions found in previous studies [17] in one dimension and already applied in physisorption phenomena [9, 12].

The physical configuration of a DSG soliton is like a bi-kink. More explicitly, a DSG soliton looks like three 'steps' which result from two superposed kinks. The physical interpretation of signs in some of the solutions obtained above means that one can consider a 'step-up' or a 'step-down' ledge when going in the positive or negative x and y directions, either simultaneously or inversely. The first of these two possibilities gives rise to a continuous deformation to the crystal surface whereas the second one leaks rather to a discontinuous deformation. Restricting ourselves to the case of a uniform deformation: an intriguing problem in this case is of whether the soliton concentration (i.e. the fraction of bi-kinks) in a dislocation train will be conserved in the two deformation directions. Discussing this problem, we first draw attention to the fact that the quantities D_x and D_y are precisely the sizes of the scaled soliton φ defined in (2). Thus we have to return to the primary variables u, l and k which allow us to write

$$l_x = \pi p(2)^{1/2} D_x \qquad l_y = \pi\beta p(2)^{1/2} D_y \tag{24}$$

so l_x and l_y are the actual sizes of soliton.

Now define the soliton fraction in a dislocation train as the ratio of the soliton (bi-kink) size, and the maximum number of atoms between any two such solitons [1, 11]. The last quantity is obtained from equations (5), integrating within the larger period of the adatom–substrate interaction potential. Results for the solutions in (i)–(v) are generalized as

$$L_0 = l_x \pi K\left(k_1^2\right) \qquad Q_0 = l_y K\left(k_2^2\right) \tag{25}$$

where we have denoted by L_0 and Q_0 the maximum number of atoms between two solitons with respect to the x and y axis, respectively. Using the appropriate expressions of D_x and D_y in (i)–(v), we can derive the soliton concentration with respect to the x axis, i.e.

$$n_x = \pi/2K\left(k_1^2\right) \qquad n_y = \pi/2K\left(k_2^2\right). \tag{26}$$

The first remark concerning these parameters is that they are dimensionless. Secondly, the number of solitons (bi-kinks) in a dislocation train is conserved in two dimensions as long as k_1^2 and k_2^2 are equal.

In the infinite-surface limit i.e. when $k_i^2/1$, relations (26) vanish. The vanishing behaviour of the soliton concentration in the infinite-surface limit can be interpreted as consequent upon an increase of the intersoliton separation. We notice that when $k_i = 0$, $n_x = n_y = 1$. In fact, in this last limit the non-linear feature of the misfit dislocation has vanished completely and only linear phenomena occur. By contrast, the first limit ($k_i^2 \to 1$) gives rise to strong non-linear phenomena. Namely, the soliton sizes gradually increase and the bi-kink sharpens until at $k_i^2 = 1$, where the sizes of the transition across a complete bi-kink structure are

$$l_1 = \lim_{k_1 \to 1} l_x \qquad l_2 = \lim_{k_2 \to 1} l_y \tag{27}$$

in the x and y directions respectively. The asymptotic behaviours given above also provide relevant information as concerns structural configurations of the misfit dislocation that are allowed to accommodate on the surface. Thus the vanishing behaviour of the soliton concentration in the infinite-surface limit can also be interpreted as a tendency to prevention of appearance of multi-step configurations. So only single dislocations are allowed and their maximum number on the crystal surface can be estimated and shown to be naturally infinite. Indeed, this can be verified by a naive estimate from the ratios L/l_x and Q/l_y, where L and Q tend to infinity when $k_t^2 \to 1$.

In conclusion, we have found some large-amplitude solutions of a 2D DSG equation. These solutions are solitons (bi-kinks) that contribute to the formation of dislocation trains in misfitting monolayers such as BCC crystals. The main result of our study is that we predict a tendency to prevention of the formation of multi-step configurations as the surface lengths tend to infinity. In fact, this is the consequence of a large separation between solitons as the surface lengths are infinite. We have also shown that the number of single dislocations that could accommodate on the infinite surface of the crystal is naturally infinite, since the dislocation can form at any step on the monolayer provided energetic conditions are favourable for creation of a soliton—that is, can promote a large-amplitude adatomic displacement. In a future work, we shall estimate some parameters associated with such large-amplitude displacements, namely the strain energy, surface tensions and the non-linear force provided by the adatom–substrate interaction that drives the misfit dislocation as well as the shear strains along the two deformation directions on the crystal surface.

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