Proceedings of Symposium on Ultrasonic Electronics, Vol. 33 (2012) pp. 313-314
13-15 November, 2012

Computer Experiments on Generation and Propagation of 1-Toda Soliton in the Nonlinear Model Crystals

非線形モデル結晶における戸田の 1 ソリトンの生成と伝播に関する計算機実験

Masanori Itaba[1†], Yuuki Yamada[2], Atsushi Minato[2], and Satoru Ozawa[2]
([1]Ibaraki Univ., [2]Grad. School of Sci. and Eng., Ibaraki Univ.)
伊多波正徳[1†]，山田祐己[2]，湊敦[2]，小澤哲[2]
([1]茨大工, [2]茨大院理工)

1. Introduction

Until now, the experiments on the propagation of acoustic soliton were carried out on some crystals. For example, giving heat strain to the edge of MgO crystal by using an optical laser pulse, the heat strains were observed as solitons which depended upon given energy. [1)] Excitation of solitons has been reported in the other crystal systems, also. [2-8)] The forms of those observed excitations were slightly different from theoretical soliton, it is considered that a state is composed of both solitons and other excitations. If it makes a theoretical soliton on actual crystal, proper initial input must give to the system. However, in arbitrary systems it is difficult to derive the initial condition for generating a theoretical soliton.

In the range where atomic position is slightly shifted from an equilibrium point and where weak nonlinear forces act, the shape of interatomic potential is almost the same on most substances, and that of Toda lattice which has soliton solutions is almost the same, also. That is to say, in the arbitrary system where weak nonlinear forces act, if it gives the Toda 1-soliton solution as the initial input, it is expected that a soliton stably propagates.

Therefore, in the present study the propagation of Toda 1-soliton on one and two-dimensional model crystals systems have been studied and the results are presented. And the ideas of ways to generate a soliton in actual crystal are mentioned later.

2. Methods

One of the model crystal adopted in the simulation is illustrated in Fig. 1. NN and NNN indicate the positions of the nearest and the next nearest neighbor atoms for the reference atom. An-harmonic forces up to the third order are taken into account, and central forces are considered between atoms. The equation of motion for the (i, j)th atom in the crystal is,

$$m\frac{d^2\boldsymbol{R}_{i,j}}{dT^2} = -\boldsymbol{grad}\phi_{i,j} \quad , \tag{1}$$

where m is the atomic mass, $\boldsymbol{R}_{i,j}$ is the coordinate of the (i, j)th atom, and T represents the time. Here, $\phi_{i,j}$ is the potential between the (i, j)th atom at $\boldsymbol{R}_{i,j}$ and other (p, q)th atom at $\boldsymbol{R}_{p,q}$,

$$\phi_{i,j} = \sum_{p,q}\sum_{n=2,3,4} [(C^{(n-1)}/n)\{|\boldsymbol{R}_{i,j} - \boldsymbol{R}_{p,q}| - |\boldsymbol{R}_{i,j}(e) - \boldsymbol{R}_{p,q}(e)|\}^n] \quad , \tag{2}$$

$$\boldsymbol{R}_{i,j} = \boldsymbol{R}_{i,j}(e) + \boldsymbol{D}_{i,j} \quad ,$$
$$\boldsymbol{R}_{p,q} = \boldsymbol{R}_{p,q}(e) + \boldsymbol{D}_{p,q} \quad . \tag{3}$$

Here (e) means that the quantity is in the equilibrium position, $\boldsymbol{D}_{i,j}$ and $\boldsymbol{D}_{q,p}$ are the displacements of the (i, j)th atom and the (p, q)th atom from their equilibrium positions, respectively.

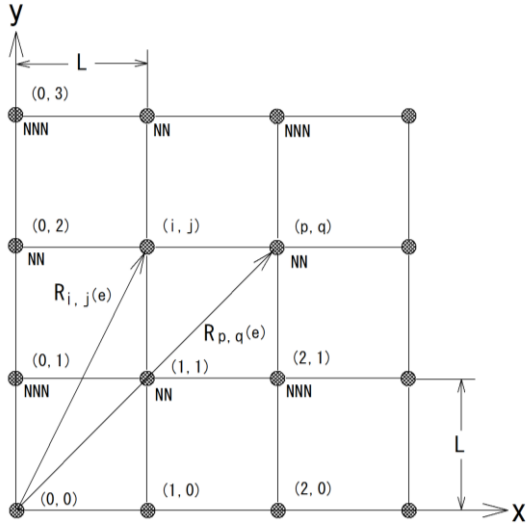

Fig. 1. Two-dimensional square lattice model crystal used in computer simulation.

Next Toda 1-soliton solution is as follows:

$$R_i = \frac{1}{b}\ln\frac{1+e^{2(ki-\omega t)}}{1+e^{2(k(i+1)-\omega t)}} \quad . \tag{4}$$

Here R, i, b, k, ω, and t are the displacement, the number of particles, the constant, the wave number, the angular velocity, and the time, respectively.

In the simulation a system of MD units is used: the atomic mass m=1, the NN distance L=1000, the time T=1. Toda potential parameters are as follows: a=1, b=1, t=50 and k=0.3, and ω is the function of a, b, m, and k. The force constants are selected as $C^{(1)}$=1, $C^{(2)}$= -0.5 and $C^{(3)}$=0.16 in order that the model potential nearly fits Toda potential. The ratio of force constants is defined as $K = C^{(n)}_{\mathrm{NNN}} / C^{(n)}_{\mathrm{NN}}$ (n =1, 2, and 3), which is a parameter that means a contribution of NNN. The experimental systems are two cases.

(S1) one-dimensional (1D) nonlinear lattice case: the number of atoms is 1200 in the x directions.

(S2) two-dimensional (2D) square lattice case: the numbers of atoms are 1200 and 32 in the x and y directions, respectively.

The initial input displacements are given to the system by modified eq. (4): the coefficient hr is multiplied to the whole of eq. (4). And the velocities of atoms can be derived from the differential of eq. (4). The experiments are carried out on parameter hr and K.

3. Results

The force F_i of the atoms as functions of the atomic position i at a definite time after the pulse application, or the snapshots of F_i, were computed. Examples of the results, (S2) case, the 16th line along the x direction in Fig. 1, are illustrated in Fig. 2(A)-(H) since the results in 1D were almost the same with 2D (K=0). (B), (D, G, H), and (F) are normalized by (A), (C), and (E), respectively. In the case of (B), the sech-type undulation has changed into the dispersive undulations since the energy of initial input was too small. In the case of (D), the sech-type undulation has stably kept its form during the propagation. In the case of (F), the sech-type undulation has changed into the nonlinear and dispersive undulations since the energy of initial input was slightly large. It can be seen from (G) and (H) that the effects of NNN contribute to the stability of soliton. Namely an increase in K contributes to an increase in the energy of an initial input. In the paper [1-3] it was given a thermal strain as initial input by using laser pulse. It is considered that it might be difficult to generate a soliton without superfluous excitations in the system. If it generates Toda 1-soliton in actual crystal, it must give proper initial input to the system. It is a step-like initial input which modified eq. (4).

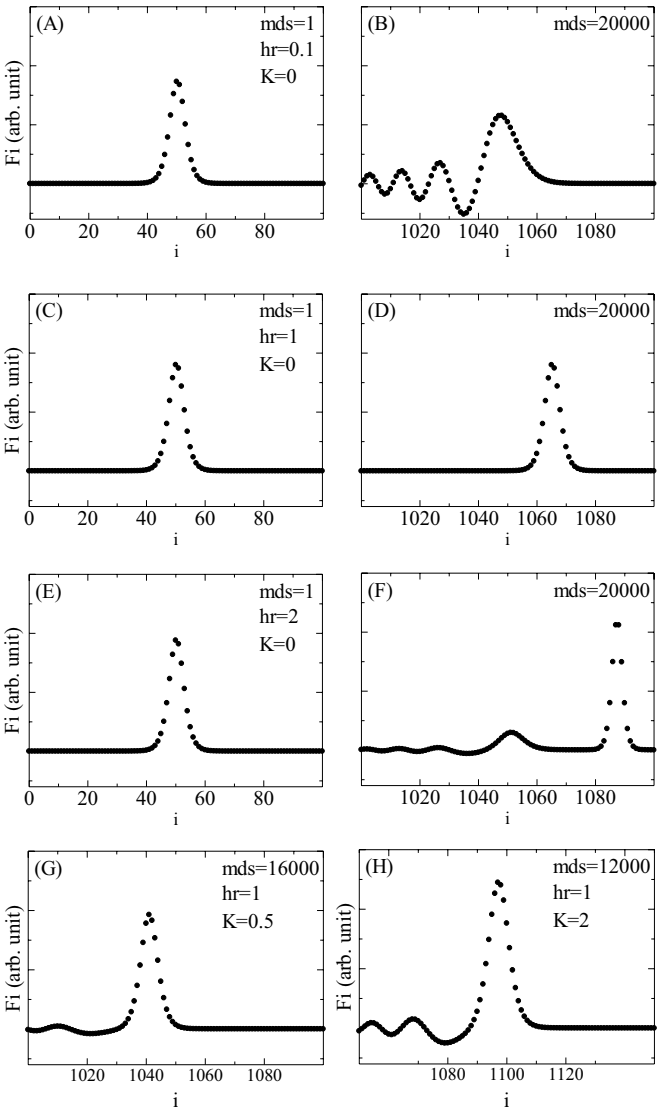

Fig. 2. Force F_i (arb.unit) of atoms vs. atomic position i for the x direction.

References

1) H. –Y. Hao, and H. J. Maris: Physica B **263-264** (1999) 670.
2) H. –Y. Hao, and H. J. Maris: Phys. Rev. B **64** (2001) 064302.
3) H. –Y. Hao, and H. J. Maris: Physica B **316-317** (2002) 147.
4) O. L. Muskens, and J. I. Dijkhuis: Phys. Rev. Lett. **89** (2002) 285504.
5) W. Singhsomroje, and H. J. Maris: Phys. Rev. B **69** (2004) 174303.
6) E. Peronne, B. Perrin: Ultrasonics **44** (2006) e1203.
7) Y. Tokunaga, M. Suzuki, and M. Imai: Jpn. J. Appl. Phys. **14** (2007) 33.
8) P. Hess, A. M. Lomonosov: Ultrasonics **50** (2010) 167.