COMPUTER EXPERIMENT ON SCATTERING OF ATOMIC EXCITATIONS BY A LATTICE DEFECT

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Abstract

A molecular dynamics computer simulation has been carried out for a monatomic, anharmonic, and two-dimensional hexagonal model crystal. Central forces between the nearest neighbor atoms are considered. Pulse input displacements are applied to atoms at an end of the crystal, and an atomic excitation propagating in the crystal is induced. Displacements, velocities, and energies of all atoms in the crystal are evaluated. A mass defect - an atom which mass is lighter or heavier than the lattice atoms - is placed at the center of the crystal. The excitation is scattered by the defect, and various aspects of the effect are studied.

Introduction

We are continuing computer simulation studies on atomic excitations in nonlinear mass-spring model crystals using the molecular dynamics (MD) method. The excitation is produced after applying pulse input displacements to certain atoms in the crystal, and the resulting displacements, velocities, and energies of all atoms in the crystal are computed. We first found that solitons or solitary waves could be produced instead of or together with phonon excitations in one-dimensional chain crystals. The study was extended to the cases of two-dimensional square crystal and three-dimensional cubic crystal. It was found that the features of the atomic excitations were sensitively dependent on the magnitude of the crystal anharmonicity and the strength of the input pulse. Our published papers concerned are cited in the references in [1].

Our study was further extended to the problem of the scattering of the atomic excitation by lattice defects in crystals. The simulation was carried out for the cases of various kinds of defects in one-dimensional crystals [2]. In the present study the computer experiment is concentrated to the scattering by a mass defect in a hexagonal two-dimensional model crystal.

Methods

The model crystal adopted in the simulation is schematically illustrated in Fig. 1. The Cartesian coordinate axes x and y are chosen as shown in the figure. These are the <2-1-10> and the <01-10> directions in the hexagonal coordinate system. Atomic positions are represented as X and Y, which are coordinate values normalized by the nearest neighbor distance L. The number of atoms are 134 and 34 in the x and y directions (201×29.4 in size). The atom at the center of the crystal (X=100.5, Y=17) is replaced by a mass defect. The input pulse displacement D_p is applied along the x direction to all atoms at the left edge of the crystal, and movements of all atoms in the crystal are induced.

The equation of motion for the (i,j)th atom is

$$m(\mathrm{d}^2\boldsymbol{R}_{i,j}/\mathrm{d}T^2) = -\,\mathbf{grad}\,\phi_{i,j}\,, \qquad (1)$$

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 atoms at $\boldsymbol{R}_{p,q}$ The potential is represented as

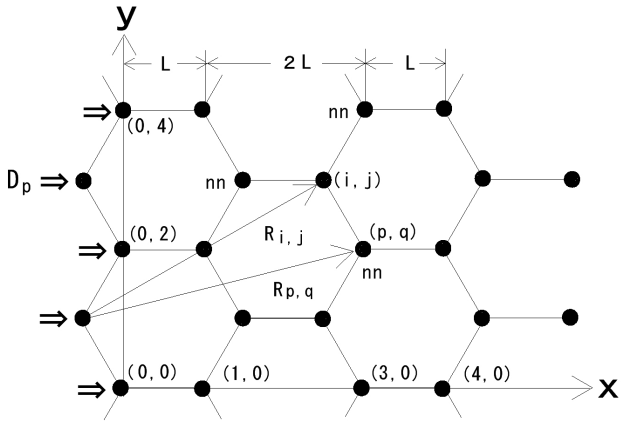

Figure 1: Two-dimensional hexagonal model crystal used in the computer simulation.

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

$$\boldsymbol{R}_{i,j} = \boldsymbol{R}_{i,j}(e) + \boldsymbol{D}_{i,j}, \quad \boldsymbol{R}_{p,q} = \boldsymbol{R}_{p,q}(e) + \boldsymbol{D}_{p,q}, \tag{2}$$

where (e) means that the quantity is in the equilibrium position, and $\boldsymbol{D}_{i,j}$ and $\boldsymbol{D}_{p,q}$ are the displacements of the (i,j)th atom and the (p,q)th atom from their equilibrium positions. Here, central forces are considered to act between the atoms, and the anharmonic force up to the third order, or the lattice anharmonic potential up to the fourth order, is taken into account. The coefficients $C^{(1)}$, $C^{(2)}$ and $C^{(3)}$ are the first-, second-, and third-order force constants, respectively.

When the atoms in the crystal are moving, the equations of motion for all atoms are numerically integrated, and the components of displacements of atoms are determined. The velocities of all atoms are also computed. Thus the total (potential + kinetic) energy E of each atom can also be determined. As described previously [1], the effect of the next nearest neighbor (nnn) interatomic interaction is not serious in the case of 2D crystal, and only the nearest neighbor (nn) interaction is taken into account.

In the simulation, a system of MD units is used [1]: atomic mass m=1, nn distance L=1000, time T=1, and force constant $C^{(1)}$=1. In addition, a discrete time interval (MD steps) is used, and in this study 1 MD step=0.05 MD unit. The MD step is chosen such that the time step is sufficiently shorter than the atomic vibration period.

In the present computation, the second- and the third-order force constants are chosen as $C^{(2)}$= - 0.1 and $C^{(3)}$=0.01 (MD units). The $C^{(2)}$ value is arbitrary, while $C^{(3)}$ is chosen according to the relation $C^{(3)}=[C^{(2)}]^2$. By this choice the contributions of the second- and the third-order anharmonicity become of the same order.

In this study, largely different values of input pulse displacement are chosen: D_p=0.5 and 10 (MD unit). The aspect of atomic excitation is expected to be very different for these two cases. As the mass defect, largely different cases are chosen: m'/m =0.02 and 50, where m' and m are the masses of the defect and lattice atoms, respectively.

Results

When the input pulse is applied, atomic excitations are induced and propagate along the x direction. The energies E of atoms in the crystal are evaluated as functions of the atomic positions and the time elapsed after the pulse application. A line of atoms situated at X=0 - 201, Y=17 are taken, and the energy E of each atom is represented as a function of coordinate X. The results for two cases, D_p=0.5 and 10 are shown in Figs. 2 and 3, respectively. Three cases of "light mass defect" m'/m=0.02, "defect-free" m'/m=1, and "heavy mass defect" m'/m=50 are shown in each figure. Several energy peaks are seen in E vs X, and the figures are snapshots at the time when the leading energy peak reaches the position X=110. Since the mass defect is at the position X=100.5, Y=17, it is seen that the excitation rather easily passes the defect. Namely, the excitations are not so strongly scattered.

The results in Figs. 2 and 3 will be compared. It has been shown that in anharmonic model crystals atomic

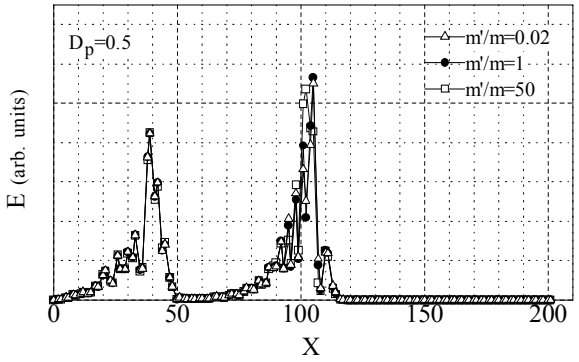

Figure 2: Snapshot of atomic excitations for small input case.

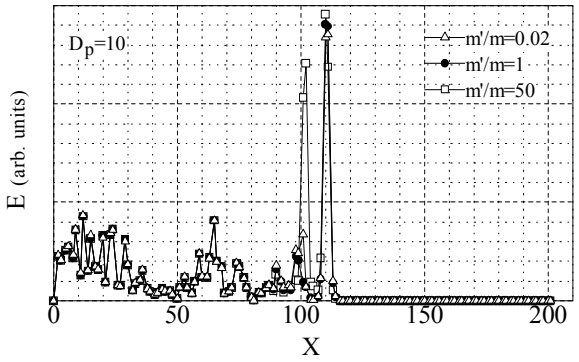

Figure 3: Snapshot of atomic excitations for large input case.

excitations are mainly phonons or solitons when the applied input pulse is relatively small or large. In our previous papers cited in [1], the appearance of soliton excitation has well been proved through the following facts: the energy of excitation is sharply concentrated in space, the characteristic feature of kink-like spatial distribution of atomic displacement in the excitation can be seen, the propagation velocity of the excitation is higher than that of phonons, when two excitations are collided there is no interaction between the two and they pass freely with each other, and so on. In the present case, we can see typical phonon and soliton excitations in Figs. 2 and 3, respectively: longitudinal and transverse phonons are seen in Fig. 2, and multiple solitons composed of two soliton peaks followed by weak phonon excitations are seen in Fig. 3. We call these the "phonon case" and the "soliton case".

In the present study, the scattering of the two kinds of excitations by a mass defect is investigated. The observation of the snapshot is not powerful to detect the scattering effect as previously mentioned. Thus, the following computer experiment was carried out. After the excitation passes through the defect at X=100.5, Y=17, the energy of each atom on the atomic line perpendicular to the propagation direction (x direction) is evaluated. The evaluation is made at two positions: X=110 (near to defect) and X=170 (far from defect). The results are shown in Figs. 4 and 5 for the phonon case and for the soliton case, respectively. Here the energy is represented as a function of position Y for the light mass (m'/m=0.02) and heavy mass (m'/m=50) cases. The energy E_n means that the value is normalized by the energy for the defect-free case (m'/m=1). In the figures also shown are the times the excitations arrive at the observed positions, X=110 and X=170. The arriving times are represented in unit of MD step (mds). The propagation velocity of soliton is higher (mds is smaller) than that of phonon.

The overall features of the scattering are almost similar for the phonon case and for the soliton case.

(a) Near to defect.

(i) For light mass case, E_n is smallest at the atomic position just behind the defect. As the atomic position leaves from here along the y direction, E_n becomes larger and approaches the unity.

(ii) For heavy mass case, the behavior is the reverse. Namely, E_n is large at the position behind the defect. Change of E_n with position is turned over compared with the light mass case.

(b) Far from defect.

For both light and heavy mass cases, the change of E_n with position becomes rather smaller and monotonous. However, still the effect of the scattering by the defect remains.

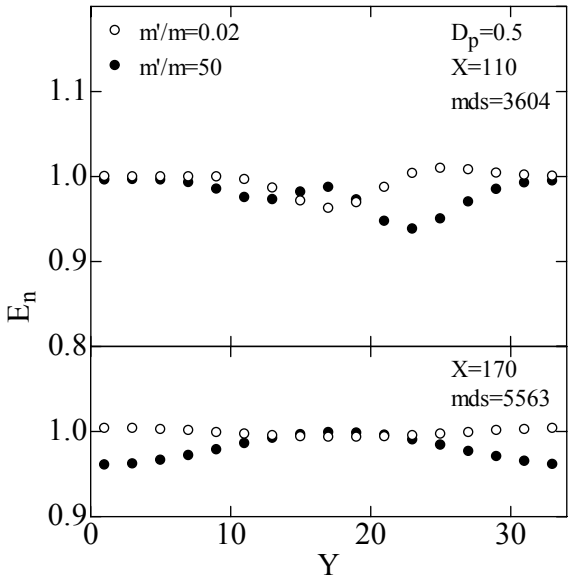

Figure 4: Distribution of energy of atoms on a line perpendicular to the propagation direction for phonons.

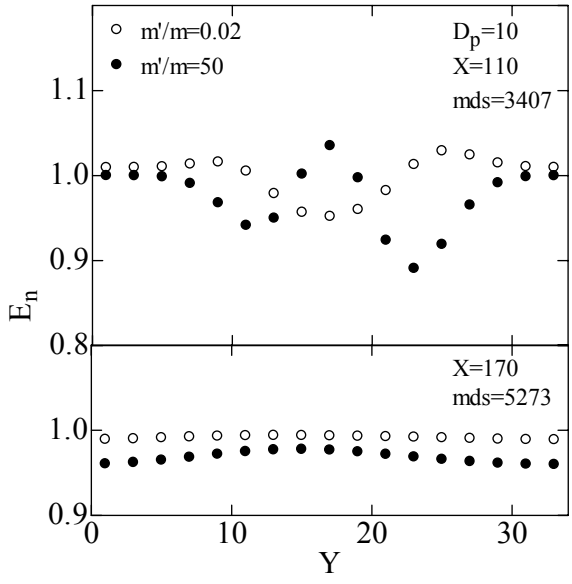

Figure 5: Distribution of energy of atoms on a line perpendicular to the propagation direction for solitons.

The above results can qualitatively explained as follows. The light mass defect is considered to act for the propagating excitation just as the case of a free surface for a propagating elastic wave. A reflection of the excitation occurs by the defect, and a decrease of the energy results behind and near the defect. The energy increase at other positions is due to the conservation of energy in the crystal. In the case of heavy mass defect, the movement of defect is induced by the incident excitation, and apparent increase of energy of atoms occurs behind and near the defect. The atomic energy of the defect atom is rather big because of the large mass. In both the light mass and heavy mass cases, the disturbance of the energy distribution becomes smaller at position far from the defect. This is due to the smoothing of energy through the interatomic interactions. Finally it is noted that the scattering effect near the defect seems to be big in the soliton case compared with the phonon case. Also noted is that the scattering occurs in an asymmetric manner near the defect. These are just the results of the simulation, and no definite interpretation can be offered at present.

Discussion

We are interested in realizing laboratory experiments of producing mechanical solitons with sufficient strength. For that purpose, 2D or quasi-2D crystals are considered to be promising as described previously in our published papers. Thus, the computer simulation of solitons in a 2D hexagonal model crystal was taken in our study. The reason why the hexagonal crystal is selected will be revealed later. In producing solitons in crystals, the strength of the input pulse is importent. This problem must be studied before the laboratory experiment is really started.

It is of primary importance to apply strong pulse input to a specimen in order to produce strong solitons. It has been shown that the strain of the applied stress pulse must be at least D_p/L=2/1000=0.2%. Usual piezoelectric transducers are not applicable for producing such a strong pulse. A shock compression technology can be used to produce a large stress pulse. However, a large-scale apparatus is required for performing such an experiment.

Currently, a method is being developed in which large-amplitude stress waves are produced in crystals through irradiation of the surface of the specimen by a strong short optical pulse [3,4]. Lattice excitation having a propagating velocity greater than that of phonons was observed, and the authors suggested that the excitation was a soliton. Their method is very interesting even if their study is still preliminary. We are planning to perform such a kind of laboratory experiment of soliton production by utilizing the knowledge obtained in our computer experiment.

The specimen material to be used in the laboratory experiment is also very important. We consider that a graphite single crystal is a powerful candidate for performing the experiment. Graphite is a very common quasi-2D hexagonal crystal, and large specimens of good quality can easily be obtained. Furthermore, the interatomic interaction in the basal plane is not of long-range type, which seems to be favorable for the soliton production. Keeping these considerations in mind, our computer experiments are carried on for a 2D hexagonal model crystal. It is also of great importance to consider the state of real specimen. Real crystals always contain various kinds of lattice defects. Typical ones are the vacancies and impurity atoms. Thus we are doing the present computer experiment, where the light mass defect and the heavy mass defect are considered to correspond to a vacancy and a heavy impurity atom. More extended studies are now in progress, and results will appear in the near future.

References

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