Computer experiments on phonons and solitons in two-dimensional hexagonal crystals

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We have studied mechanical excitations in one-dimensional (chain), two-dimensional (square lattice), and three-dimensional (cubic lattice) crystals using the molecular dynamic simulation method. When the lattice anharmonicity of the crystals is not small, solitons as well as phonons can be produced in these crystals [1-3]. It was found that the solitons could most remarkably be observed in two-dimensional (2D) crystals [3]. In the present study, hexagonal crystals are chosen as the model crystal after considering possible utility of the results of the simulation for realizing laboratory experiments using quasi-2D crystals, for example, such as graphite single crystals.

A mass-spring model crystal including anharmonic potential up to the forth order is chosen, and central forces between the nearest neighbor (nn) and the next nearest neighbor (nnn) atoms are considered. The size of the crystal is 64×32 atoms. The anharmonicity of the lattice is medium in its size. An input pulse displacement is given to the atoms on an end of the crystal, and induced displacements, velocities, and energies (potential+kinetic) of all atoms in the crystal are computed.

Examples of the results of the simulation are shown in the figures. In these figures, the displacement D and the energy E of atoms are shown in arbitrary units as functions of the atomic position X along the input pulse direction. The figures show snapshots of propagating excitations at certain time after the pulse application. In figures (a) and (b), the input pulse amplitudes are 5 and 30 (in a certain unit), respectively. In figure (a), the propagating excitations are phonons. Meanwhile, in figure (b), the characteristics of propagating soliton excitation can be seen: the step-like shape of D-vs-X and the concentration of energy at the step position in E-vs-X. Namely, large enough input is required for producing solitons. Also note that the propagation velocity of solitons is larger than that of phonons. The study is carrying on under various conditions of the simulation, and the obtained results will be presented soon.

[1] S.Ozawa, Y.Hiki, Physica B 219&220 (1996) 473.
[2] S.Ozawa, R.Komuro, Y.Hiki, Physica B 263-264 (1999) 90.
[3] Md.M.A.Joarder, A.Minato, S.Ozawa, Y.Hiki, Jpn. J. Appl. Phys. 40 (2001) in press.