CONDENSED-STATE PHYSICS

DISCRETE BREATHERS IN CRYSTALS WITH THE NaCl STRUCTURE

J. A. Baimova,1 S. V. Dmitriev,1 A. A. Kistanov,1 and A. I. Potekaev2

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In the recent decade, the spatially localized large-amplitude vibrational modes in defect-free crystals, referred to as discrete breathers (DBs), are intensively investigated in the materials science. This review reports the main results on gap DBs in crystals with the NaCl structure. The experimental proof of their existence in a NaI crystal is described. A number of molecular dynamics simulation results are presented, including new so far unpublished data. The properties of crystals potentially affected by the DBs are discussed.

Keywords: crystal lattice vibrations, phonon spectrum, discrete breather, family of NaCl crystals.

INTRODUCTION

Discrete breathers are large-amplitude excitations localized in space and periodic in time, which are common in non-linear discrete systems [4–10] and in materials science [2, 11]. The term “breather” originates from the English word breathe, which indicates their periodicity in time. Let us briefly describe the physical conditions of the existence of DBs in crystals and their peculiarities distinguishing them from other vibrational modes, using the literature data [1–3].

Crystal lattice excitations can be divided into linear (low-amplitude) and non-linear, where the deviations of atoms from their crystal lattice positions are so large that one has to take into account the non-linear interatomic-force component. The linear excitations include, for instance, low-amplitude plane phonon waves and linear modes localized on the crystal-structure defects. An important feature of the linear modes is their independence of each other, which results from the fact that they represent exact solutions to the atomic motion equations linearized with respect to their equilibrium positions, and for the linear equations the solution superposition principle holds. An increase in the excitation amplitude results in the inclusion of non-linear terms of the extension of interatomic forces over displacements, which results in interaction of different vibrational modes with each other.

The reason, for which DBs exist as localized vibrational modes in defect-free crystals and radiate no energy, consists in the fact that their oscillation frequency lies outside the crystal phonon spectrum. The departure of the DB frequency from the phonon spectrum is due to the dependence of the nonlinear oscillator frequency on its amplitude. In the case of rigid-type nonlinearity, the oscillator frequency increases with the amplitude, and in the case of a soft type of nonlinearity the reverse situation is observed. In the crystals with rigid-type nonlinearity, the DB frequency at sufficiently large amplitudes lies above the phonon spectrum. In the soft-type nonlinearity, the DB frequency would enter the gap of the phonon spectrum, so in this case the presence of a gap in the latter is a necessary condition for a DB to exist.

It was shown in [12] that in nonlinear lattices of a dimensionality higher than 1, the DB amplitude generally exceeded a certain threshold value to let its frequency depart from the spectrum. In this connection, the question has to
be answered as concerns the DB generation mechanisms, since they cannot result from slow energy pumping, starting from the zero level, but only as a result of delivering a certain portion of the energy to a local region of the crystal.

It should be noted that despite a considerable progress in the theoretical description of DBs, the issues of their practical application in the condensed matter physics and materials science have been hardly studied. A certain progress has been achieved in the experimental and theoretical description of DB properties in crystals with the NaCl structure (see Fig. 1). In particular, DBs were experimentally observed in a NaI crystal [4] after their existence had been predicted by the method of molecular dynamics [5]. The purpose of this work is to provide a systematized representation of the well-known data on DBs in the family of crystals under study and to describe new results obtained by the authors, in particular, concerning a possible energy exchange between DBs.

1. EXPERIMENTAL OBSERVATION OF DBs IN A NaI CRYSTAL

Today one of the few experimental proofs of existence of DBs in crystals is their presence in the vibration spectrum of a NaI crystal obtained by the method of inelastic neutron scattering [4]. The experiments were performed at the temperature 555 K. The DB’s frequency was close to the bandgap center of the crystal phonon spectrum; DBs were spatially localized and polarized along <111>. It was also shown that the peak intensity in the phonon spectrum, which corresponded to DBs, increased with the temperature, which was expected, taking into account the nonlinear nature of these vibrational modes. In addition, the energy necessary for a DB to appear was estimated to be 0.3 eV. Finally, the authors of [4] arrived at a conclusion that DBs in an alkali halide NaI crystal contribute into the vibrational spectrum of the crystal and can play a significant role in the formation of physical properties at high temperatures.

The experimental investigations of DB’s properties in a NaI crystal were continued in [13], where the authors came to a conclusion of an ordered arrangement of discrete breathers in a state of thermal equilibrium. According to the data obtained by neutron scattering, at comparatively low temperatures the polarization of DBs fluctuates between <011> and <111>. At the temperature 636 K, however, they acquire a stable <011> polarization, and in so doing the transverse optical mode splits into three modes, which is generally observed during investigations of the superstructures, while the Bragg reflections do not demonstrate any superstructures. The authors argue that observation of a transverse optical mode is associated with ordering of the DB system, which does not disturb the crystal lattice topology.