Conditions for exciting soliton-type waves in A_3B stoichiometry crystals

P.V. Zakharov[1*], *I.S. Lucenko*[1], *M.O. Sysoeva*[2], *A.M. Eremin*[1]

[1]Shukshin Altai State Humanities Pedagogical University
[2]Biysk Technological Institute (branch) of the Altay State Technical University
*e-mail: zakharovpvl@rambler.ru

In work by method of molecular dynamics process of excitement of soliton-type waves and her distribution on a crystal of stoichiometric structure of A_3B is studied. Solitons are capable to move on crystals to considerable distances without change of a form and speed of the movement. This fact stimulates interest in such objects from a position of search of mechanisms of their excitement and studying of their properties.

Modeling is carried out with use of a package of molecular dynamics of LAMMPS[1]. As the potential of interatomic interaction the potential received by method of the embedded atom offered Zhou[2] was used.

Modeling of excitement of solitonic waves is closely connected with a concept of the nonlinear supratransmission[3] caused by external influence at frequencies outside of a phonon range of a crystal. The defining factor in excitement of such objects is the possibility of existence of discrete breather in the considered crystals. Discrete breather accumulate energy near area of influence and at achievement of some value of amplitude let out soliton-type wave. In fig. 1 the example of distribution of waves for two crystals of structure of A_3B is given: Pt_3Al and Ni_3Al. The crystal of Ni_3Al does not support existence of discrete breather unlike Pt_3Al.

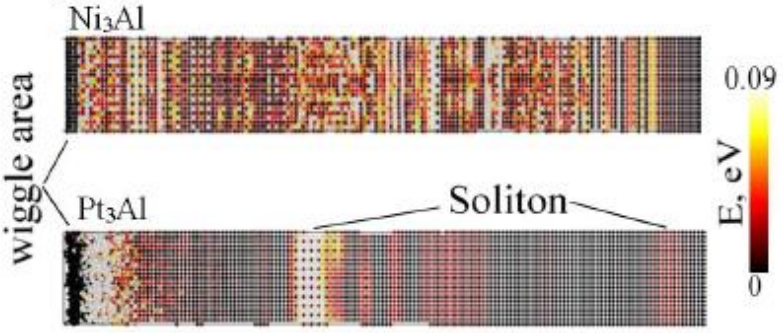

Fig. 1. Distribution of energy along model of crystals Ni_3Al and Pt_3Al

The received results demonstrate that formation of such waves is possible in crystals which are supported by slot-hole discrete breather, i.e. in this case in Pt_3Al. Waves are generated by discrete breather and extend from area of influence deep into of a crystal.

These solitary waves are capable to propagate to hundreds of nanometers without change of a form and speed. At the same time on each of atoms it can be concentrated the energy about 0.02 eV. The energy total volume transferred by a wave is defined by quantity of rows of the atoms involved in fluctuations and can be estimated at hundreds electron-volt.

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[1] LAMMPS Molecular Dynamics Simulator. URL: *http://lammps.sandia.gov/*
[2] Zhou X.W., Johnson R.A. and Wadley H.N.G. *Physical Review B*. 2004, **69**, 144113.
[3] Geniet F., Leon J. *Phys. Rev. Lett*. 2002, **89**, 134102.