Conditional for exciting soliton-type waves in $A_2B$ stoichiometry crystals

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In work by method of molecular dynamics process of excitation of soliton-type waves and her distribution on a crystal of stoichiometric structure of $A_2B$ 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 excitation 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 excitation of solitonic waves is closely connected with a concept of the nonlinear photon transmission[3] caused by external influence at frequencies outside of a phonon range of a crystal. The defining factor in excitation 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 $A_2B$ is given: Pt$_3$Al and Ni$_3$Al. The crystal of Ni$_3$Al does not support existence of discrete breather unlike Pt$_3$Al.

![Energy distribution](image)

**Fig. 1. Distribution of energy along model of crystals Ni$_3$Al and Pt$_3$Al**

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$_3$Al. 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 0.62 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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