Interaction of a soliton wave with nanopores in stoichiometry crystals $A_3B$

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Abstract. Solitons are essentially nonlinear and stable objects in various environments. In this work, the molecular dynamics method is used to study the propagation of solitary waves in a discrete medium in the form of an $A_3B$ stoichiometry crystal and their interaction with nanopores. The model under consideration was a Pt$_3$Al crystal, the atoms of which interacted through the potential obtained by the immersed atom method. Such waves can propagate to hundreds of nanometers across the crystal. We have studied the passage of waves through a cell containing nanopores of various diameters. The mechanisms of energy dissipation in the process under consideration are shown. The distance after the obstacle at which the wave front is restored is estimated. The energy characteristics of a solitary wave after interaction with a topological defect in the form of a cylindrical nanopore are calculated. The results obtained can be useful both from a fundamental point of view in studying the properties of solitons, and from practical for non-destructive testing methods.

1. Introduction
The mechanisms of generation and propagation of solitary waves have been of interest since their discovery in the middle of the XIX century to the present. The second birth of these objects, called solitons, received with the beginning of the use of computer technology to study them. Such objects can have a different nature, but their structural stability and existence in nonlinear media unite. Among the whole variety of solitons, one can distinguish discrete breathers that were discovered a little more than 30 years ago [1]. Interest in these objects is quite high due to their potential practical application in various fields [2].

In one of our recent works [3], the role of discrete breathers in the excitation of a solitary wave, which was produced by external harmonic influence on crystals of composition $A_3B$, was demonstrated. Such waves can propagate to tens of micrometers without changing their shape and speed. The estimate of the energy concentrated by the wave is of the order of 2-5 eV per atomic row. Thus, such a wave, propagating through the crystal, can have a significant effect on processes occurring at the atomic level.
Solitons attract the attention of scientists from various fields of physics. Further, we consider a number of recent publications devoted to solitary waves in various media. Obviously, solitary waves are able to propagate over considerable distances, preserving their characteristics, as evidenced by field and model tests [4]. So the authors of [4-6] describe the propagation of solitary waves in granular structures and layered composite materials. At the same time, emphasis is placed on the fact that such waves can act as a diagnostic tool. The authors showed that this non-destructive method can be used to measure the basic elastic properties of structural composites, offering a reliable and economical alternative to existing destructive and non-destructive testing methods.

Traditionally, attention to solitons is given in the study of magnetic materials. In [7], waves are considered on the surface of a ferromagnetic fluid, which is affected by a magnetic field. For uniaxial ferromagnets, an autoresonant method was developed in [8] for exciting the magnetizer breather with magnetic fields of variable frequency and small amplitude. The authors determined the conditions for the excitation of nonlinear pulsation oscillations of the domain wall in the autoresonance mode in rhombic antiferromagnets and the conditions for controlling its nonlinear dynamics with frequency-modulated variable fields of small amplitude. Also in [9], the one-dimensional nonlinear dynamics of a domain wall under the action of an external constant magnetic field in a three-layer ferromagnet was theoretically studied. In this case, there is good agreement between the analytical and numerical results for the case of small defects. The authors demonstrated the dependence of the minimum speed required by the domain boundary for the transition from one layer to another on the material parameters [9].

The classical theoretical approach to the study of solitons is presented in [10–13]. Here, solutions of differential equations are considered; single-soliton and multisoliton solutions are obtained. Attention is paid to issues of self-organization in such systems [11].

For us, discrete structures supporting soliton solutions are most interesting. For example, in [14], the authors found that for hexagonal lattices, solitary wave solutions exist in certain directions related to the basic symmetries of the lattice. It is also emphasized that such studies can be useful in the development of shock absorbers, acoustic lenses or devices for non-destructive testing of structures [14]. The papers [15–17] discuss the excitation, propagation, and destruction of solitary waves in discrete structures of various dimensions and nature.

In this work, we study the interaction of solitary waves with structural defects in a Pt3Al crystal in the form of nanopores of various sizes.

2. Methods and Approaches

Modeling was carried out using the LAMMPS package [19]. The model we are considering is a bulk fcc A1B stoichiometry crystal with the L12 superstructure containing up to \(3.5 \times 10^6\) particles interacting via the potential obtained by the immersed atom method for a Pt3Al crystal [18]. The model used is similar to the model considered in [3]. The total energy \(E\) of the crystal can be expressed as

\[
E = \frac{1}{2} \sum_{i,j \neq i} \varphi_{ij}(\mathbf{r}_{ij}) + \sum_i F_i(\rho_i),
\]

where \(\varphi_{ij}\) represents the pair energy between atoms \(i\) and \(j\) separated by a distance \(\mathbf{r}_{ij}\), and \(F_i\) is the embedding energy associated with the embedded atom \(i\) in a local location with electron density \(\rho_i\). The electron density can be calculated by the formula

\[
\rho_i = \sum_{j \neq i} f_j(\mathbf{r}_{ij}),
\]

where \(f_j(\mathbf{r}_{ij})\) is the electron density in the area of atom \(j\) located at a distance \(\mathbf{r}_{ij}\) from atom \(i\). The temperature of the computational cell was set by assigning random speeds to the atoms in accordance with the Maxwell-Boltzmann distribution. The step of numerical integration of the equations of motion was 1 fs.

The Cartesian XYZ coordinate axes are oriented along the crystallographic directions \(<100>\), \(<010>\) and \(<001>\), respectively. In the model along the X and Y axes, periodic boundary conditions were imposed. The boundary conditions on the surfaces of the Z axis were set stringent. Note that the cell size changed only along the Z axis, thereby achieving linear cell sizes up to 2,5 micrometers. The calculation cell was a parallelepiped elongated along the Z axis. The number of particles reached...
1.2 × 10^6 particles. The initial temperature was set at 0 K. The final temperature did not exceed several tens of Kelvin due to the massiveness of the computational cell. The models used an NVE ensemble.

The solitary wave generation mechanism corresponded to our work [3], and was ensured by external harmonic action at frequencies outside the phonon spectrum of the crystal under consideration. This action excites discrete breathers near the crystal surface. Forming a cluster, they are a source of secondary waves in the form of a solitary wave.

Figure 1. Fragment of a model cell of a Pt_3Al crystal with a nanopore of different radius: a) 5 Å, b) 10 Å, c) 15 Å, d) 20 Å.

Figure 1 shows the appearance of the nanopores under consideration. For modeling, we chose the cylindrical shape of the pores with the axis of the cylinder parallel to the Y axis. To ensure the stability of the model, preliminary relaxation was performed. Since an external periodic effect could affect the pores, the generation of waves occurred at a distance of 50 nm from the defects. The analysis of the obtained structures was carried out using various visualizers [20].

3. The results and the discussions

Solitary waves are able to be reflected from obstacles in the form of interphase boundaries or crystal surfaces. Interaction with topological lattice defects, the sizes of which are comparable to the long wavelength, affect the wave front, leading to its distortion and energy dissipation.

Figure 2 shows the distribution of the kinetic energy of atoms before and after the passage of a nanopore wave. In general, the picture is classical for elastic waves during the passage of discrete structures.

Figure 2. Distribution of kinetic energy before and after the interaction of a solitary wave with a nanopore of radius 15 Å.
It is important to note that wave front reconstruction occurs rather quickly for all considered nanopore diameters. After 50 nanometers, the wave fronts took a shape close to the original form. Figure 3a shows the energy distribution along one atomic series of platinum in the case of an ideal crystal and in the presence of nanopores of different radii. The decisive role in the dissipation of energy is played by the form of the model itself, which is done intentionally. The size of the model along the X and Y axes was of the same order as the pore sizes, and the presence of periodic conditions did not allow the manifestation of surface effects. Significant attenuation of the wave also occurs if the pore size is larger than the wavelength, as evidenced by the curves for pores with a radius of 15 and 20 Å. The total energy stored in a single atomic row of platinum in the defect-free case was 0.047 eV, in the presence of pores it decreased linearly, and for the case of passage of a pore with a radius of 20 Å, it amounted to 0.022 eV.

![Figure 3](image)

**Figure 3.** Distribution of energy (a) and force (b) along a series of Pt atoms before and after the passage of pores, where N is the ordinal number of an atom in a row

Figure 3b shows the distribution of force along the direction of propagation of a solitary wave for the atomic series of platinum in a defect-free crystal and in the presence of cylindrical nanopores. For example, pore graphs with a radius of 10 and 20 Å are shown. Unlike energy distribution, peaks here can be more pronounced after the passage of pores. In this case, the sign of force can be reversed. This indicates the instability of the solitary wave front despite its apparent recovery. Obviously, this is due to the fact that the main analysis of the data was performed after the wave passed 50 nanometers after the obstacle. In the future, the characteristics considered behaved more predictably, the energy and force distribution plots did not have pronounced peaks.

4. Conclusion
The molecular dynamics method was used to study the interaction of solitary waves with nanopores in a Pt$_3$Al crystal. It was shown that the waves under consideration are able to overcome obstacles whose linear dimensions are greater than their length. The characteristics of the wave under consideration are obtained, the processes of structural-energy transformations during interaction with the considered crystal defects are studied. The energy profile of a solitary wave after the passage of cylindrical pores of various diameters was calculated.

The results of the work can be useful both from a fundamental point of view in studying the properties of solitons in discrete media, and from practical for non-destructive testing and development methods.

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