Stability of supratransmission waves in a crystal of A\textsubscript{3}B stoichiometry upon interaction with single dislocations

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Abstract. Supratransmission waves are stable objects that can exist in different discrete environments. In this paper, we consider the interaction of such waves with single edge dislocations of various configurations in a crystal with A\textsubscript{3}B stoichiometry. The model was a Pt\textsubscript{3}Al crystal, the potential obtained by the embedded atom method was used to describe the interaction of its atoms. Quantitative characteristics of the wave were obtained before and after the interaction. It is found that the degree of energy dissipation by dislocations depends on the mutual orientation of the wave front and the extra plane of the dislocation. Numerical estimates are made for four different configurations. The results obtained can be useful in studying the propagation of soliton-type waves in defect crystals of various compositions.

1. Introduction

The mechanisms of energy propagation through crystals under various intense influences play a decisive role in possible structural transformations of the material. Effects associated with atypical mechanisms are of particular interest. First of all, these include the manifestation of nonlinearity in the transfer of energy during the formation of wave packets under external influences at frequencies outside the spectrum. In the literature, this effect is called supratransmission. It is well studied for various one-dimensional systems. The most widespread are studies of supratransmission in one-dimensional oscillator circuits. The work [1] shows the possibility of exciting such objects with periodic action on one of the ends of the circuit. In this case, energy transfer is observed in the forbidden zones, which may be due to the nonlinearity of the system. A similar result was obtained for nonlinear sine-Gordon circuits in [2]. Good agreement between theoretical predictions and experimental data is demonstrated, and calculations of the threshold values required to trigger waves are presented. There are also works in which the effect of supratransmission is observed in other systems. An example is [3], where studies of one-dimensional lattices of Hamiltonian particles were carried out. The authors of [4] discovered the transmission of wave packets in a metastructure based on the concept of origami.

The nature and behavior of the described phenomena can be considered from the point of view of the theory of solitons. There are a number of works [5-7] with a detailed mathematical analysis of these
objects. Also in [7], a comparison of analytical and numerical solutions is made, with high agreement degree. The similarity of its behavior with solitons makes it possible to predict the possibility of interaction of these waves with various topological and dynamic defects. Supratransmission waves can be excited by harmonic action on intermetallics crystal [8, 9], and they can qualitatively be represented as a solution to the sine-Gordon equation.

In [10], the interaction of supratransmission waves with nanopores of various diameters is shown. Linear defects in crystals, in turn, occur no less frequently and have a significant effect on the properties of a substance, which makes their study an urgent task. Computer simulations, and in particular the molecular dynamics method, make it possible to consider different types of nonlinear effects [11-18], including those inside a crystal. Of great interest in this aspect is the study of the regularities of the propagation of waves of various natures in a solid with dislocations. In the presence of interrelationships between the characteristics of the wave and the parameters of the dislocation structure, it becomes possible to use waves as non-destructive methods of studying the material. Mathematically similar dependences were demonstrated in works [19, 20].

2. Methods and Approaches

Modeling was carried out by the molecular dynamics method using the LAMMPS software package [22]. The well-proven potential obtained by the embedded atom method (EAM) [21] was used to describe the interaction. The boundary conditions for modeling are free along the Z axis; for the X and Y axes, both free and periodic boundary conditions were used, depending on the specific problem. Visualization was carried out using the Ovito software package [23].

Pt₃Al crystals containing up to 1.5 million atoms were used for modeling. A single dislocation was located in the lower half of the crystal. Various variants of the defect were considered: with Burgers vectors, \( \vec{b} \), both parallel to the direction of wave propagation, and perpendicular to it. Variants of the dislocation arrangement in which a layer containing only platinum and simultaneously platinum and aluminum was broken were also considered separately. Figure 1 shows the appearance of the dislocations for which the simulation was performed. Figures 1a-1b show dislocations parallel to the wave propagation; in the first case, the defect was obtained by removing an atomic row containing only platinum atoms, in the second, a row consisting of atoms of both types was removed. Figures 1c-1d show similar patterns for dislocations perpendicular to wave propagation.

![Figure 1](image)

**Figure 1.** Fragment of a model cell of a Pt₃Al crystal with a different single dislocation: a) the extra plane contains Pt and Al atoms, \( \vec{b} \) along <100>; b) extra plane contains Pt atoms, \( \vec{b} \) along <100>; c) extra plane contains Pt and Al atoms, \( \vec{b} \) along <010>; d) extra plane contains Pt atoms, \( \vec{b} \) along <010>. The arrows show the direction of wave propagation.

The wave was launched according to the method described in [8], by means of an external harmonic action with frequencies outside the phonon spectrum. The main data set was obtained for a wave generated by an action with a frequency of 7.4 THz and an amplitude of 0.2 Å, at which the wave profile is most pronounced. To control the wave, data were taken at three points: before the interaction, immediately after the interaction, and at a distance from the dislocation.
3. The results and the discussions
The resulting wave is a combination of two waves of the Pt and Al sublattices. Thus, the main energy is localized on platinum atoms, but the average velocity is higher for aluminum atoms. The wave profiles for the sublattices are shown in Figure 2. (a) shows the dependence of the kinetic energy of the wave particles on the coordinate, and (b) the dependence of the particle velocity. Next, we will study the interaction for these components of the wave separately.

Let us consider a variant of the arrangement of a dislocation with the Burgers vector \( \vec{b} \) along the <010> direction. In this case, the wave will travel on one side of the defect-free crystal and, on the other, overcome the dislocation.

![Wave profiles for Pt and Al sublattices](image)

**Figure 2.** Distribution of energy (a) and velocity (b) along the atomic row before interaction, (c) and (d) after interaction, respectively. N - atom number in a row.

When a wave passes through a dislocation, energy dissipates, the main contribution to which is made by the region near the cutoff of the extra plane of the dislocation. Note the fact that all the transfer of energy by a wave to static atoms occurs in the platinum sublattice. After passing through, the wave profiles take the form shown in Fig. 2 s, d. Changes in wave profiles also confirm the fact of energy transfer in only one sublattice. However, it should be noted that despite significant changes, the resulting wave is not completely destroyed and continues to move along the crystal with a lower speed and energy reserve.

The energy loss on average over the wave is less than 9%, while the average velocity of the wave particles has decreased by 5%. Since only half of the wave interacts directly with the dislocation, after the interaction the wave loses its symmetry; however, the difference in velocity and energy for the halves is no more than 0.9% of the average value. This indicates the restoration of a single wave profile, which,
in turn, indicates its stability. In this case, it does not matter which atomic series was interrupted, the data on the interaction remain the same.

A different picture arises for a dislocation with the Burgers vector along <010>. In this case, direct interaction occurs only in the narrow central part of the wave. In this case, energy dissipation of an identical nature also occurs, however, the losses in this case are 37%. After overcoming the edge of the extra plane, the wave continues its motion, but at the same time the left and right parts are separated, which causes a "step" in the wave profile. In this case, the form of the row interrupted by the dislocation has a greater effect on the parameters of the wave after interaction. In fig. 3 shows the supratransmission wave after passing the edge of the dislocation extra plane. With such a dislocation, after the primary dissipation of energy at the edge, it is localized on Pt atoms along the dislocation line.

![Figure 3](image)

**Figure 3.** Visualization of the energy distribution in the wave after passing the edge dislocation with the Burgers vector along the <010> direction.

Thus, one can judge about the high stability of the supratransmission wave with lattice distortions perpendicular to the direction of wave propagation and lower stability for parallel distortions. The determining factors are the anisotropic properties of the crystal. Also, in the first case, the linear dimensions of the defect turn out to be significantly less than the wavelength, while in the second case, the grating distortion affects distances comparable to the wavelength of the supratransmission.

4. Conclusion

The molecular dynamics method was used to simulate the interaction of supratransmission waves with single dislocations in a Pt₃Al crystal. It was shown that the waves under consideration are capable of overcoming various single dislocations. The quantitative characteristics of the wave before and after the interaction are calculated. The stability of waves is demonstrated for the case when a linear defect is located parallel to the wave front. The results of this work can be useful both from a fundamental point of view in studying the properties of solitons in discrete media, and from a practical point of view for methods of non-destructive testing and development.

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