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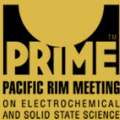
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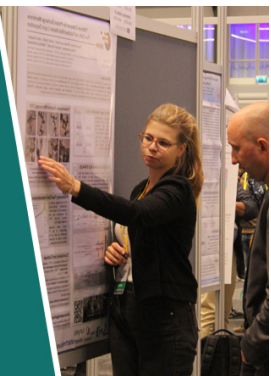
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Localized modes in platinum aluminides

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Abstract. Platinum aluminides have the prospect of being used as both functional and structural materials for a range of scientific and technical tasks. They possess unique properties that make them effective catalysts. The dynamics of the crystal lattice play an important role in the manifestation of these properties. In this study, an analysis of the density of phonon states of crystals and the possibility of the existence of localized lattice vibrations in Al and Pt alloys is conducted using atomistic modeling. The following compounds are considered: AlPt, Al₂Pt, Al₃Pt, AlPt₂, Al₃Pt₅, AlPt₃ (four types of lattices). The calculated phonon spectra allow for the assessment of the possibility of the existence of nonlinear localized modes in the forbidden zone of the spectrum, if it is present. It is shown that a number of crystals within the framework of the considered formalism and interatomic potential can have a forbidden zone. This condition, together with the nonlinearity of the bonds, ensures the existence of highly-amplitude localized modes in the following compounds: AlPt₃, AlPt₃(1), AlPt₃(2), AlPt₃(3). It is also established that in the Al₃Pt₅ alloy, the existence of prolonged high-amplitude excitations on the Al atom is possible.

1. Introduction

The dynamics of the crystal lattice determine many properties of crystals. For example, a number of energy transport mechanisms within a crystal are related to the peculiarities of its crystalline structure and interatomic bonds. Therefore, studying the behavior of the crystal structure as a whole, as well as locally, allows for a more detailed understanding of energy transfer processes in crystals, their localization, and their influence on macro properties. One notable example is thermal conductivity, such as the effect of ballistic heat transfer in discrete structures [1]. Another interesting phenomenon is the effect of nonlinear supratransmission [2, 3], which enables the transfer of energy at frequencies outside the forbidden region of the spectrum of the system under consideration. All of these are promising subtle effects that can significantly enhance the efficiency of existing devices and lay the foundation for new ones operating on different physical principles. Primarily, these include sensitive sensors, frequency filters, thermal diodes, and energy flow valves in discrete structures.

This study focuses on Pt and Al compounds, as listed in table 1. The aim is to search for nonlinear high-amplitude modes in these crystals. Special attention is given to localized modes, such as discrete



breathers. To achieve this goal, an atomistic modeling method based on molecular dynamics is applied. The choice of the Pt-Al system is primarily driven by the unique properties of these materials. They combine chemical activity with high strength characteristics. Furthermore, our previous work has shown that a range of crystals based on these elements can sustain discrete breathers and soliton-like waves [4-6].

Let's take a closer look at the terms discrete breather and localized mode [7-11]. Generally speaking, when it comes to such objects, it should be noted that in realistic models of crystals, as well as in natural experiments, it is impossible to provide ideal conditions for their existence. This leads to the fact that exact mathematical nonlinear objects (exact solutions of differential equations) cannot exist in such systems. In this case, the concept of quasi-breather would be more appropriate. However, due to established terminology, they are often referred to as similar to exact solutions in mathematical models. Therefore, in this work, these two terms will be used as synonyms.

Table 1. Alloys Al_nPt_m .

Alloys	Syngony	Spatial group
AlPt	cubic	$Pm\bar{3}m$
AlPt(1)	cubic	$P2_1\bar{3}$
Al_2Pt	cubic	$Fm\bar{3}m$
Al_3Pt	tetragonal	$I4/mmm$
Al_3Pt_2	Trigonal	$P\bar{3}m1$
$Al_3Pt_2(1)$	Trigonal	$P\bar{3}m1$
Al_3Pt_5	orthorhombic	$Pbam$
$Al_{21}Pt_8$	tetragonal	$I4_1/a$
$AlPt_2$	orthorhombic	$Pmma$
$AlPt_2(1)$	orthorhombic	$Pnma$
$AlPt_3$	tetragonal	$P4/mbm$
$AlPt_3(1)$	cubic	$Pm\bar{3}m$
$AlPt_3(2)$	tetragonal	$I4/mcm$
$AlPt_3(3)$	tetragonal	$P4/mbm$

And so, a discrete breather is a periodic oscillatory mode that manifests itself in a spatially localized form and has a significantly larger amplitude than the thermal vibrations of atoms. The existence of such modes in various physical systems is supported by experimental evidence. There are two types of nonlinearity in discrete breathers - soft and hard. The soft type is characterized by a decrease in frequency with increasing amplitude and can be realized in crystals with a gap in the phonon spectrum. Such discrete breathers are called gap breathers. Discrete breathers of the hard type have frequencies that can fall within the phonon spectrum gap or lie above the spectrum.

2. Model and experimental technique

One of the main methods for studying lattice dynamics is molecular dynamics. This classical method is widely used to solve the problems mentioned above [12-15]. It is based on solving the differential equations of motion for each particle in the system, where the choice of interatomic potential plays a crucial role in determining the interactions between particles. This method allows for the study of the kinetics of processes in real-time, which is important for a more accurate and comprehensive analysis of lattice dynamics. Furthermore, all thermodynamic micro- and macroparameters are available for analysis, providing a more complete understanding of the processes at hand. Here, we created models of Al and Pt alloys with different crystal structures. The data from The Materials Project database [16] were used as a basis. The alloy crystals Al_nPt_m have parameters presented in Table 1. The necessary configurations of the calculation cells were formed using the AtomsK program. The elementary cell fragments are shown in figure 1. The models themselves contained from 52,000 to 130,000 atoms, which

is sufficient for studying the properties of the lattices mentioned. Phonon spectra were calculated for each of the alloys (figure 2). The calculations were performed using two methods: our own methodology and the methodology discussed in [17].

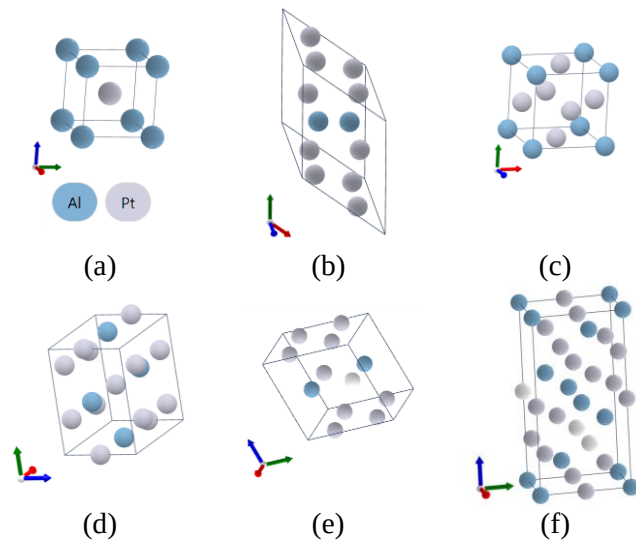


Figure 1. Unit cells of alloys: (a) AlPt, (b) AlPt₃, (c) AlPt₃(1), (d) AlPt₃(2), (e) AlPt₃(3), (f) Al₃Pt₅.

The LAMMPS Molecular Dynamics Simulator computer program was utilized for modeling. Calculations were performed using the EAM interatomic potential. The embedded atom method was employed to calculate the interaction energy between atoms. This method relies on the construction function H , which is the summation of functions dependent on the distance between the i -th atom and its j -th neighbors. The function ρ represents the electronic density of the structure under consideration.

$$E_i = H_a[\sum_{i \neq j} \rho_a(r_{ij})] + \frac{1}{2} \sum_{i \neq j} \varphi_{\alpha\beta}(r_{ij}) \quad (1)$$

Within the functional relationship (1), the symbol r_{ij} denotes the distance between the i -th and j -th atoms, ρ_a represents the contribution to the electron charge density originating from the j -th atom at the position of the i -th atom, and $\varphi_{\alpha\beta}$ is the pairwise potential function. The function H is referred to as the “embedding” function, and it quantifies the energy necessary to position the i -th atom of type α within the electron cloud. The EAM potential is a many-body potential. The sum of contributions from a large number of atoms forms the electron density. In practice, to reduce the complexity and computation time, the number of neighbors is often reduced. In this case, the cutoff radius was set to 10 Å. Next, within the volume of each crystal, the atoms of the light sublattice were given displacements along the following crystallographic directions corresponding to the axes: X-<100>, Y-<010>, Z-<001>. This allowed for the excitation of high-amplitude vibrations. A displacement magnitude of 0.8 Å ensured the manifestation of the nonlinear component in the atom dynamics.

3. Results and discussion

To analyze the possibility of exciting localized modes, the phonon spectra of selected models were examined. In the phonon spectra of Al₃Pt, AlPt(1), AlPt₂, AlPt₂(1), AlPt₃, Al₃Pt₅ alloys, a gap can be observed (figure 2). This makes them promising candidates for searching for discrete breathers with a soft type of nonlinearity. However, it should be noted that the presence of a band gap in the spectrum is only a necessary condition, but not sufficient. The width of the band gap also plays an important role.

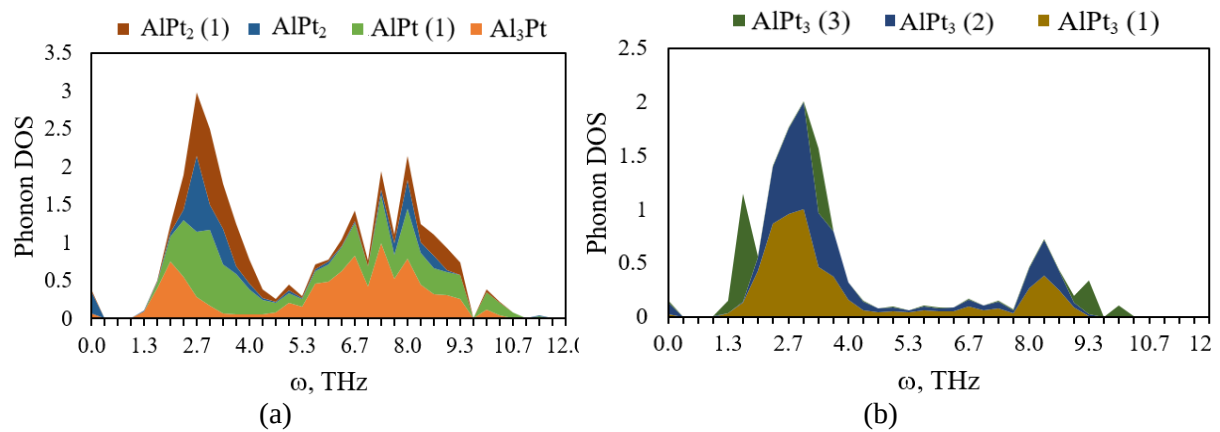


Figure 2. Phonon spectra: (a) Al_3Pt , $\text{AlPt}(1)$, AlPt_2 , $\text{AlPt}_2(1)$; (b) $\text{AlPt}_3(1)$, $\text{AlPt}_3(2)$, $\text{AlPt}_3(3)$.

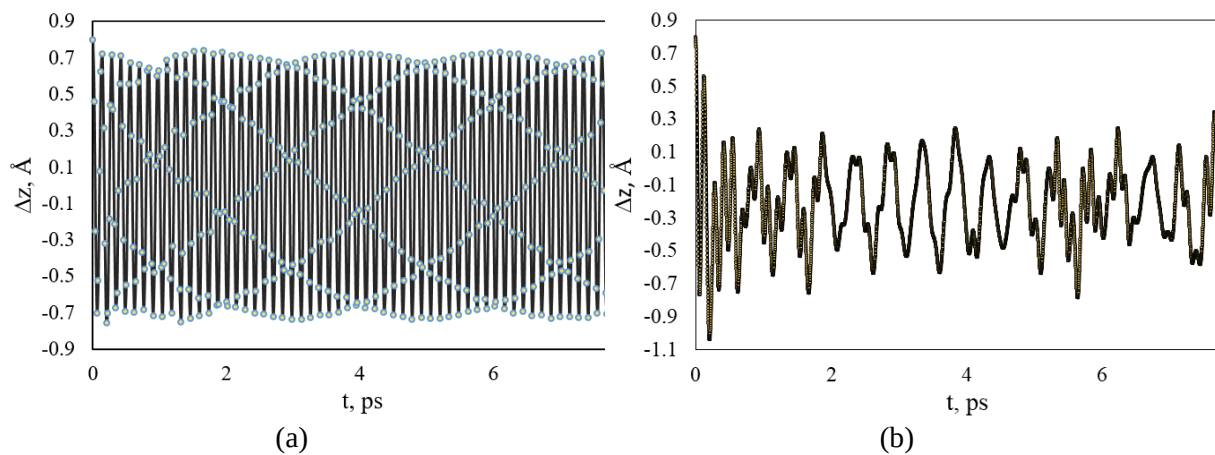


Figure 3. Dependence of the coordinate of the Al atom along the Z axis on time in the crystal: (a) AlPt_3 , (b) Al_3Pt_5 .

After analyzing the spectra in the selected materials, attempts were made to excite highly-amplitude nonlinear modes. The results revealed that discrete breathers launched along the X, Y, Z axes in the alloys AlPt_3 , $\text{AlPt}_3(1)$, $\text{AlPt}_3(2)$, $\text{AlPt}_3(3)$ were sufficiently stable and existed for a time significantly exceeding 10 ps (figure 3). This is due to the extremely wide band gap in these crystals. The discrete breathers exhibit a soft type of nonlinearity, with a frequency on the order of 7 THz, falling within the phonon spectrum gap. These results are in good agreement with our previous findings for crystals with this stoichiometry. In the Al_3Pt_5 alloy, the oscillator launched along the Z axis can be described as highly-amplitude nonlinear vibrations. Its frequency is 5 THz, which also corresponds to the gap in the spectrum for this crystal. The instability of the vibrations is due to a narrower gap in the spectrum and the more complex geometry of the material. In the remaining alloys, the vibrations were unstable and quickly decayed.

4. Conclusion

The nonlinear nature of interatomic interactions can manifest in different types of lattice vibrations, as reflected in the analyzed dispersion curves. The molecular dynamics method employed allows for the consideration of various factors. By examining a series of crystals with the composition Al_nPt_m , it has been shown that some of them, within the framework of the considered formalism and interatomic potential, may have a phonon spectrum with a band gap. This condition, combined with the nonlinearity of the bonds, can ensure the existence of highly-amplitude localized modes, such as discrete breathers.

This has been demonstrated for the corresponding alloys listed in table 1: AlPt₃, AlPt₃(1), AlPt₃(2), AlPt₃(3). This confirms our previous work specifically on this alloy. It has also been established that in the Al₃Pt₅ alloy, the existence of prolonged high-amplitude excitations on the Al atom is possible. These vibrations cannot be referred to as discrete breathers due to their non-periodicity.

Acknowledgment

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