



Comparison of Peridynamics and Lattice Dynamics Wave Dispersion Relationships

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Abstract

Peridynamics is a non-local continuum formulation and material points inside an influence domain, named horizon, can interact with each other. Peridynamics also has a capability to represent wave dispersion which is observed in real materials especially at shorter wave lengths. Therefore, wave frequency and wave number have a nonlinear relationship in peridynamics. In this study, we present wave dispersion characteristics of peridynamics and compare with lattice dynamics to determine the horizon size for different materials including copper, gold, silver and platinum through an iterative process for the first time in the literature. This study also shows the superiority of peridynamics over classical continuum mechanics by having a length scale parameter, horizon, which allows peridynamics to represent the entire range of dispersion curves for both short and long wave lengths as opposed to limitation of classical mechanics to long wave lengths.

Keywords Peridynamics · Dispersion relationship · Lattice model · Non-local

1 Introduction

Peridynamics is a new continuum mechanics formulation [1]. Peridynamic equations of motion are integro-differential equations and they do not contain spatial derivatives as opposed to classical continuum mechanics which uses partial differential equations. As opposed to semi-analytical approaches [2] and finite element methodology, this brings a significant advantage to predict crack initiation and propagation since the displacement field is discontinuous if cracks exist in the structure and spatial derivatives are not defined along the crack surfaces. Moreover, peridynamics is a non-local continuum formulation so that material points inside an influence domain, named horizon, can interact with each other. Horizon is a length scale parameter which does not exist in classical continuum mechanics. Peridynamics also has a capability to represent wave dispersion which is observed in real materials especially at shorter wave lengths. Therefore, wave frequency and wave number have a nonlinear relationship in peridynamics.

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There has been a significant progress on peridynamics. Amongst these, Alpay and Madenci [3] performed fully coupled thermomechanical peridynamic analysis to predict crack growth. Basoglu et al. [4] investigated the potential of micro-cracks to deflect crack propagation. Celik et al. [5] utilised peridynamics to simulate nanoindentation experiments for thin films. De Meo et al. [6] predicted how cracks initiate and propagate from corrosion pits by using peridynamics. Diyaroglu et al. [7] developed peridynamic wetness approach to determine moisture concentration in electronic packages. In order to reduce computational time of peridynamic simulations, Guski et al. [8] performed peridynamic investigation of the microstructural behaviour of plasma sprayed coatings. Huang et al. [9] developed a new peridynamic model for visco-hyperelastic materials. Imachi et al. [10] investigated dynamic crack arrest in peridynamic framework. Karpenko et al. [11] investigated the effect of small defects such as holes and micro-cracks on crack propagation. Kefal et al. [12] performed peridynamic topology optimisation study of structures with cracks. Liu et al. [13] studied fracture of graphene sheets by using peridynamics. Madenci et al. [14] developed weak form of peridynamics for nonlocal essential and natural boundary conditions. Naumenko and Eremeyev [15] presented a non-linear direct peridynamic plate theory. Oterkus and Madenci [16] demonstrated peridynamic formulation to consider torsional and antiplane shear deformations. Ren et al. [17] introduced dual horizon peridynamics to take into account variable horizons in the solution domain. Vazic et al. and Candas et al. [18–20] studied the interaction of macro and micro-crack under dynamic conditions. In another study, Vazic et al. [21] presented peridynamic Mindlin plate formulation by considering Winkler elastic foundation. Vazic et al. [22] compared different family member search algorithms that can be used in peridynamic simulations. Peridynamic Timoshenko beam and Kirchhoff plate formulations are provided in Yang et al. [23] and [24], respectively. Peridynamic formulations for higher-order beams and plates are given in Yang et al. [25] and [26], respectively. Zhu et al. [27] studied polycrystalline fracture by using peridynamics.

Dispersion relationships were also investigated in peridynamic framework. Butt et al. [28] presented wave dispersion and propagation in state-based peridynamics. Bazant et al. [29] compared wave dispersion and basic concepts of peridynamics to classical nonlocal damage models. Gu et al. [30] performed peridynamic wave dispersion analysis for concrete. Dayal [31] used strain-gradient expansions to approximate peridynamic dispersion relation using Taylor series. Mutnuri and Gopalakrishnan [32] examined the wave dispersion properties in bond-based peridynamics. Wildman [33] presented discrete micromodulus functions for reducing wave dispersion in linearized peridynamics. Zhang et al. [34] investigated wave dispersion and propagation in linear peridynamic media. However, none of these studies utilised dispersion relationships to calculate the horizon size. Therefore, in this study, peridynamic dispersion relationships for bond-based peridynamics are compared with the ones obtained from lattice dynamics and optimum values of horizon sizes for different materials are obtained including copper, gold, silver and platinum for the first time in the literature.

2 Dispersion Relationships in Peridynamic Theory

Peridynamics is a non-local continuum mechanics formulation since a material point can interact with other material points inside a region called horizon. The peridynamic equation of motion for a material point located at \mathbf{x} can be written as follows:

$$\rho \ddot{\mathbf{u}}(\mathbf{x}, t) = \int_{H_{\mathbf{x}}} \mathbf{f}(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) dV' + \mathbf{b}(\mathbf{x}, t) \quad (1)$$

where ρ is mass density, t is time, \mathbf{u} and $\ddot{\mathbf{u}}$ represent the displacement and acceleration of the material point located at \mathbf{x} , and \mathbf{b} is the body load acting on the material point at \mathbf{x} . \mathbf{x}' is the location of the material point inside the horizon of the material point located at \mathbf{x} , $H_{\mathbf{x}}$. Peridynamic force density, \mathbf{f} , between material points located at \mathbf{x} and \mathbf{x}' can be expressed as follows:

$$\mathbf{f} = c s \frac{(\mathbf{x}' + \mathbf{u}') - (\mathbf{x} + \mathbf{u})}{|(\mathbf{x}' + \mathbf{u}') - (\mathbf{x} + \mathbf{u})|} \quad (2)$$

where c is the bond constant and the stretch, s , can be defined as follows:

$$s = \frac{|(\mathbf{x}' + \mathbf{u}') - (\mathbf{x} + \mathbf{u})| - |\mathbf{x}' - \mathbf{x}|}{|\mathbf{x}' - \mathbf{x}|} \quad (3)$$

Next, both one- and two-dimensional dispersion relationships in peridynamic theory will be presented.

2.1 One-Dimensional Dispersion Relationships

To obtain the dispersion relationship for one-dimensional structures, the plane wave solution

$$u(x, t) = U e^{i(kx - \omega t)} \quad (4)$$

can be utilised where ω is the angular frequency, k is the wave number and U is the constant amplitude.

Substituting the plane wave solution given in Eq. (4) into the peridynamic equation of motion given in Eq. (1) yields the dispersion relationship as follows:

$$\omega_{pd}^2 = \frac{4E}{\rho \delta^2} (\gamma - \text{cosintegral}(k\delta) + \ln(k\delta)) \quad (5)$$

where $c = 2E/(A\delta^2)$, E is the elastic modulus, δ is the horizon size, A is the cross-sectional area and γ is the Euler gamma constant.

2.2 Two-Dimensional Dispersion Relationships

To obtain the dispersion relationship for two-dimensional structures, first, the plane wave solution for the longitudinal (x -) direction can be considered as follows:

$$u(\mathbf{x}, t) = U e^{i(k\mathbf{x} \cdot \mathbf{n} - \omega t)} \quad (6)$$

where \mathbf{n} is the unit vector of the wave propagation direction. For a wave propagating in the longitudinal direction, the unit vector is $\mathbf{n} = \mathbf{e}_x$. Moreover, the tangential displacements are specified as zero, i.e. $v(\mathbf{x}, t) = 0$.

Substituting the plane wave solution given in Eq. (6) into the peridynamic equation of motion given in Eq. (1) yields the dispersion relationship in the longitudinal direction as follows:

$$\omega_L = \sqrt{\frac{9E}{\rho \delta^3} \left(\delta - \frac{2\text{BesselJ}[1, \delta k]}{k} \right)} \quad (7)$$

where $c = 9E/(\pi h \delta^3)$, h is plate thickness and $\text{BesselJ}[m, \dots]$ is Bessel function of the m kind. The dispersion relationship for the transverse (y -) direction can be obtained similarly as follows:

$$\omega_T = \sqrt{\frac{9E}{\rho \delta^3} \left(\delta - \frac{\text{BesselJ}[1, \delta k](-2 + \delta k \pi \text{StruveH}[0, \delta k])}{k} + \frac{\delta \text{BesselJ}[0, \delta k](-2 + \pi \text{StruveH}[1, \delta k])}{k} \right)} \quad (8)$$

where $\text{StruveH}[m, \dots]$ is Struve function of the m kind.

3 Dispersion Relationships in Lattice Dynamics

The nature of the crystal vibration and their interactions has been described with various methodologies. Born-von Karman (BvK) proposed a BvK model [35, 36] which assumes the ion-ion central interactions acting between one atom and its neighbours. Thus, the potential energy is a function of the distance between atomic pairs, where the displacements that change between the atoms will contribute to the force constants.

A monatomic, face centred cubic (FCC) structural lattice with lattice constant ‘ a ’ has been studied, in which central forces are assumed to act between one atom and its first second and second nearest neighbours. This is due to the potential decays rather rapidly beyond the first few neighbours.

The determinant for calculating phonon frequencies for the normal modes of the vibrations of the lattices is written as [36] follows:

$$|D - \omega^2 MI| = 0 \quad (9)$$

where D is the 3×3 element of the determinant (dynamic matrix), M is the atomic mass, I is the unit matrix and ω is the angular frequency of phonons in rad/sec. The explicit expression for the various element of the various diagonal and non-diagonal elements is given by the following:

$$D_{ii} = 2A_1 [2 - C_i(C - C_i)] + 4A_2 S_i^2 \quad (10)$$

and

$$D_{ij} = 2A_1 S_i S_j \quad (11)$$

where A_1 and A_2 are the central force constants in first and second nearest neighbours, respectively.

$$S_i = \sin\left(\frac{1}{2} a q_n\right), C_i = \cos\left(\frac{1}{2} a q_n\right), C = C_i + C_j + C_k \quad (12)$$

where q_n is the phonon wave vector and $n = i, j, k$.

Suppose $q_i = q$, $q_j = q_k = 0$, (1,0,0) axis, in this case, the non-diagonal elements are $D_{ij} = 0$, and

$$D_{xx} = 4A_1 \left[1 - \cos \left(\frac{1}{2}aq \right) \right] + 4A_2 \sin^2 \left(\frac{1}{2}aq \right) = 8A_1 \sin^2 \left(\frac{1}{4}aq \right) + 4A_2 \sin^2 \left(\frac{1}{2}aq \right) \tag{13}$$

$$D_{yy} = D_{zz} = 4A_1 \sin^2 \left(\frac{1}{4}aq \right) \tag{14}$$

Therefore, dispersion relationships can be written as follows:

$$\begin{cases} \omega_1^2 = \frac{8A_1}{M} \sin^2 \left(\frac{1}{4}aq \right) + \frac{4A_2}{M} \sin^2 \left(\frac{1}{2}aq \right) \\ \omega_2^2 = \omega_3^2 = \frac{4A_1}{M} \sin^2 \left(\frac{1}{4}aq \right) \end{cases} \tag{15}$$

The central force constants A_1 and A_2 can be related to the elastic constants as follows:

$$A_1 = aC_{44} \tag{16}$$

$$A_2 = \frac{a}{4} (C_{11} - C_{12} - C_{44}) \tag{17}$$

4 Numerical Results

In this section, dispersion relationships for four different materials obtained from peridynamics and lattice dynamics will be presented. By comparing the dispersion relationships obtained from peridynamics and lattice dynamics approaches through an iterative process will provide the horizon size value for a particular material.

4.1 Copper

In the first case, copper material is considered. The material properties of the copper are presented in Table 1.

Peridynamic dispersion curves for copper can be obtained using the 1-Dimensional dispersion relationship given in Eq. (4). By comparing peridynamic relationship with the one obtained from lattice dynamics given in Eq. (15), the horizon size can be obtained as $\delta = 2.405 \times 10^{-10}$ m (Fig. 1a).

Table 1 Material properties of copper

Parameters	Value	Units
Atomic mass	1.055e-25	kg
Density	8960	Kg/m ³
Lattice constant	3.598	Å
Young’s modulus	130	GPa
Poisson’s ratio	0.34	-
Elastic constant, C_{11} [37]	1.69	10 ¹² dyn/cm ²
Elastic constants, C_{12} [37]	1.22	10 ¹² dyn/cm ²
Elastic constants, C_{44} [37]	0.754	10 ¹² dyn/cm ²

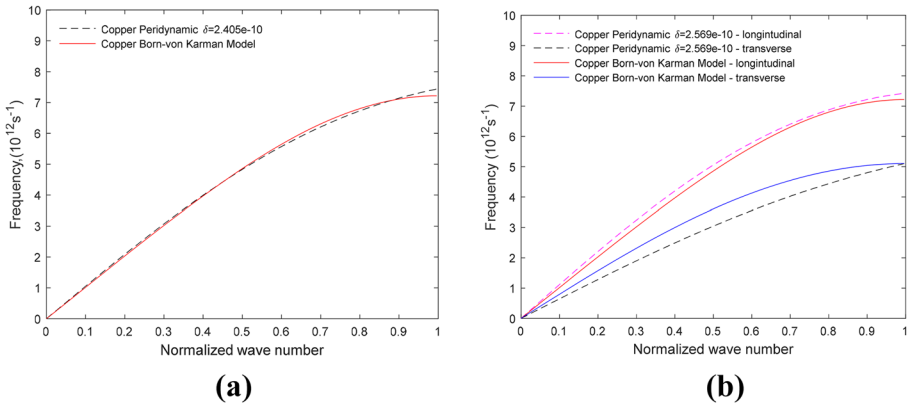


Fig. 1 Dispersion relationships for copper: **a** 1-D; **b** 2-D

Peridynamic dispersion curves for copper for both longitudinal and transverse directions can be obtained from Eqs. (7) and (8), respectively. By comparing peridynamic relationships with the ones obtained from lattice dynamics given in Eq. (15), the horizon size can be obtained as $\delta = 2.569 \times 10^{-10}$ m (Fig. 1b).

4.2 Gold

In the second case, gold material is considered. The material properties of the gold are presented in Table 2.

Peridynamic dispersion curves for gold can be obtained using the 1-dimensional dispersion relationship given in Eq. (4). By comparing peridynamic relationship with the one obtained from lattice dynamics given in Eq. (15), the horizon size can be obtained as $\delta = 2.903 \times 10^{-10}$ m (Fig. 2a).

Peridynamic dispersion curves for gold for both longitudinal and transverse directions can be obtained from Eqs. (7) and (8), respectively. By comparing peridynamic relationships with the ones obtained from lattice dynamics given in Eq. (15), the horizon size can be obtained as $\delta = 3.0875 \times 10^{-10}$ m (Fig. 2b).

Table 2 Material properties of gold

Parameters	Value	Units
Atomic mass	3.2707137e-25	kg
Density	19,320	Kg/m ³
Lattice constant	4.064	Å
Young’s modulus	79	GPa
Poisson’s ratio	0.42	-
Elastic constant, C ₁₁ [37]	1.89	10 ¹² dyn/cm ²
Elastic constant, C ₁₂ [37]	1.59	10 ¹² dyn/cm ²
Elastic constant, C ₄₄ [37]	0.426	10 ¹² dyn/cm ²

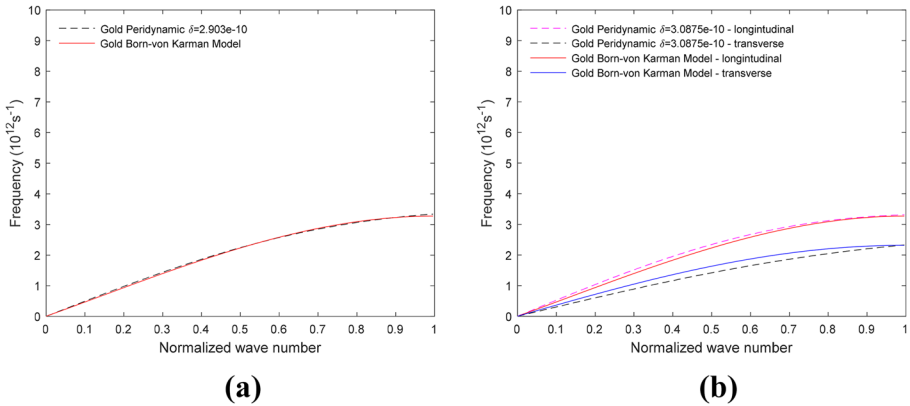


Fig. 2 Dispersion relationships for gold: **a** 1-D; **b** 2-D

4.3 Silver

In the third case, silver material is considered. The material properties of the silver are presented in Table 3.

Peridynamic dispersion curves for silver can be obtained using the 1-dimensional dispersion relationship given in Eq. (4). By comparing peridynamic relationship with the one obtained from lattice dynamics given in Eq. (15), the horizon size can be obtained as $\delta = 2.991 \times 10^{-10}$ m (Fig. 3a).

Peridynamic dispersion curves for silver for both longitudinal and transverse directions can be obtained from Eqs. (7) and (8), respectively. By comparing peridynamic relationships with the ones obtained from lattice dynamics given in Eq. (15), the horizon size can be obtained as $\delta = 3.173 \times 10^{-10}$ m (Fig. 3b).

4.4 Platinum

In the final case, platinum material is considered. The material properties of the platinum are presented in Table 4.

Peridynamic dispersion curves for platinum can be obtained using the 1-Dimensional dispersion relationship given in Eq. (4). By comparing peridynamic relationship with the

Table 3 Material properties of silver

Parameters	Value	Units
Atomic mass	1.7911901e-25	kg
Density	10,490	Kg/m ³
Lattice constant	4.079	Å
Young’s modulus	85	GPa
Poisson’s ratio	0.37	-
Elastic constant, C ₁₁ [37]	1.22	10 ¹² dyn/cm ²
Elastic constant, C ₁₂ [37]	0.92	10 ¹² dyn/cm ²
Elastic constant, C ₄₄ [37]	0.446	10 ¹² dyn/cm ²

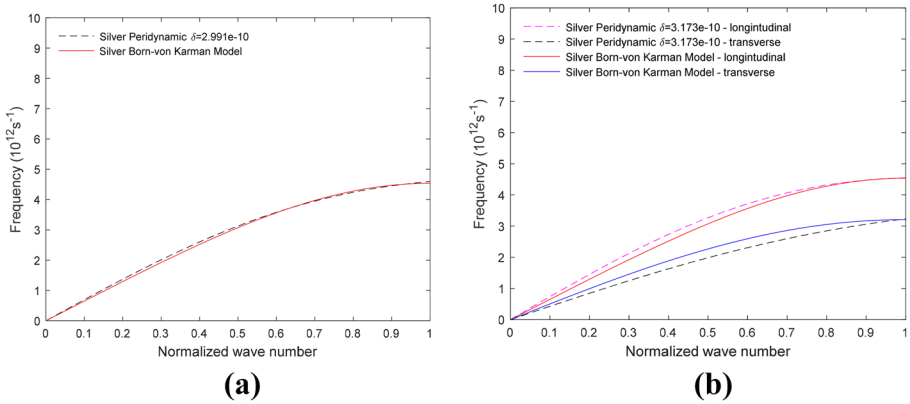


Fig. 3 Dispersion relationships for silver: **a** 1-D; **b** 2-D

one obtained from lattice dynamics given in Eq. (15), the horizon size can be obtained as $\delta = 3.185 \times 10^{-10}$ m (Fig. 4a).

Peridynamic dispersion curves for platinum for both longitudinal and transverse directions can be obtained from Eqs. (7) and (8), respectively. By comparing peridynamic relationships with the ones obtained from lattice dynamics given in Eq. (15), the horizon size can be obtained as $\delta = 3.375 \times 10^{-10}$ (Fig. 4b).

By considering all comparisons between peridynamic dispersion curves and those obtained from lattice dynamics, a very good match was obtained for 1-dimensional peridynamic model for all four materials considered in this study. However, for 2-dimensional peridynamic models, the difference between peridynamics and lattice model results is slightly higher for copper with respect to gold, silver and platinum. By comparing the material properties of all four materials, atomic mass, density and lattice constant of copper are lower with respect to other three materials which may be the reason behind this difference.

Table 4 Material properties of platinum

Parameters	Value	Units
Atomic mass	3.2394457e-25	kg
Density	21,450	Kg/m ³
Lattice constant	3.912	Å
Young’s modulus	171	GPa
Poisson’s ratio	0.38	-
Elastic constant, C11 [37]	3.467	10 ¹² dyn/cm ²
Elastic constant, C12 [37]	2.507	10 ¹² dyn/cm ²
Elastic constant, C44 [37]	0.756	10 ¹² dyn/cm ²

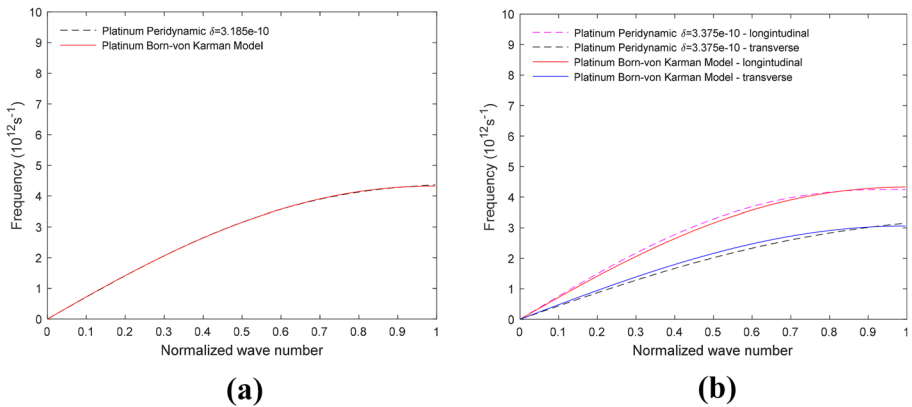


Fig. 4 Dispersion relationships for platinum: **a** 1-D; **b** 2-D

5 Conclusion

In this study, one-dimensional and two-dimensional dispersion relationships were obtained from peridynamics and lattice dynamics. Dispersion relationships from both approaches have nonlinear characteristic as observed in real materials. Finally, optimum horizon sizes for peridynamics for different materials including copper, gold, silver and platinum were obtained by comparing peridynamic dispersion curves against dispersion curves obtained from lattice dynamics through an iterative process for the first time in the literature. This study also shows the superiority of peridynamics over classical continuum mechanics by having a length scale parameter, horizon, which allows peridynamics to represent the entire range of dispersion curves for both short and long wave lengths as opposed to limitation of classical mechanics to long wave lengths.

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Data availability The datasets generated during and/or analysed during the current study are available from the corresponding author on reasonable request.

Declarations

Conflict of Interest The authors declare no competing interests.

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