Abstract. In this paper, we propose accurate numerical boundary conditions for atomic simulations of twin boundary. The heterogeneity of the lattice structure induces physical reflection across the twin boundary. When numerical boundary and the twin boundary coincide, the goal is to reproduce the correct amount of physical reflection. In particular, we consider waves periodic in the direction parallel to the twin boundary and reduce the problem into a complex-valued chain motion. Using Laplace transform, we design time history kernel (THK) treatment. We further design matching boundary conditions (MBC) by reproducing physical reflection at long wave limit and a specific wave number. Reflection analysis and numerical tests demonstrate the effectiveness of the proposed THK and MBC treatments.

AMS subject classifications: 74J05, 74M25, 37N15

Key words: Twin boundary, artificial boundary condition, dispersion relation, reflection coefficient, atomic simulation.

1 Introduction

Atomic simulations provide a standard toolkit nowadays for explorations at nano up to micron scales [10]. Though the computing power has grown continuously in the past several decades, it never catches up with the even faster growth of human desire to simulate bigger systems in more details. Hence it is still, if not more, important to suitably formulate a numerical model that represents real applications. One aspect we are concerned with is heterogeneous atomic structures. In metallic materials, the precipitation hardening effects are greatly influenced by numerous deformation, such as twinning [6]. In twin lattices, the same type of atoms may form heterogeneous structure due to different orientations [2]. Atomic simulations are indispensable tools for understanding their mechanical and thermal properties. In many applications, one type of lattice A is embedded

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in another type of lattice B, which is much bigger in size. The vast surrounding lattice B is usually assumed to be homogeneous, and often at equilibrium initially. Then one may include the response of sub-lattice B by boundary conditions when the sub-lattice A is modeled and simulated.

In the reduced case of a homogeneous lattice, namely, when the sub-lattices A and B are identical, there incurs no reflection across the boundary. A transparent boundary condition is the ideal goal, which is usually expensive to realize numerically [1]. Cost-effective boundary conditions are then designed in terms of artificial boundary conditions, absorbing boundary conditions and various buffer-zone treatments, e.g. [8, 11]. In contrast, there indeed incurs reflection across the boundary in a heterogeneous lattice. Hence, in the design of an accurate boundary condition for a heterogeneous lattice, the challenge lies in reproducing the physical reflection to the correct amount numerically. As we shall see in this study, it is far more complicated than for a homogeneous lattice. To our best knowledge of state-of-the-art, there is yet no result along this direction.

In this work, we develop some accurate boundary conditions, including time history kernel (THK) treatment and matching boundary conditions (MBC), for treating the numerical boundary in a heterogeneous lattice with twin boundary.

The rest of this paper is organized as follows. First we describe the problem set-up of atomic dynamics with twin boundary. Then we propose THK treatment, and MBC to approximate the physical reflection. For a special choice of parameters, MBC’s are given explicitly. Numerical tests are then presented to verify the effectiveness. Finally we make some concluding remarks.

2 Governing equations

We consider a heterogeneous lattice with twin boundary as shown in Fig. 1. It consists of an upper half lattice, denoted by \( n \geq 0 \), and a lower lattice with \( n \leq 0 \). Under the assigned coordinate system, for even layers \( (n \text{ even}) \), atoms are labeled in horizontal direction with even indices \( (m \text{ even}) \) only; whereas for odd layers, \( m \) takes odd number only. Away from the boundary, we have perfect square lattice, with atomic mass \( m_a \), lattice constant \( h_a \). For simplicity, we consider out-of-plane waves only, and assume nearest neighboring interaction. The out-of-plane displacement away from equilibrium at \((m,n)\)-atom is denoted as \( u_{m,n}(t) \). The interatomic potential between atoms numbered \((m_1,n_1)\) and \((m_2,n_2)\) is \( V(u_{m_1,n_1} - u_{m_2,n_2}, h_a) \). The governing equation for \((m,n)\)-atom in the upper lattice then reads (\(m,n\) with the same parity)

\[
m_a \ddot{u}_{m,n} = -\partial_{u_{m,n}} V(u_{m,n} - u_{m,n+2}, h_a) - \partial_{u_{m,n}} V(u_{m,n} - u_{m-1,n+1}, h_a) - \partial_{u_{m,n}} V(u_{m,n} - u_{m-1,n-1}, h_a) - \partial_{u_{m,n}} V(u_{m,n} - u_{m-2,n-2}, h_a), \quad n \geq 3. \tag{2.1}
\]

By a harmonic approximation of the interatomic potential, the governing linearized equation reads

\[
m_a \ddot{u}_{m,n} = k(u_{m,n+2} + u_{m-1,n+1} - 4u_{m,n} + u_{m+1,n-1} + u_{m,n-2}), \quad n \geq 3. \tag{2.2}
\]
Here \( k = -\frac{\partial^2 V}{\partial u_{\alpha}^2}(0, h_0) \) is the elastic constant. Rescaling time by \( \sqrt{k/m_\alpha} \) and displacement by \( h_0 \) gives a dimensionless equation

\[
\ddot{u}_{m,n} = u_{m,n+2} + u_{m-1,n+1} - 4u_{m,n} + u_{m+1,n-1} + u_{m,n-2}, \quad n \geq 3. \tag{2.3}
\]

Similarly, for an atom in the lower lattice, the dimensionless governing equation is \((m,n)\) with the same parity

\[
\ddot{u}_{m,n} = u_{m,n+2} + u_{m+1,n+1} - 4u_{m,n} + u_{m-1,n-1} + u_{m,n-2}, \quad n \leq -3. \tag{2.4}
\]

For the layers across the twin boundary, there usually appears distortion in the lattice structure. Let the elastic constant under the distortion be \( h_1k, h_2k \) and \( h_3k \) for the atom pairs \((m,-1)-(m,1), (m,0)-(m-1,\pm 1)\) and \((m,0)-(m,\pm 2)\), respectively. The dimensionless governing equations then follow.

\[
\begin{align*}
\ddot{u}_{m,2} &= u_{m,4} + u_{m-1,3} - (3 + h_3)u_{m,2} + u_{m+1,1} + h_3u_{m,0}, & m \text{ even}, \\
\ddot{u}_{m,1} &= u_{m,3} + u_{m-1,2} - (2 + h_1 + h_2)u_{m,1} + h_2u_{m+1,0} + h_1u_{m-1,1}, & m \text{ odd}, \\
\ddot{u}_{m,0} &= h_3u_{m,2} + h_2u_{m-1,1} - 2(h_2 + h_3)u_{m,0} + h_2u_{m-1,-1} + h_3u_{m,-2}, & m \text{ even}, \\
\ddot{u}_{m,-1} &= h_1u_{m,1} + h_2u_{m+1,0} - (2 + h_1 + h_2)u_{m,-1} + u_{m-1,-2} + u_{m,-3}, & m \text{ odd}, \\
\ddot{u}_{m,-2} &= h_3u_{m,0} + u_{m+1,-1} - (3 + h_3)u_{m,-2} + u_{m-1,-3} + u_{m,-4}, & m \text{ even}.
\end{align*}
\tag{2.5-2.9}
\]

We denote for each fixed \( n \) and wave number \( \xi \in [-\pi/2, \pi/2] \),

\[
u_{m,n} = U_n(t, \xi) e^{im_\xi}.
\tag{2.10}
Here $m$ has the same parity as the fixed $n$. We suppress the dependence for $U_n(t; \xi)$ on $\xi$ in the sequel, and invoke it again only when the inverse transform is considered.

From (2.3)-(2.9), we derive the governing equations for the transformed variable $U_n(t)$

$$
\ddot{U}_n = U_{n-2} + e^{i\xi}U_{n-1} - 4U_n + e^{-i\xi}U_{n+1} + U_{n+2}, \quad n \geq 3,
$$

$$
\ddot{U}_2 = h_3U_0 + e^{i\xi}U_1 - (3 + h_3)U_2 + e^{-i\xi}U_3 + U_4,
$$

$$
\ddot{U}_1 = h_1U_{-1} + h_2e^{i\xi}U_0 - (2 + h_1 + h_2)U_1 + e^{-i\xi}U_2 + U_3,
$$

$$
\ddot{U}_0 = h_3U_{-2} + h_2e^{-i\xi}U_{-1} - 2(h_2 + h_3)U_0 + h_2e^{-i\xi}U_1 + h_3U_2,
$$

$$
\ddot{U}_{-1} = U_{-3} + e^{-i\xi}U_{-2} - (2 + h_1 + h_2)U_{-1} + h_2e^{i\xi}U_0 + h_1U_1,
$$

$$
\ddot{U}_{-2} = U_{-4} + e^{-i\xi}U_{-3} - (3 + h_3)U_{-2} + e^{i\xi}U_{-1} + h_3U_0,
$$

$$
\ddot{U}_n = U_{n-2} + e^{-i\xi}U_{n-1} - 4U_n + e^{i\xi}U_{n+1} + U_{n+2}, \quad n \leq -3.
$$

We remark that the original atomic system (2.3)-(2.9) involves only nearest-neighboring interaction, while the transformed problem (2.11)-(2.17) involves non-nearest neighboring interaction. This induces challenges in addition to the twin boundary.

### 3 Time history kernel functions

There is a class of exact boundary conditions for lattice dynamics, under the framework of time history kernel treatment [9]. The basic assumptions include the linearity of the governing Newton laws, which holds true for our current circumstance, and the initial equilibrium state for a semi-infinite lattice toward where the waves propagate.

We assume the lower semi-lattice be homogeneous and infinite ($m \in \mathbb{Z}, n \in \mathbb{Z}^-$). If initially the lattice is at equilibrium for all atoms below a certain $N$, then due to the non-nearest neighboring interaction, we may express $U_n$ by $U_{n+1}$ and $U_{n+2}$ by convolutions with corresponding kernel functions $a_n(t)$ and $b_n(t)$.

$$
U_n(t) = a_n(t) * U_{n+1}(t) + b_n(t) * U_{n+2}(t),
$$

where $f(t) * g(t) = \int_0^t f(t-\tau)g(\tau) d\tau$.

In fact, there is a recursive relation for these kernel functions. For each $U_n(t)$, we formally denote its governing equation (one of (2.11)-(2.17) depending on $n$) to be

$$
\ddot{U}_n(t) = aU_{n-2} + bU_{n-1} + cU_n + dU_{n+1} + eU_{n+2}.
$$

Under the Laplace transform, we have

$$
a\hat{U}_{n-2} + b\hat{U}_{n-1} + (c - s^2)\hat{U}_n + d\hat{U}_{n+1} + e\hat{U}_{n+2} = 0,
$$

where $\hat{\cdot}$ denotes the transformed quantity, and $s$ is the Laplace transform variable. Direct calculations show that

$$
[(c - s^2) + b\hat{a}_{n-1} + a(\hat{a}_{n-2}\hat{a}_{n-1} + \hat{b}_{n-2})]\hat{U}_n
= -(d + b\hat{b}_{n-1} + a\hat{a}_{n-2}\hat{b}_{n-1})\hat{U}_{n+1} - e\hat{U}_{n+2}.
$$
Accordingly, we have recursive relations
\[
\hat{\alpha}_n = -\frac{d + b\hat{\beta}_{n-1} + a\hat{\alpha}_{n-2}\hat{\beta}_{n-1}}{(c - s^2) + b\hat{\alpha}_{n-1} + a(\hat{\alpha}_{n-2}\hat{\alpha}_{n-1} + \hat{\beta}_{n-2})}, \tag{3.5}
\]
\[
\hat{\beta}_n = -\frac{e}{(c - s^2) + b\hat{\alpha}_{n-1} + a(\hat{\alpha}_{n-2}\hat{\alpha}_{n-1} + \hat{\beta}_{n-2})}. \tag{3.6}
\]

In particular, the Newton equations are uniform for \( n \leq -3 \), hence so are the kernel functions \( \alpha_n = a, \beta_n = \beta \). Using the Laplace transform of (2.17), we find that
\[
-(s^2 + 4)\hat{\alpha} + \hat{\alpha}^3 + 2\hat{\alpha}\hat{\beta} + e^{-i\xi}(\hat{\alpha}^2 + \hat{\beta}) + e^{i\xi} = 0, \tag{3.7}
\]
\[
-(s^2 + 4)\hat{\beta} + \hat{\alpha}^2 \hat{\beta} + \hat{\beta}^2 + e^{-i\xi}\hat{\alpha}\hat{\beta} + 1 = 0. \tag{3.8}
\]

The Laplace inverse transform is not easy to evaluate in general. Following [12], we propose to obtain the kernel functions by solving the corresponding ordinary differential equations.
\[
\ddot{\alpha} = -4a + a*(a\alpha + 2\beta + e^{-i\xi}\alpha) + e^{-i\xi}\beta, \tag{3.9}
\]
\[
\ddot{\beta} = -4\beta + \beta*(a\alpha + \beta + e^{-i\xi}\alpha), \tag{3.10}
\]
\[
\alpha(0) = 0, \quad \dot{\alpha}(0) = e^{i\xi}, \quad \beta(0) = 0, \quad \dot{\beta}(0) = 1. \tag{3.11}
\]

Other kernel functions may be obtained recursively as follows.
\[
\dot{\alpha}_{-2} = -(3 + h_3)\alpha_{-2} + \alpha_{-2}*(a\alpha + \beta + e^{-i\xi}\alpha) + a\beta + e^{-i\xi}\beta, \tag{3.12}
\]
\[
\dot{\beta}_{-2} = -(3 + h_3)\beta_{-2} + \beta_{-2}*(a\alpha + \beta + e^{-i\xi}\alpha), \tag{3.13}
\]
\[
\dot{\alpha}_{-1} = -(2 + h_1 + h_2)\alpha_{-1} + \alpha_{-1}*(a_2*\alpha + \beta + e^{-i\xi}\alpha_{-2}) + a\beta_{-2} + e^{-i\xi}\beta_{-2}, \tag{3.14}
\]
\[
\dot{\beta}_{-1} = -(2 + h_1 + h_2)\beta_{-1} + \beta_{-1}*(a_2*\alpha + \beta + e^{-i\xi}\alpha_{-2}), \tag{3.15}
\]
\[
\alpha_0 = -(2h_2 + h_3)a_0 + a_0*(h_3(\alpha_{-1}\alpha_{-2} + \beta_{-2}) + h_2e^{-i\xi}\alpha_{-1})
+ h_3\alpha_{-2}\beta_{-2} + h_2e^{-i\xi}\beta_{-1}, \tag{3.16}
\]
\[
\beta_0 = -(2h_2 + h_3)\beta_{0} + \beta_0*(h_3(\alpha_{-1}\alpha_{-2} + \beta_{-2}) + h_2e^{-i\xi}\alpha_{-1}), \tag{3.17}
\]
\[
\alpha_{-1}(0) = a_{-1}(0) = e^{i\xi}, \quad \beta_{-2}(0) = 0, \quad \dot{\beta}_{-2}(0) = h_3, \tag{3.18}
\]
\[
\alpha_{-1}(0) = 0, \quad \dot{\alpha}_{-1}(0) = h_2e^{i\xi}, \quad \beta_{-1}(0) = 0, \quad \dot{\beta}_{-1}(0) = h_1, \tag{3.19}
\]
\[
\alpha_{0}(0) = 0, \quad \dot{\alpha}_{0}(0) = h_2e^{i\xi}, \quad \beta_{0}(0) = 0, \quad \dot{\beta}_{0}(0) = h_3, \tag{3.20}
\]
\[
\alpha_{1}(0) = 0, \quad \dot{\alpha}_{1}(0) = e^{-i\xi}, \quad \beta_{n}(0) = 0, \quad \dot{\beta}_{n}(0) = 1. \tag{3.21}
\]

To better illustrate time history kernel treatment, we show a specific case with \( h_1 = 1.2, h_2 = h_3 = 1 \), and \( \xi = \pi/5 \). The kernel functions with (3.9)-(3.23) shown in Figs. 2-3 are
Figure 2: Time history kernel functions for $h_1 = 1.2$, $h_2 = h_3 = 1$, $\xi = \pi/5$: (a) $\alpha(t)$; (b) $\beta(t)$; (c) $\alpha_{-2}(t)$; (d) $\beta_{-2}(t)$; (e) $\alpha_{-1}(t)$; (f) $\beta_{-1}(t)$; (g) $\alpha_0(t)$; (h) $\beta_0(t)$; (i) $\alpha_1(t)$; (j) $\beta_1(t)$. The solid lines represent the real part of coefficients, and dotted for the imaginary part.
Figure 3: Time history kernel functions for \( h_1 = 1.2, h_2 = h_3 = 1 \): (a) \( \alpha(t) \) for \( \xi = 0 \); (b) \( \beta(t) \) for \( \xi = 0 \); (c) \( \alpha(t) \) for \( \xi = \pi / 5 \); (d) \( \beta(t) \) for \( \xi = \pi / 5 \); (e) \( \alpha(t) \) for \( \xi = 2\pi / 5 \); (f) \( \beta(t) \) for \( \xi = 2\pi / 5 \); (g) \( \alpha(t) \) for \( \xi = 3\pi / 5 \); (h) \( \beta(t) \) for \( \xi = 3\pi / 5 \); (i) \( \alpha(t) \) for \( \xi = 4\pi / 5 \); (j) \( \beta(t) \) for \( \xi = 4\pi / 5 \). The solid lines represent the real part of coefficients, and dotted for the imaginary part.
computed with the Velocity Verlet algorithm and a time step size $\delta t = 0.002$. We remark that smaller time step size improves the accuracy yet with heavier computing load.

There are several observations. All kernel functions decay rather quickly toward 0, except $a_1$ and $b_1$. The oscillations for $a_1$, $b_1$ maintain at a certain level for the computed time period, which correspond to the physical reflection at the twin boundary. This implies a heavy computing load if we adopt this boundary condition.

Next, we compare the kernel functions for various $\xi$ in Fig. 3. We observe that $b(t)$ is real, while $a(t)$ is complex. Moreover, for $\xi$ and $\pi - \xi$, we find the corresponding $a$’s are negative complex conjugate, while $b$’s are the same.

Because of the non-nearest neighboring interaction for the lattice dynamics in (2.11)-(2.17), one needs to adopt boundary conditions for two consequent layers. For instance, we may use (3.1) for $n = -3$ and $n = -4$, where the corresponding kernel functions are $a(t)$ and $b(t)$. This choice for boundary treatments is indeed a homogeneous lattice boundary treatment, not reflecting the twin boundary feature. As they are exact boundary conditions, the error in a numerical simulation may come mainly from discretization error.

4 Matching boundary conditions

Time history kernel treatment provides exact boundary conditions, yet with heavy computing load particularly for long time simulations. We design a class of more efficient ones in terms of matching boundary conditions (MBC).

First, for an oscillatory wave $U_n(t) \sim e^{-i\omega t} z^n$ in the upper lattice ($n \geq 3$) with frequency $\omega$, it may be readily found that $z$ solves ($\zeta = e^{-i\xi}$)

$$z^4 + \zeta z^3 + (\omega^2 - 4)z^2 + \zeta^{-1}z + 1 = 0. \quad (4.1)$$

When all four roots are of modulus 1, they give four wave numbers $\eta_p = \arg(z_p)$. The wave is a Fourier mode then with $U_n(t) \sim e^{-i(\omega t - \eta n)}$. The above quartic equation is equivalent to the dispersion relation

$$\omega(\eta) = \sqrt{4 - 2\cos(\eta - \zeta) - 2\cos 2\eta}. \quad (4.2)$$

The group velocity is defined as $v(\eta) = d\omega / d\eta$.

We notice that $\omega$ remains unchanged under transform $(\zeta, \eta) \rightarrow (\pi - \zeta, \pi - \eta)$. The dispersion relations are therefore depicted in Fig. 4 only for several $\zeta$ between 0 and $\pi/2$. As a notation, we let $\eta_1$ and $\eta_3$ be with positive group velocity $v_1$ and $v_3$, namely, the dispersion relation curve takes an increasing slope.

On the other hand, for a range of $\omega$, there are two different $\eta$’s rendering the same frequency. This corresponds to the case when only two roots for (4.1) are of modulus one. The other two are complex in general, and of reciprocal modulus, giving rise to surface modes. In this case, we denote $z_1 = e^{i\eta_1}$ to be the one with positive group velocity, and $z_3$ with modulus less than 1 ($|z_4| = 1/|z_3|$).
In the lower lattice, \( z \) solves
\[
z^4 + \xi^{-1}z^3 + (\omega^2 - 4)z^2 + \xi z + 1 = 0. \tag{4.3}
\]
The dispersion relation reads
\[
\omega(\eta) = \sqrt{4 - 2\cos(\eta + \xi) - 2\cos 2\eta}. \tag{4.4}
\]
We notice that if \( z \) satisfies (4.1), then \( z^{-1} \) satisfies (4.3), and their group velocities are of opposite sign.

For a monochromatic incident wave with wave number \( \eta \) (\( z = e^{i\eta} \) either be \( z_2 \) or \( z_4 \)) from top to bottom, reflection occurs and results in
\[
U_n(t) = \begin{cases} 
  e^{-i\omega t}(z^n + R_1z^n_R + R_3z_3^n), & n \geq 1, \\
  e^{-i\omega t}V_0, & n = 0, \\
  e^{-i\omega t}(T_1z_1^{-n} + T_3z_3^{-n}), & n \leq -1.
\end{cases} \tag{4.5}
\]
Substituting this into the governing equations (2.12)-(2.16), we obtain
\[
B \begin{pmatrix} T_1 \\ T_3 \\ V_0 \\ R_1 \\ R_3 \end{pmatrix} + d = 0, \tag{4.6}
\]
A vector residual function is then defined as follows

\[
\Delta(\eta) = DX,
\]

with

\[
\begin{bmatrix}
  z_4 & z_4 & 0 & 0 & 0 \\
  z_3 & z_3 & 0 & 0 & 0 \\
  z_2 & z_2 & 0 & 0 & 0 \\
  z_1 & z_3 & 0 & 0 & 0 \\
  0 & 0 & 1 & 0 & 0 \\
  0 & 0 & z_1 & z_3 & 0 \\
  0 & 0 & z_2^2 & z_2^3 & z_2 \\
  0 & 0 & z_1^4 & z_3^3 & z_3 \\
  0 & 0 & 0 & 0 & 1 \\
  \vdots & \vdots & \vdots & \vdots & \vdots \\
  \end{bmatrix}, \quad d = 0,
\]

(4.7)

\[
B = \begin{bmatrix}
1 & \xi & \Omega_2 & \xi^{-1} & h_3 & 0 & 0 & 0 & 0 \\
0 & 1 & \xi & \Omega_1 & h_2\xi^{-1} & h_1 & 0 & 0 & 0 \\
0 & 0 & h_3 & h_2 & \Omega_0 & h_2\xi & h_3 & 0 & 0 \\
0 & 0 & h_1 & h_2\xi^{-1} & \Omega_1 & \xi & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & h_3 & \xi^{-1} & \Omega_2 & \xi & 1
\end{bmatrix},
\]

(4.8)

and \( \Omega_2 = -(3 + h_3 - \omega^2) \), \( \Omega_1 = -(2 + h_1 + h_2 - \omega^2) \), \( \Omega_0 = -(2h_2 + 2h_3 - \omega^2) \).

The solution to this algebraic system gives

\[X = e^{-i\omega t} \begin{bmatrix} T_1 \\ T_3 \\ V_0 \\ R_1 \\ R_3 \end{bmatrix} + d,\]

(4.9)

with

\[X = [U_{-4}, U_{-3}, U_{-2}, U_{-1}, U_0, U_1, U_2, U_3, U_4]^T.\]

(4.10)

Following [13], we propose an MBC, which takes the form of a linear constraint among the displacements and velocities of \( N \) atoms near the physical boundary. Because of the non-nearest neighboring interaction, two equations together form such an MBC. For instance, inspired by experiences with a heterogeneous one-dimensional chain [4], we consider the following form

\[
\begin{aligned}
c_{-2}U_{-2} + c_{-1}U_{-1} + c_0U_0 + c_1U_1 &= d_{-2}U_{-2} + d_{-1}U_{-1} + d_0U_0 + d_1U_1, \\
a_{-1}U_{-1} + a_0U_0 + a_1U_1 + a_2U_2 &= b_{-1}U_{-1} + b_0U_0 + b_1U_1 + b_2U_2.
\end{aligned}
\]

(4.11)

A vector residual function is then defined as follows

\[
\Delta(\eta) = DX,
\]

(4.12)

with

\[
D = \begin{bmatrix}
  0 & 0 & \alpha_{-2} & \alpha_{-1} & \alpha_0 & \alpha_1 & 0 & 0 & 0 \\
  0 & 0 & \beta_{-1} & \beta_0 & \beta_1 & \beta_2 & 0 & 0 & 0
\end{bmatrix},
\]

(4.13)
and
\[
\alpha_j = -i\omega c_j - d_j, \quad \beta_j = -i\omega a_j - b_j, \quad j = -2, -1, 0, 1, 2.
\] (4.14)

It is noticed that if \( \Delta(\eta) \) vanishes at a certain \( \eta \neq 0 \), then the wave of the form (4.5) satisfies this boundary condition. In another word, the MBC (4.11) reproduces exactly the correct amount of physical reflection across the boundary. Notice that the complex equation \( \Delta(\eta) = 0 \) gives rise to two pairs of linear equations on \( a_j, b_j, c_j, d_j \) in general. We therefore can only afford finite many wave numbers to be precisely resolved. The more atoms we include, the more wave numbers we can accommodate. There is then a trade-off between cost and accuracy. This generalizes the matching boundary condition construction in [13].

In the MBC (4.11), we propose to determine the coefficients by requiring
\[
\Delta(\eta) = \mathcal{O}(\eta^3), \quad \Delta(\eta^*) = 0.
\] (4.15)

Here \( \eta^* \) is chosen empirically. We recommend to select it according to the geometry, or the group velocity, or the initial data. The real and imaginary parts of the above conditions lead to eight linear equations, which uniquely determine the parameters in the proposed MBC.

To illustrate the effectiveness of an MBC, we consider the reflection coefficient for the reduced system.

Notice that for a slowly varying wavetrain \( u(x, t) \sim Ae^{i(\omega t + kx)} \), the average energy density \( \mathcal{E} \sim |A|^2 \), and the average energy flux density \( \mathcal{F} \sim \omega'(k) \mathcal{E} \) [14]. Accordingly, we let
\[
|R(\eta)|^2 = \frac{|R_1(\eta)|^2 |v(\eta_1)| + |R_3(\eta)|^2 |v(\eta_3)|}{|v(\eta)|}.
\] (4.16)

Because we consider incident waves from top to bottom, they admit wave numbers with negative group velocity. Further more, for \( |z_3| < 1 \), reflected surface modes do not propagate, hence correspondingly \( v_3 = 0 \). In terms of the original atomic dynamics, they are the Rayleigh waves [3].

While the physical reflection is given by (4.16), numerical reflection under MBC (4.11) is expected to approximate the physical one.

To better illustrate MBC, we consider a specific case with \( h_1 = 1.2, h_2 = 1, h_3 = 1, \xi = \pi/5 \) again. We require \( \Delta(0) = 0, \Delta'(0) = 0, \text{Re} (\Delta''(0)) = 0 \), and pick \( \eta^* = -\arctan 1/2 \). By solving these linear equations, we determine all coefficients as follows
\[
c_{-2} = 1, \quad d_{-2} = -6.824792826237971, \\
c_{-1} = 10.026745875570885, \quad d_{-1} = -5.509562906975846, \\
c_0 = -3.353089371187660, \quad d_0 = 22.618777135973342, \\
c_1 = 5.636379265513604, \quad d_1 = -8.763689070105501, \\
a_{-1} = 1, \quad b_{-1} = -3.19679715575866, \\
a_0 = -1.15802334198124, \quad b_0 = 4.277583919456105, \\
a_1 = 3.511775793592538, \quad b_1 = -0.264246928363208, \\
a_2 = -0.984400830864901, \quad b_2 = -0.451823229996202. \]

(4.17)
Reflection analysis result is displayed in Fig. 5. For reference, we plot also the dispersion relation (dash-dotted line). The physical reflection is shown by solid line. Incident wave number ranges between $-1.747$ to $0.1194$, and $1.813$ to $2.953$. At each end of these two intervals, group velocity is 0. It is not surprising that the reflection coefficient is 1 there, as the wave propagation direction vanishes. For $\eta$ between $-1.747$ to $-1.225$, the reflection maintains a high level. As a matter of fact, our choice of $\xi = \pi/5$ implies that when $\eta = -\sqrt{5}\xi \approx -1.405$, wave vector is perpendicular to horizontal line, and total reflection occurs. There is also a relatively smaller spike at $\xi = -0.7571$ where the group velocity of one of the reflected wave is 0. Similarly, one of the reflected wave propagation direction vanishes.

The MBC reflection is plotted by dashed line. In the long wave limit, namely, for small $\eta$, it agrees very well with the physical one. There is an intersection point of the two curves at $\eta^* = -\arctan 1/2 \approx -0.464$. This is the position where we enforce agreement. MBC reflection is relatively smaller in $[-1.747, -0.7571]$. Moreover, it is bigger than 1 in the short wave interval $[1.813, 2.953]$. In designing MBC in (4.11) with 4 layers, we do not have enough freedom to control this part of waves. Nevertheless, our numerical experiments do not incur instability. This might be explained from a previous analysis on linear boundary conditions in [7].

5 Numerical tests

In the following, we take $h_1 = 1.2$, $h_2 = 1$, $h_3 = 1$, $\xi = \pi/5$ and simulate under initial data
The boundary at \( n = -1000 \) and \( n = 1000 \) are not specially treated, as the wave does not reach the boundary by \( t = 220 \). In Fig. 6, we plot a part of \( u_{m,n}(t) = \text{Re}(U_n(t)e^{im\pi/5}) \) for \( 0 \leq m \leq 20, -100 \leq n \leq 400 \). At \( t = 80 \) in subplot (b), the wave profile splits and one wave front is close to the twin boundary. Then at \( t = 150 \) in subplot (c), it goes across the twin boundary, partially reflected. At \( t = 220 \), most parts of the reflected wave leave the boundary with some residual, seemingly of higher wave numbers. Notice that the group velocity is smaller for such waves, we further plot \( |U_n(t)| \) in Fig. 7 to show the wave propagation in an amplitude manner.

Then we present the THK results with \( n = -4, \cdots, 1000 \). We depict several snapshots in Fig. 8. Comparing with the reference solution in Fig. 6, the approximation of wave propagation and reflection are quite good. Because it offers an exact boundary treatment,
numerical errors arise only from the ODE solver. The amplitude of $U_n(t)$ is shown in Fig. 9, which agrees with the reference solution in Fig. 7. A more careful comparison of $|U_n(t)|$ is shown in Fig. 10, showing a minor deviation near the twin boundary.
Next, we show the MBC results with $n = -2, \cdots, 1000$. We depict several snap shots in Fig. 11. Comparing with the reference solution in Fig. 6, the approximation of wave propagation and reflection are also quite good. The amplitude of $U_n(t)$ is displayed in Fig. 12, which agrees with the reference solution in Fig. 7. A more careful comparison of $|U_n(t)|$ is shown in Fig. 13, where we see again a minor deviation near the twin boundary.

If we select $\eta^* = -0.395$ according to the biggest group velocity, we can get another sets of coefficients. Wave propagation simulation comparison is shown in Fig. 14.

To compare THK and MBC, we devise the following two metrics.

$$
\varepsilon_1 = \left( \frac{\sum_{n=0}^{200} (|U_{n}^{ref}(220)| - |U_{n}^{num}(220)|)^2}{\sum_{n=0}^{200} |U_{n}^{ref}(220)|^2} \right)^{\frac{1}{2}},
$$

(5.2)
Figure 11: Wave propagation simulation with MBC: (a) $u_{m,n}(0)$; (b) $u_{m,n}(80)$; (c) $u_{m,n}(150)$; (d) $u_{m,n}(220)$.

Figure 12: Wave propagation simulation with MBC: amplitude of $U_n(t)$.

$$\varepsilon_2 = \left( \frac{\sum_{t=100}^{220} (|U_3^{ref}(t)| - |U_3^{num}(t)|)^2}{\sum_{t=100}^{220} |U_3^{ref}(t)|^2} \right)^{\frac{1}{2}}.$$  \hspace{1cm} (5.3)

Here $U_n^{ref}(t)$ is the reference solution, and $U_n^{num}(t)$ is the numerical solution with THK or
Figure 13: Wave propagation simulation comparison between MBC and reference solution: $|U_n(220)|$ (left) and $|U_3(t)|$ (right).

Figure 14: Wave propagation simulation comparison between MBC ($\eta^*$ is selected according to group velocity) and reference solution: $|U_n(220)|$ (left) and $|U_3(t)|$ (right).

Table 1: Comparison between time history kernel and matching boundary conditions.

<table>
<thead>
<tr>
<th>Boundary conditions</th>
<th>$\Delta t = 0.05$</th>
<th>$\Delta t = 0.01$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPU time</td>
<td>THK</td>
<td>MBC</td>
</tr>
<tr>
<td></td>
<td>549.7s</td>
<td>8.3s</td>
</tr>
<tr>
<td>$\epsilon_1$</td>
<td>4.37%</td>
<td>6.43%</td>
</tr>
<tr>
<td>$\epsilon_2$</td>
<td>1.56%</td>
<td>4.99%</td>
</tr>
</tbody>
</table>

MBC. We choose the terminal time $T = 220$ and atom $n = 3$ near the boundary to define the errors, respectively. The results are shown in Table 1. Furthermore, we perform the same computation with another time step size $\Delta t = 0.01$ ($\delta t = \Delta t/25 = 0.004$ is adopted to compute the kernel functions) to illustrate the numerical convergence.

As shown in Table 1, THK attains a higher accuracy than MBC. This is well expected, as in the design of MBC, we only control a few wave numbers. But waves with other
group velocity also hit the boundary and reflect as time elapses. We remark that the choice of controlled wave number influences the accuracy of MBC. If not appropriately chosen, numerical simulations may even diverge.

On the other hand, the accuracy improves if a smaller time step size is taken. As mentioned above, numerical error in THK arises only from the ODE solver. It can be driven toward zero with enough computational effort. For MBC, however, we can not control all wave numbers. As a result, for a given MBC, the error approaches to a certain level instead, even the time step size decreases. In fact, the reflection coefficient analysis may help understanding the asymptotes.

There is a trade-off between accuracy and numerical cost. In THK, the kernel functions and boundary displacements are computed with convolutions, which are numerically expensive. In MBC, the coefficients are calculated from the linear algebraic system, and the boundary displacements/velocities are computed with linear relations. Thus MBC is numerically more efficient than THK, which we observe from the computing time directly from afore-mentioned numerical tests.

6 Conclusion

In summary, we have proposed accurate numerical boundary conditions for twin lattices. On the one hand, THK treatment is developed using Laplace transform. On the other hand, we design effective MBC. When wave hits the twin boundary, reflection occurs at different wave numbers simultaneously. We formulate the entire wave field by analyzing the physical process. By matching the residual functions at the long wave limit, and a specific wave number, we obtain matching boundary conditions which reproduce the physical reflections to decent accuracy. The accuracy may be further improved at the cost of more layers of atoms. The design is arduous and routinary, extensible to more general lattices and in higher space dimensions. In this way, we successfully treat the system with heterogeneity and non-nearest neighboring interaction. We verify the effectiveness by reflection analysis. Finally, we illustrate the effectiveness of THK treatment and MBC with numerical tests, compared with the reference solution.

Atomic simulations for heterogeneous structures have many applications. The method used in twin lattices may provide clues in the design of effective boundary treatments in those specific applications, including plasticity [5,6].

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Appendix

A.1 Time history kernel

For an atomic chain with non-nearest neighboring interaction, the translational symmetry asserts that the kernel function expression takes the same form for each atom. This may be shown by the following argument for infinite series.

For a series satisfying the recursive relation

\[ ax_{n-2} + bx_{n-1} + cx_n + dx_{n+1} + ex_{n+2} = 0, \]  
(A.1)

we may reformulate it in a pairwise manner

\[
\begin{bmatrix}
  a & b \\
  0 & a
\end{bmatrix}
\begin{bmatrix}
  x_{2n-2} \\
  x_{2n-1}
\end{bmatrix}
+ \begin{bmatrix}
  c & d \\
  b & c
\end{bmatrix}
\begin{bmatrix}
  x_{2n} \\
  x_{2n+1}
\end{bmatrix}
+ \begin{bmatrix}
  e & 0 \\
  d & e
\end{bmatrix}
\begin{bmatrix}
  x_{2n+2} \\
  x_{2n+3}
\end{bmatrix} = 0. \]
(A.2)

This may be regarded as a nearest-neighboring interaction for a diatomic-molecular chain. If a unidirectional relation holds

\[
\begin{bmatrix}
  x_{2n} \\
  x_{2n+1}
\end{bmatrix} = \begin{bmatrix}
  A & B \\
  C & D
\end{bmatrix}\begin{bmatrix}
  x_{2n-2} \\
  x_{2n-1}
\end{bmatrix}, \]  
(A.3)

we may obtain a matrix equation for the entries A, B, C and D as follows

\[
\begin{bmatrix}
  a & b \\
  0 & a
\end{bmatrix} + \begin{bmatrix}
  c & d \\
  b & c
\end{bmatrix}\begin{bmatrix}
  A & B \\
  C & D
\end{bmatrix} + \begin{bmatrix}
  e & 0 \\
  d & e
\end{bmatrix}\begin{bmatrix}
  A & B \\
  C & D
\end{bmatrix}^2 = 0. \]  
(A.4)

In general, these two equations require

\[ C = AB, \quad D = A + B^2. \]  
(A.5)

They agree with the unidirectional relation

\[ u_{2n+1} = Au_{2n-1} + Bu_{2n} = Au_{2n-2} + B(Au_{2n-2} + Bu_{2n-1}) = ABu_{2n-2} + (A + B^2)u_{2n-1}. \]  
(A.6)

A.2 Matching boundary conditions

Let \( V = [T_1 T_3 V_0 R_1 R_3]^T \), then the residual function

\[ \Delta(\eta) = DX = e^{-i\omega t}D(\beta V + d) = e^{-i\omega t}D(-A(BA)^{-1}Bd + d). \]  
(A.7)

At some particular wave number \( \xi = \xi^* \), the determinant of \( BA \) may be 0. We recommend to use polynomial division to get perturbation terms. According to the Cramer’s rule, \( V \) can be expressed as

\[ V = f(z, z_1, z_2, \omega) g(z, z_1, z_2, \omega), \]  
(A.8)
According to perturbation method, we can get

\[
V_0 + V_1 \eta + V_2 \eta^2 + \cdots = \frac{f_0 + f_1 \eta + f_2 \eta^2 + \cdots}{g_0 + g_1 \eta + g_2 \eta^2 + \cdots}
\]
\[
= \frac{f_0}{g_0} + \left( \frac{f_1}{g_0} - \frac{g_1 f_0}{g_0 g_0} \right) \eta + \left( \frac{f_2}{g_0} - \frac{g_2 f_0}{g_0 g_0} - \frac{g_1 f_1}{g_0 g_0} + \frac{g_1 g_2 f_0}{g_0 g_0} \right) \eta^2 + \cdots. \tag{A.9}
\]

If \(f_0 = 0\) and \(g_0 = 0\), then

\[
V_0 + V_1 \eta + V_2 \eta^2 + \cdots = \frac{f_0 + f_1 \eta + f_2 \eta^2 + \cdots}{g_0 + g_1 \eta + g_2 \eta^2 + \cdots}
\]
\[
= \frac{f_1 + f_2 \eta + f_3 \eta^2 + \cdots}{g_1 + g_2 \eta + g_3 \eta^2 + \cdots}
\]
\[
= \frac{f_1}{g_1} + \left( \frac{f_2}{g_1} - \frac{g_2 f_1}{g_1 g_1} \right) \eta + \left( \frac{f_3}{g_1} - \frac{g_3 f_1}{g_1 g_1} - \frac{g_2 f_2}{g_1 g_1} + \frac{g_2 g_3 f_1}{g_1 g_1} \right) \eta^2 + \cdots. \tag{A.10}
\]

**A.3 Reflection coefficient**

Under the condition of \(h_1 = 1.2\), \(h_2 = 1\), \(h_3 = 1\), \(\xi = \pi/5\), reflection coefficient defined with average energy flux density is shown in (4.16). We can also define transmission coefficient

\[
|T(\eta)|^2 = \frac{|T_1(\eta)|^2 |v_1(-\eta_1)| + |T_3(\eta)|^2 |v_1(-\eta_3)|}{|v(\eta)|},
\]
where $v_l$ is the group velocity of lower lattice, and it holds that
\[ v_l(-\eta) = v(\eta). \] (A.12)

According to the conservation law of energy, we have $|R|^2 + |T|^2 = 1$, and numerically verified in Fig. 15.

References