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Accurate Boundary Conditions for Twin Boundary

Shaoqiang Tang[1,*] and Xi Zhu[1]

[1] *HEDPS and LTCS, College of Engineering, Peking University, Beijing 100871, China.*

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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

*Corresponding author. *Email addresses:* maotang@pku.edu.cn (S. Tang), zhuxi@pku.edu.cn (X. Zhu)

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 even), atoms are labeled in horizontal direction with even indices (m 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)

$$\begin{aligned} m_a\ddot{u}_{m,n} =& -\partial_{u_{m,n}}V(u_{m,n}-u_{m,n+2},h_a)-\partial_{u_{m,n}}V(u_{m,n}-u_{m-1,n+1},h_a)\\ &-\partial_{u_{m,n}}V(u_{m,n}-u_{m+1,n-1},h_a)-\partial_{u_{m,n}}V(u_{m,n}-u_{m,n-2},h_a),\quad n\geq 3. \end{aligned} \tag{2.1}$$

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

$$m_a\ddot{u}_{m,n}=k(u_{m,n+2}+u_{m-1,n+1}-4u_{m,n}+u_{m+1,n-1}+u_{m,n-2}),\quad n\geq 3. \tag{2.2}$$