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Matching Boundary Conditions for Scalar Waves in Body-Centered-Cubic Lattices

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Abstract. Matching boundary conditions (MBC's) are proposed to treat scalar waves in the body-centered-cubic lattices. By matching the dispersion relation, we construct MBC's for normal incidence and incidence with an angle α. Multiplication of MBC operators then leads to multi-directional absorbing boundary conditions. The effectiveness are illustrated by the reflection coefficient analysis and wave packet tests. In particular, the designed M1M1 treats the scalar waves in a satisfactory manner.

AMS subject classifications: 65Z05, 70-08

Key words: Body-centered-cubic (BCC) crystalline solids, dispersion relation, matching boundary condition, reflection coefficient, scalar waves.

1 Introduction

Atomic simulations play an increasingly important role in exploring fundamental issues of materials science and their applications to micro, nano and multiscale physics for emerging technologies [21]. In such simulations, artificial boundary treatment is one of the core techniques to avoid non-physical results due to spurious reflections [29]. Due to the discrete features and dispersion [13, 30], artificial boundary conditions [2, 6, 10, 14] developed for continuous wave propagation problems can not be adopted directly here.

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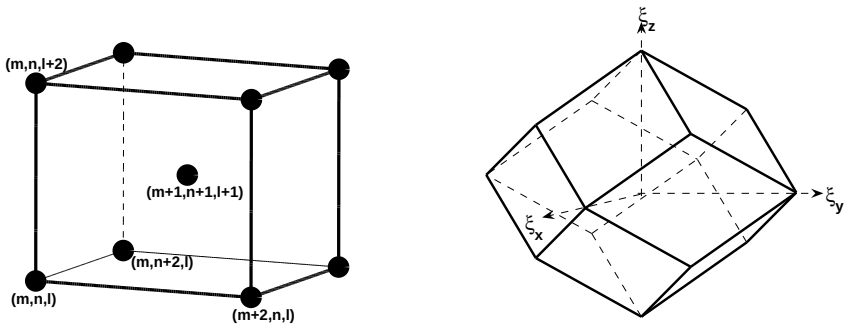

Figure 1: Unit cell (left) and first Brillouin zone (right) of BCC lattice.

Therefore effective absorbing boundary conditions are demanded to suppress effectively the reflections in atomic simulations.

In this paper, we consider a body-centered-cubic (BCC) lattice. As shown in Fig. 1, its unit cell has one lattice point in the center in addition to eight corner points. Many metals, such as Li, Na, K, Rb, W, Cs and Fe, take the BCC structure.

The simplest boundary condition for numerical simulations is the periodic boundary condition [4, 5, 7, 12, 16, 35]. As periodicity does not hold in most applications that require multiscale simulations, other boundary treatments have been developed for the BCC lattice. For instance, a flexible boundary condition was developed for simulating dislocations [25–27]. It is an iterative method using the superposition of Green's functions computed for plenty of atoms. Along this line, exact lattice Green's function may be computed for a semi-infinite lattice, leading to the time history kernel treatment and the bridging scale method [8, 15, 23, 24]. However, for the three dimensional BCC lattice, the calculation of the kernel functions is complicated, involving the inverse Laplace transforms and the Fourier transforms. Furthermore, the trade-off of the convolution cut-off time and the accuracy should be made according to specific applications. We also notice that a discrete boundary treatment was developed in terms of variational boundary conditions [17,18]. It considerably reduces the computing cost. Yet the design of such conditions requires to solve an optimization problem, which is time-step dependent and complicated for the three dimensional lattice.

As an alternative, matching boundary conditions (MBC's) were proposed recently [32–34]. Such conditions take the form of linear combinations of displacements and velocities at selected atoms near the artificial boundary. The combination coefficients are determined by matching the dispersion relation. MBC's perform very well in one-dimensional monoatomic chains, one-dimensional diatomic chains, two-dimensional square lattices and two-dimensional hexagonal lattices. Simplicity and essentially no additional computing load are the two major advantages for this class of boundary conditions.

In this paper, we extend the MBC's to treat scalar waves in the BCC lattice. By