CAUCHY-BORN RULE AND THE STABILITY OF CRYSTALLINE SOLIDS: DYNAMIC PROBLEMS

WEINAN E AND PINGBING MING

Abstract. We study continuum and atomistic models for the elastodynamics of crystalline solids at zero temperature. We establish sharp criterion for the regime of validity of the nonlinear elastic wave equations derived from the well-known Cauchy-Born rule.

1. Introduction

This is the second of a series papers devoted to a mathematical study of the Cauchy-Born rule [7, 4, 5, 12], which establishes a connection between atomistic and the continuum models of crystalline solids. The Cauchy-Born rule is the most fundamental hypothesis in the molecular theory of crystal elasticity. Cauchy derived the expression of elastic moduli from pairwise atomistic potentials and the well-known Cauchy relations [29, 18]. In the context of elasticity theory for crystalline solids, there are extensive discussions on the validity of the Cauchy-Born rule. These discussions are mainly based on the underlying lattice symmetry, see [12, 23, 25, 34, 35] and the references therein. In the mathematics literature, Braides, Dal Maso and Garroni [6] studied an atomistic model with pairwise potential and proved it converges to a continuum model using the concept of $\Gamma-$convergence. Blanc, Le Bris and Lions made the assumption that the microscopic displacement of the atoms follows a smooth macroscopic displacement field, and derived, in the continuum limit, expressions for both the bulk and surface energies from atomistic models [3]. Their leading order bulk energy term is given by the Cauchy-Born rule. Friesecke and Theil [13] examined a special two-dimensional mass-spring model. By extending the work on convexity for continuous functionals to discrete models, they succeeded in proving that in certain parameter regimes, the Cauchy-Born rule does give the energy of the global minimizer in the thermodynamic limit. They also identified parameter regimes for which this statement fails and they interpreted this as being the failure of the Cauchy-Born rule. More recently, Conti, Dolzmann, Kirchheim and Müller [8] generalized the results of Friesecke and Theil to an $n-$dimensional mass-spring model.

In the first paper [11] of this series, we focused on the static problem. The main result is that if a stability condition, expressed in terms of the spectra of the dynamical matrix associated with the atomistic model, is satisfied, then continuum model given by the Cauchy-Born rule has a classical local minimizer, and the atomistic model has a local minimizer nearby. This result was established for general crystal structures, including complex lattices. We note that even though the stability conditions are linear in nature, the results we established are optimal in

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the sense that if the stability condition is violated, then either crystal defects develop in which case the material exits the elastic regime, or phase transformation occurs in which case the crystal structure changes and hence the Cauchy-Born rule has to be reformulated. In fact, from a philosophical viewpoint, the main result of [11] is to establish an interplay between Cauchy-Born elasticity and the stability of crystals. This is displayed more clearly in the present paper which focuses on the dynamic case and identifies sharp conditions on how the material exits dynamically the regime of Cauchy-Born elasticity. From a technical viewpoint, our approach is to view the atomistic model as a finite difference scheme for the continuum model given by the Cauchy-Born rule, and follows the general strategy established in Strang's proof of convergence of finite difference schemes for nonlinear partial differential equations [30]. The key components of that proof are stability of the linearized problem and asymptotic analysis of the finite difference schemes. These are indeed the main technical issues handled in [11] for general complex lattices. From this viewpoint, the difference between the results proved in [3] and [11] is that [3] proves consistency, whereas [11] proves convergence. The origin of this difference is stability. Indeed [11] gives counterexamples for which the results of [3] are valid but the Cauchy-Born elastic model is not valid, due to the fact that the crystal structure is unstable.

The present paper follows the strategy established in [11]. We will consider the molecular dynamic models at zero temperature on one hand, and the nonlinear elastodynamics models obtained from the Cauchy-Born rule on the other. The main conclusion is that as long as the deformation gradient stays inside the stability region, then the solutions of the two models are close to each other. We will give sharp conditions that characterize this stability region in the space of deformation gradients (or displacement gradients). In subsequent papers [33, 17], we will give a detailed classification of what happens when the material system exits this stability region: what kind of instability develops and how does it evolve subsequently?

2. Preliminaries

2.1. **Some prerequisites.** We first establish several prerequisites which are needed for understanding the main results of the present paper: the atomistic model, the crystal lattice, the Cauchy-Born rule, and the phonon analysis. Below we will give a very quick summary of these ingredients. More detailed discussion can be found in standard textbooks for solid state physics (see for example [2]).

Atoms in a crystal are usually arranged on the sites of some lattice. We will denote the lattice by L. Lattices are divided into simple and complex lattices ($\nu+1-$lattices in the terminology of [24]). A complex lattice can be viewed as the union of congruent simple lattices. For simplicity, we will restrict ourselves to the situation when the complex lattice is the union of two congruent simple lattices and we will denote by $\boldsymbol{p}_0$ the shift between the two congruent lattices for the undeformed configuration.

We will consider only classical models, in which the interaction between atoms are described by an atomistic potential, which usually takes the following form:

$$V(\boldsymbol{y}_1,\dots,\boldsymbol{y}_N)=\sum_{i,j}V_2(\boldsymbol{y}_i/\varepsilon,\boldsymbol{y}_j/\varepsilon)+\sum_{i,j,k}V_3(\boldsymbol{y}_i/\varepsilon,\boldsymbol{y}_j/\varepsilon,\boldsymbol{y}_k/\varepsilon)+\dots, \tag{2.1}$$

where ε is the lattice constant, $\boldsymbol{y}_i$ is the deformed position of i^{th} atom. Throughout this paper, we will make the following assumptions on the potential function V.

(1) V is translation invariant.
(2) V is invariant with respect to rigid-body motion.
(3) V is smooth in a neighborhood of the equilibrium state.

(4) V has a finite range and the right hand side of (2.1) has finite number of terms.

Several interesting conclusions follow from these assumptions. For example, by translation invariance, we may fix one atom at the origin and all other atoms can be viewed as translation of the origin. To be more precise, we write $V_2(\mathbf{0}, \boldsymbol{s}) = V_2(\boldsymbol{s})$ and $V_3(\mathbf{0}, \boldsymbol{s}_1, \boldsymbol{s}_2) = V_3(\boldsymbol{s}_1, \boldsymbol{s}_2)$. We assume that V is zero if one of the $\boldsymbol{s}_i$ is zero. Usually, $(\boldsymbol{s}_1, \ldots, \boldsymbol{s}_d)$ is a fixed basis for the lattice. We refer to [11] for the discussion of other assumptions. Similar discussions can also be found in [15] and [26, §3]

Cauchy-Born rule is the standard recipe for computing the stored energy function W in the continuum model of solids from the atomistic potential V. We will denote such stored energy function by W_{CB}. For simple lattices, given a $d \times d$ matrix A, $W_{\mathrm{CB}}(\mathsf{A})$ is computed by first deforming an infinite crystal uniformly with displacement gradient A, and then setting $W_{\mathrm{CB}}(\mathsf{A})$ to be the energy density of the deformed unit cell. For example, for a three-body potential, we have

$$W_{\mathrm{CB}}(\mathsf{A}) = \frac{1}{\vartheta_0} \sum_{\langle \boldsymbol{s}_1, \boldsymbol{s}_2 \rangle} \frac{1}{3!} V_3\big((\mathsf{1} + \mathsf{A})\boldsymbol{s}_1, (\mathsf{1} + \mathsf{A})\boldsymbol{s}_2\big), \tag{2.2}$$

where ϑ_0 is the volume of the unit cell, and $\boldsymbol{s}_1, \boldsymbol{s}_2$ run over the range of V_3.

For complex lattices, we first deform one of the Bravais sublattice uniformly with displacement gradient A. We then relax the shift vector $\boldsymbol{p}$ for the other Bravais sublattice, keeping the position of the deformed Bravais sublattice fixed, namely,

$$W_{\mathrm{CB}}(\mathsf{A}) = \min_{\boldsymbol{p}} W(\mathsf{A}, \boldsymbol{p}),$$

where, assuming a three-body potential,

$$W(\mathsf{A}, \boldsymbol{p}) = \lim_{m \to \infty} \frac{1}{|\, mD \,|} \sum V_3(\boldsymbol{y}_i + z_i \boldsymbol{p}, \boldsymbol{y}_j + z_j \boldsymbol{p}).$$

Here the summation is carried out for $\boldsymbol{y}_i, \boldsymbol{y}_j \in (\mathsf{1} + \mathsf{A})L \cap mD$ and $z_i, z_j = 0, 1$, D is the unit cube.

Given any stored energy function W_{CB} and the displacement gradient A, the elastic stiffness tensor C [18, 32] at A may be expressed as

$$\mathsf{C}_{\alpha\beta\gamma\delta}(\mathsf{A}) = \frac{\partial^2 W_{\mathrm{CB}}}{\partial \mathsf{A}_{\alpha\gamma} \partial \mathsf{A}_{\beta\delta}}(\mathsf{A}) \qquad \alpha, \beta, \gamma, \delta = 1, \ldots, d.$$

A lot can be learned about the lattice statics and lattice dynamics from the phonon analysis, which is the discrete Fourier analysis of lattice waves at the equilibrium or uniformly deformed state. This is standard textbook material on solid state physics (e.g. [31] and [2]). Since we need to establish some terminologies, we will briefly discuss a simple example of a one-dimensional chain.

Consider the following example:

$$M \frac{d^2 y_j}{dt^2} = -\frac{\partial V}{\partial y_j} = V'(y_{j+1} - y_j) - V'(y_j - y_{j-1}),$$

where M is the mass of the atom. Let $y_j = j\varepsilon + \widetilde{y}_j$, linearizing the above equation, we get

$$M \frac{d^2 \widetilde{y}_j}{dt^2} = V''(\varepsilon)(\widetilde{y}_{j+1} - 2\widetilde{y}_j + \widetilde{y}_{j-1}). \tag{2.3}$$

Let $\widetilde{y}_j(k) = e^{i(k\, x_j - \omega\, t)}$, we obtain

$$\omega^2(k) = \frac{4}{M} V''(\varepsilon) \sin^2 \frac{k\varepsilon}{2},$$

where $k=\frac{2\pi\ell}{N\varepsilon}$ with $\ell=-[N/2],\dots,[N/2]$.

For the more general case, it is useful to define the reciprocal lattice $\widehat{L}$, which is the lattice of points in the k-space that satisfy $e^{i\,k\cdot\,x_j}=1$ for all $x_j\in L$. The first Brillouin zone in the k-space is defined to be the subset of points that are closer to the origin than to any other point on the reciprocal lattice [2].

$$\Gamma_L=\{\,\boldsymbol{x}\in\widehat{L}\mid\|\,\boldsymbol{x}\,\|_{\ell_2}<\|\,\boldsymbol{x}-\boldsymbol{y}\,\|_{\ell_2}\quad\forall\boldsymbol{y}\in\widehat{L}\,\},$$

where $\|\cdot\|_{\ell_2}$ is the ℓ_2 norm of a vector.

For complex lattices, the phonon spectrum contains both acoustic and optical branches [2], which will be denoted by $\omega^a_{\mathsf{A}}(\boldsymbol{k})$ and $\omega^o_{\mathsf{A}}(\boldsymbol{k})$ respectively at any given deformation gradient A. At the equilibrium state ($\mathsf{A}=\mathbf{0}$), we simply denote by $\omega_a(k)$ and $\omega_o(k)$ the acoustic and optical branches of the phonon spectrum. We refer to [31] for the definition of phonon spectrum for these general cases.

2.2. **Notation.** For any nonnegative integer m, we denote by $H^m(\mathbb{R}^d;\mathbb{R}^d)$ the Sobolev space of mappings $\boldsymbol{y}$: $\mathbb{R}^d\to\mathbb{R}^d$ such that $\|\boldsymbol{y}\|_{H^m}<\infty$ (see [1] for the definition). We write $H^1(\mathbb{R}^d)$ for $H^1(\mathbb{R}^d;\mathbb{R}^1)$. For any Banach space U with norm $\|\cdot\|_U$, the space $L^2(0,T;U)$ consists of all measurable functions $\boldsymbol{v}:[0,T]\to U$ with

$$\|\boldsymbol{v}\|_{L^2(0,T;U)}=\Big(\int_0^T\|\boldsymbol{v}(t)\|_U^2\,\mathrm{d}\,t\Big)^{1/2}.$$

The space $H^m(0,T;U)$ consists of all functions $d^k\boldsymbol{v}/dt^k\in L^2(0,T;U)$ for $k=0,\dots,m$, which is equipped with the norm

$$\|\boldsymbol{v}\|_{H^m(0,T;U)}=\Big(\int_0^T\sum_{k=0}^m\|d^k\boldsymbol{v}/dt^k\|_U^2\,\mathrm{d}\,t\Big)^{1/2}.$$

The space $C([0,T];U)$ contains all continuous functions $\boldsymbol{v}:[0,T]\to U$ with

$$\|\boldsymbol{v}\|_{C([0,T];U)}=\max_{t\in[0,T]}\|\boldsymbol{v}(t)\|_U.$$

Summation convention will be used. We will use $|\cdot|$ to denote the absolute value of a scalar quantity, the Euclidean norm of a vector and the volume of a set. In several places we denote by $\|\cdot\|_{\ell_2}$ the ℓ_2 norm of a vector to avoid confusion. For any $\boldsymbol{z}\in\mathbb{R}^{N\times d}$ excluding the constant vector, we define $\|\,\boldsymbol{z}\,\|_d=\varepsilon^{d/2}\big(\boldsymbol{z}^T\mathsf{H}_0\boldsymbol{z}\big)^{1/2}$ with H_0 the Hessian matrix of the atomistic potential V at the undeformed state. For any $\boldsymbol{x}_i\in\mathbb{R}^d$, we let

$$D^+_\ell\boldsymbol{x}_i=\boldsymbol{x}_{i+\boldsymbol{s}_\ell}-\boldsymbol{x}_i,\qquad D^-_\ell\boldsymbol{x}_i=\boldsymbol{x}_i-\boldsymbol{x}_{i-\boldsymbol{s}_\ell}\qquad\text{for}\quad\ell=1,2,\dots,d.$$

We denote by $D\boldsymbol{x}_i=(D^+_\ell\boldsymbol{x}_i,D^-_\ell\boldsymbol{x}_i)$ for $\ell=1,2,\dots,d$.

For a vector $\boldsymbol{v}$, $\nabla\boldsymbol{v}$ is the tensor with components $(\nabla\boldsymbol{v})_{ij}=\partial_jv_i$; for a tensor field S, $\operatorname{div}\mathsf{S}$ is the vector with components ∂_jS_{ij}. Given any function y: $\mathbb{R}^{d\times d}\to\mathbb{R}$, we define

$$D_{\mathsf{A}}y(\mathsf{A})=\Big(\frac{\partial y}{\partial\mathsf{A}_{ij}}\Big)\quad\text{and}\quad D^2_{\mathsf{A}}y(\mathsf{A})=\Big(\frac{\partial^2y}{\partial\mathsf{A}_{ij}\partial\mathsf{A}_{kl}}\Big),$$

where $\mathbb{R}^{d\times d}$ denotes the set of real $d\times d$ matrices. For a matrix $\mathsf{A}=\{\mathsf{A}_{ij}\}\in\mathbb{R}^{d\times d}$, we define the norm $\|\mathsf{A}\|=\big(\sum_{i=1}^d\sum_{j=1}^d\mathsf{A}_{ij}^2\big)^{1/2}$. We denote by $\mathsf{1}_{k\times k}$ the $k\times k$ identity matrix.

We will also use the standard notation $\partial=(\partial_t,\nabla)$, and for any set A, we denote by $\overset{\circ}{A}$ the interior of A.

3. Main Results

A typical problem of interest in elastodynamics is to determine the motion of a solid material when its initial configuration and the initial velocity are known. We will denote by $\boldsymbol{y}$ and $\boldsymbol{x}$ the deformed and undeformed position of a material point respectively. The displacement field $\boldsymbol{u} : \mathbb{R}^d \times [0,T] \to \mathbb{R}^d$ is defined by

$$\boldsymbol{u}(\boldsymbol{x},t) = \boldsymbol{y}(\boldsymbol{x},t) - \boldsymbol{x}.$$

In continuum elasticity, we seek for a function $\boldsymbol{u}$ that satisfies the system

$$\rho\partial_t^2\boldsymbol{u} - \operatorname{div}\big(D_{\mathsf{A}}W_{\mathrm{CB}}(\nabla\boldsymbol{u})\big) = \boldsymbol{0} \quad \text{in} \quad \mathbb{R}^d$$

with the initial conditions

$$\boldsymbol{u}|_{t=0} = \boldsymbol{u}^0, \quad \partial_t\boldsymbol{u}|_{t=0} = \boldsymbol{u}^1,$$

where $\boldsymbol{u}^0, \boldsymbol{u}^1$ are given smooth functions and ρ is the density of the reference configuration. We multiply both sides of the above equation by ϑ_0 to get

$$\begin{cases} m\partial_t^2\boldsymbol{u} - \operatorname{div}\big(D_{\mathsf{A}}(\vartheta_0 W_{\mathrm{CB}})(\nabla\boldsymbol{u})\big) = \boldsymbol{0} & \text{in} \quad \mathbb{R}^d, \\ \boldsymbol{u}|_{t=0} = \boldsymbol{u}^0, \quad \partial_t\boldsymbol{u}|_{t=0} = \boldsymbol{u}^1, \end{cases}$$

where $m = \rho\vartheta_0$. In what follows, we simply denote $\vartheta_0 W_{\mathrm{CB}}$ by W_{CB}.

Turning to the atomistic model, for definiteness, we will only consider the case of complex lattices which are made up of two species of atoms. Extension to more general complex lattices and simple lattices is straightforward. Given a total of $2N$ atoms with equal number of A-specie of atoms with mass m_A and B-specie of atoms with mass m_B, we look for the positions $\boldsymbol{y} = (\boldsymbol{y}^A, \boldsymbol{y}^B)$ of the $2N$ atoms, which satisfy

$$\begin{cases} \mathsf{M}\partial_t^2\boldsymbol{y} + \dfrac{\partial V}{\partial \boldsymbol{y}} = \boldsymbol{0}, \\ \boldsymbol{y}|_{t=0} = \boldsymbol{x} + \boldsymbol{u}^0(\boldsymbol{x}), \quad \partial_t\boldsymbol{y}|_{t=0} = \boldsymbol{u}^1(\boldsymbol{x}), \end{cases} \tag{3.1}$$

where M is the mass matrix that takes the form:

$$\mathsf{M} = \begin{pmatrix} m_A \mathbf{1}_{dN\times dN} & \boldsymbol{0} \\ \boldsymbol{0} & m_B \mathbf{1}_{dN\times dN} \end{pmatrix}.$$

We will let

$$m_{\mathrm{a}} = \frac{1}{2}(m_A + m_B).$$

With this, we can write the continuum model as:

$$\begin{cases} m_{\mathrm{a}}\partial_t^2\boldsymbol{u} - \operatorname{div}\big(D_{\mathsf{A}}W_{\mathrm{CB}}(\nabla\boldsymbol{u})\big) = \boldsymbol{0} & \text{in} \quad \mathbb{R}^d, \\ \boldsymbol{u}|_{t=0} = \boldsymbol{u}^0, \quad \partial_t\boldsymbol{u}|_{t=0} = \boldsymbol{u}^1. \end{cases} \tag{3.2}$$

For complex lattices, it is also useful to consider the following system that describes both the displacement field $\boldsymbol{u}$ and the shift vector field $\boldsymbol{p} : \mathbb{R}^d \times [0,T] \to \mathbb{R}^d$ explicitly:

$$\begin{cases} m_{\mathrm{a}}\partial_t^2\boldsymbol{u} - \operatorname{div}\big(D_{\mathsf{A}}W(\nabla\boldsymbol{u},\boldsymbol{p})\big) = \boldsymbol{0} & \text{in} \quad \mathbb{R}^d, \\ D_{\boldsymbol{p}}W(\nabla\boldsymbol{u},\boldsymbol{p}) = \boldsymbol{0} & \text{in} \quad \mathbb{R}^d, \\ \boldsymbol{u}|_{t=0} = \boldsymbol{u}^0, \quad \partial_t\boldsymbol{u}|_{t=0} = \boldsymbol{u}^1 \end{cases} \tag{3.3}$$

with given smooth functions $\boldsymbol{u}^0, \boldsymbol{u}^1$. The initial condition for $\boldsymbol{p}$ is obtained as follows. By $(3.3)_2$, we may derive formally $\boldsymbol{p}(\boldsymbol{x},t) = \boldsymbol{p}(\nabla\boldsymbol{u}(\boldsymbol{x},t))$, where

$$\boldsymbol{p}(A) = \operatorname*{argmin}_{\boldsymbol{p}} W(\mathsf{A},\boldsymbol{p}),$$

which is obtained by (3.17). Hence, we must have

$$\boldsymbol{p}^0 = \boldsymbol{p}|_{t=0} = \boldsymbol{p}(\nabla \boldsymbol{u}^0). \tag{3.4}$$

Differentiating $(3.3)_2$ with respect to t, we get

$$\frac{\partial^2}{\partial \boldsymbol{p}\,\partial \mathsf{A}} W(\nabla \boldsymbol{u}, p)\nabla \partial_t \boldsymbol{u} + \frac{\partial^2}{\partial \boldsymbol{p}^2} W(\nabla \boldsymbol{u}, \boldsymbol{p})\partial_t \boldsymbol{p} = \boldsymbol{0},$$

which gives the second compatibility condition:

$$\boldsymbol{p}^1 = (\partial_t \boldsymbol{p})|_{t=0} = -\Big[\frac{\partial^2 W}{\partial \boldsymbol{p}^2}\Big]^{-1} \frac{\partial^2 W}{\partial \boldsymbol{p}\,\partial \mathsf{A}}\Big|_{(\nabla \boldsymbol{u}, \boldsymbol{p}) = (\nabla \boldsymbol{u}^0, \boldsymbol{p}^0)} \nabla \boldsymbol{u}^1. \tag{3.5}$$

It follows from (3.4) and (3.5) that the initial data for the shift vector field is completely determined by the initial condition imposed on the displacement field.

It is easy to see that any solution $\boldsymbol{u}$ of (3.3) also solves (3.2). Indeed, using $(3.3)_1$ and $(3.3)_2$, we obtain

$$\begin{aligned} D_{\mathsf{A}} W_{\mathrm{CB}}(\mathsf{A})|_{\mathsf{A}=\nabla \boldsymbol{u}} &= D_{\mathsf{A}} W(\mathsf{A}, \boldsymbol{p}(\mathsf{A}))|_{\mathsf{A}=\nabla \boldsymbol{u}} = (D_{\mathsf{A}} W + D_{\boldsymbol{p}} W)(\mathsf{A}, \boldsymbol{p}(\mathsf{A}))|_{\mathsf{A}=\nabla \boldsymbol{u}} \\ &= D_{\mathsf{A}} W(\nabla \boldsymbol{u}, \boldsymbol{p}(\nabla \boldsymbol{u})). \end{aligned}$$

Let

$$\mathscr{R} = \{\, \mathsf{A} \in \mathbb{R}^{d\times d} \mid \det(\mathsf{1} + \mathsf{A}) > 0 \,\}.$$

We define

$$\lambda(\mathsf{A}) = \min_{\substack{|\boldsymbol{\xi}| = |\boldsymbol{\eta}| = 1 \\ \boldsymbol{\xi}, \boldsymbol{\eta} \in \mathbb{R}^d}} \mathsf{C}(\mathsf{A})(\boldsymbol{\xi} \otimes \boldsymbol{\eta}, \boldsymbol{\xi} \otimes \boldsymbol{\eta}),$$

$$\lambda_1(\mathsf{A}) = \min_{\substack{\boldsymbol{k} \in \Gamma_{\mathsf{A}L} \\ \boldsymbol{k} \neq \boldsymbol{0}}} \frac{\omega_{\mathsf{A}}^a(\boldsymbol{k})}{|\boldsymbol{k}|},$$

and

$$\lambda_2(\mathsf{A}) = \min_{\boldsymbol{k} \in \Gamma_{\mathsf{A}L}} \varepsilon \omega_{\mathsf{A}}^o(\boldsymbol{k}).$$

Given three non-negative constants $\varLambda, \varLambda_1, \varLambda_2$, we define two subsets of $\mathscr{R}$ as

$$\mathscr{O}_1(\varLambda) = \{\, \mathsf{A} \in \mathscr{R} \mid \lambda(\mathsf{A}) > \varLambda \,\}. \tag{3.6}$$

$$\mathscr{O}_2(\varLambda_1, \varLambda_2) = \{\, \mathsf{A} \in \mathscr{R} \mid \lambda_1(\mathsf{A}) > \varLambda_1 \ \ \&\ \ \lambda_2(\mathsf{A}) > \varLambda_2 \,\}. \tag{3.7}$$

For the case when L is a simple lattice, there is only the acoustic branch of the phonon spectrum, the definition of $\mathscr{O}_2$ is changed into

$$\mathscr{O}_2(\varLambda_1) = \{\, \mathsf{A} \in \mathscr{R} \mid \lambda_1(\mathsf{A}) > \varLambda_1 \,\}.$$

Our main results are the following:

Theorem 3.1. *Assume that the initial data* $(\boldsymbol{u}^0, \boldsymbol{u}^1) \in H^{s+1} \times H^s$ *for some integer* $s > d/2 + 1$ *and there exists* $\varLambda > 0$ *such that* $\nabla \boldsymbol{u}^0 \in \mathscr{O}_1(\varLambda)$*. Then there exists* T_1^* $(0 < T_1^* \le \infty)$ *depending on the norm of the initial data, and a unique strong solution* $\boldsymbol{u}_{CB}$ *of* (3.2) *on the time interval* $[0, T_1^*)$ *such that* $\nabla \boldsymbol{u}_{CB}(\cdot, t) \in \mathring{\mathscr{O}}_1(\varLambda_t)$ *for some positive number* $\varLambda_t$*. Moreover,*

$$\boldsymbol{u}_{CB}(\cdot, t) \in C^0\big([0, T_1^*); H^{s+1}\big) \cap C^1\big([0, T_1^*); H^s\big).$$

The interval $[0, T_1^*)$ *is maximal in the sense that if* $T_1^* < \infty$*, then either*

$$\limsup_{t \to T_1^*} \int_0^t \|\partial \nabla \boldsymbol{u}_{CB}(\cdot, \tau)\|_{L^\infty} \mathrm{d}\tau = +\infty \tag{3.8}$$

or

$$\lim_{t\to T_1^*} dist\,(\nabla \boldsymbol{u}_{CB}(\cdot,t), \partial \overset{\circ}{\mathscr{O}}_1(0)) = 0, \tag{3.9}$$

where dist denotes distance between two sets.

To state the corresponding results for the atomistic model, we distinguish the cases when L is a simple lattice or a complex lattice.

Theorem 3.2. *Assume that $\|\boldsymbol{u}^0\|_{H^{s+1}}$ and $\|\boldsymbol{u}^1\|_{H^s}$ are bounded for some integer $s > d/2+6$, and there exist two positive constants Λ and Λ_1 such that $\mathbf{0} \in \mathscr{O}_2(\Lambda_1)$, and $\nabla \boldsymbol{u}^0 \in \mathscr{O}_1(\Lambda) \cap \mathscr{O}_2(\Lambda_1)$. Then there exists $T_2^* (0 < T_2^* \le \infty)$ and a locally unique solution $\boldsymbol{y}^\varepsilon(t)$ of* (3.1) *on the interval $[0, T_2^*)$. The interval $[0, T_2^*)$ is maximal in the sense that if $T_2^* < \infty$, then*

$$\lim_{t\to T_2^*} dist\,(D\boldsymbol{y}^\varepsilon(t), \partial \overset{\circ}{\mathscr{O}}_2(0)) = 0. \tag{3.10}$$

Moreover, let $T^* = T_2^*$, for any δ $(0 < \delta < T^*)$, there exists $C(\delta) > 0$ such that

$$\|\,\boldsymbol{y}^\varepsilon(t) - \boldsymbol{y}_{CB}(t)\,\|_d \le C(\delta)\,\varepsilon \qquad \text{for } \ 0 \le t \le T^* - \delta, \tag{3.11}$$

where $\boldsymbol{y}_{CB}(t) = \boldsymbol{x} + \boldsymbol{u}_{CB}(\boldsymbol{x}, t)$.

For complex lattices, the initial data has to satisfy two compatibility conditions:

$$\|\nabla\big((\boldsymbol{p}_0/\varepsilon\cdot\nabla)\boldsymbol{u}^0 - \boldsymbol{p}^0\big)\|_{L^\infty} \le C\varepsilon, \tag{3.12}$$

$$\|\big(\boldsymbol{p}_0/\varepsilon\cdot\nabla\big)\boldsymbol{u}^1 - \boldsymbol{p}^1\|_{L^\infty} \le C\varepsilon, \tag{3.13}$$

where $\boldsymbol{p}^0$ and $\boldsymbol{p}^1$ are given by (3.4) and (3.5), respectively.

Theorem 3.3. *Assume that the initial data satisfies the compatibility conditions* (3.12) *and* (3.13)*, $\|\boldsymbol{u}^0\|_{H^{s+1}}$ and $\|\boldsymbol{u}^1\|_{H^s}$ are bounded for some integer $s > d/2+6$. Assume also that there exist three positive constants Λ, Λ_1 and Λ_2 such that $\mathbf{0} \in \mathscr{O}_2(\Lambda_1, \Lambda_2)$, and $\nabla \boldsymbol{u}^0 \in \mathscr{O}_1(\Lambda) \cap \mathscr{O}_2(\Lambda_1, \Lambda_2)$. Then there exists $T_2^* (0 < T_2^* \le \infty)$ and a locally unique solution $\boldsymbol{y}^\varepsilon(t)$ of the atomistic model* (3.1) *over the interval $[0, T_2^*)$. The interval $[0, T_2^*)$ is maximal in the sense that if $T_2^* < \infty$ then*

$$\lim_{t\to T_2^*} dist\,(D\boldsymbol{y}^\varepsilon(t), \partial \overset{\circ}{\mathscr{O}}_2(0,0)) = 0. \tag{3.14}$$

Moreover, let $T^* = T_2^*$, for any δ $(0 < \delta < T^*)$, there exists $C(\delta) > 0$ such that

$$\|\,\boldsymbol{y}^\varepsilon(t) - \boldsymbol{y}_{CB}(t)\,\|_d \le C(\delta)\,\varepsilon \qquad \text{for } 0 \le t \le T^* - \delta, \tag{3.15}$$

where $\boldsymbol{y}_{CB}(t) = (\boldsymbol{x}^A + \boldsymbol{u}_{CB}(\boldsymbol{x}^A, t), \boldsymbol{x}^B + \boldsymbol{u}_{CB}(\boldsymbol{x}^B, t))$ with $\boldsymbol{x}^B = \boldsymbol{x}^A + \boldsymbol{p}_0$, and $\{\boldsymbol{x}^A\}$ denotes the equilibrium position for atoms of species A.

A direct consequence of the above theorem is

Corollary 3.4. *Under the same condition of Theorem 3.3, we have*

$$\|\,\boldsymbol{p}^\varepsilon(t) - \boldsymbol{p}_{CB}(t)\,\|_{\ell_2} \le C(\delta)\,\varepsilon^2 \qquad \text{for any } 0 \le t \le T^* - \delta,$$

where $\{\boldsymbol{p}^\varepsilon\}(t) = \{\boldsymbol{y}^\varepsilon\}^B(t) - \{\boldsymbol{y}^\varepsilon\}^A(t)$ and $\boldsymbol{p}_{CB}(t) = \boldsymbol{p}_0 + \boldsymbol{u}_{CB}(\boldsymbol{x}^B, t) - \boldsymbol{u}_{CB}(\boldsymbol{x}^A, t)$.

In this paper, we only prove the case when L is a simple lattice, and leave the case when L is a complex lattice to another paper since the technicalities in that case are much more involved.

If we were to consider the system (3.3), it is more convenient to define $\mathscr{O}_1$ in terms of W as follows: we define

$$\lambda(\mathsf{A},\boldsymbol{p}) = \min_{\substack{|\boldsymbol{\xi}|=|\boldsymbol{\eta}|=|\boldsymbol{\zeta}|=1\\ \boldsymbol{\xi},\boldsymbol{\eta},\boldsymbol{\zeta}\in\mathbb{R}^d}} (\boldsymbol{\xi}\otimes\boldsymbol{\eta},\boldsymbol{\zeta}) D^2W(\mathsf{A},\boldsymbol{p})(\boldsymbol{\xi}\otimes\boldsymbol{\eta},\boldsymbol{\zeta})^T,$$

where

$$D^2W(\mathsf{A},\boldsymbol{p}) = \begin{pmatrix} \dfrac{\partial^2 W}{\partial \mathsf{A}^2} & \dfrac{\partial^2 W}{\partial \mathsf{A}\partial \boldsymbol{p}} \\ \dfrac{\partial^2 W}{\partial \mathsf{A}\partial \boldsymbol{p}} & \dfrac{\partial^2 W}{\partial \boldsymbol{p}^2} \end{pmatrix}.$$

Given a non-negative constant Λ, the set $\mathscr{O}_1$ is defined as

$$\mathscr{O}_1(\Lambda) = \{\, (\mathsf{A},\boldsymbol{p}) \in \mathscr{R}\times\mathbb{R}^d \mid \lambda(\mathsf{A},\boldsymbol{p}) > \Lambda \,\}.$$

If we impose Dirichlet boundary condition on the system (3.2), then the definition of $\mathscr{O}_1$ is the same as (3.6). If we impose Neumann boundary condition or mixed boundary condition on the system (3.2), then we firstly change λ to

$$\widetilde{\lambda}(\mathsf{A}) = \min_{\|\mathsf{B}\|=1,\mathsf{B}\in\mathbb{R}^{d\times d}} \mathsf{C}(\mathsf{A})(\mathsf{B},\mathsf{B}). \tag{3.16}$$

Next, given a non-negative constant Λ, we define

$$\widetilde{\mathscr{O}}_1(\Lambda) = \{\, \mathsf{A}\in\mathscr{R} \mid \widetilde{\lambda}(\mathsf{A}) > \Lambda \,\}.$$

Or, we may define $\widetilde{\mathscr{O}}_1$ in terms of W as

$$\widetilde{\mathscr{O}}_1(\Lambda) = \{\, (\mathsf{A},\boldsymbol{p}) \in \mathscr{R}\times\mathbb{R}^d \mid \widetilde{\lambda}(\mathsf{A},\boldsymbol{p}) > \Lambda \,\},$$

where

$$\widetilde{\lambda}(\mathsf{A},\boldsymbol{p}) = \min_{\substack{\|\mathsf{B}\|=|\boldsymbol{\zeta}|=1\\ \mathsf{B}\in\mathbb{R}^{d\times d},\boldsymbol{\zeta}\in\mathbb{R}^d}} (\mathsf{B},\boldsymbol{\zeta}) D^2W(\mathsf{A},\boldsymbol{p})(\mathsf{B},\boldsymbol{\zeta})^T.$$

We shall give an example in next section to illustrate the difference between $\mathscr{O}_1$ and $\widetilde{\mathscr{O}}_1$.

It follows from the definition of $\mathscr{O}_1$ that for any $(\mathsf{A},\boldsymbol{p})\in\mathscr{O}_1(\Lambda)$, there exists $\Lambda_3>0$ such that

$$\boldsymbol{\zeta}\frac{\partial^2 W}{\partial \boldsymbol{p}^2}(\mathsf{A},\boldsymbol{p})\boldsymbol{\zeta}^T \ge \Lambda_3 \qquad \text{for all } \boldsymbol{\zeta}\in\mathbb{R}^d \text{ with } |\boldsymbol{\zeta}| = 1. \tag{3.17}$$

Note that the shift vector $\boldsymbol{p}$ that solves $(3.3)_2$ is usually not unique. There are several branches of solutions for $\boldsymbol{p}$, Theorem 3.3 is applicable to each branch.

4. Discussions and Explicit Examples

In this section, we will discuss several explicit examples for the stability regions.

4.1. **Stability assumptions.** The results in [11] depend heavily on the stability conditions **Assumption A** and **Assumption B**, which can be formulated in terms of the stability regions $\mathscr{O}_1$ and $\mathscr{O}_2$ as

$$\begin{aligned} &\text{Assumption A holds} \quad \text{if and only if} \quad \mathbf{0} \in \mathscr{O}_2(\Lambda_1, \Lambda_2),\\ &\text{Assumption B holds} \quad \text{if and only if} \quad \mathbf{0} \in \mathscr{O}_1(\Lambda). \end{aligned}$$

for certain positive constants $\Lambda, \Lambda_1, \Lambda_2$. In what follows, we give two examples for the stability assumptions. We first consider a simple one-dimensional chain with the Lennard-Jones potential [16]. As in [11], we have

$$W_{\mathrm{CB}}(A) = \frac{\zeta^2(6)}{\zeta(12)} \left(\frac{1}{4} | 1 + A |^{-12} - \frac{1}{2} | 1 + A |^{-6} \right), \tag{4.1}$$

where ζ is the Riemann-zeta function. Therefore, the continuum problem is

$$\begin{cases} m\, \partial_t^2 u - \dfrac{3\zeta^2(6)}{\zeta(12)} \dfrac{d}{dx} \left(-\Big(1 + \dfrac{du}{dx}\Big)^{-13} + \Big(1 + \dfrac{du}{dx}\Big)^{-7} \right) = 0 \qquad x \in \mathbb{R}, \\ \qquad\qquad\qquad\qquad u|_{t=0} = u^0, \quad \partial_t u|_{t=0} = u^1. \end{cases} \tag{4.2}$$

A straightforward calculation gives that

$$D_A^2 W_{\mathrm{CB}}(0) = 18\zeta^2(6)/\zeta(12) > 0.$$

Therefore, $0 \in \mathscr{O}_1(\Lambda)$ for any $0 < \Lambda < 18\zeta^2(6)/\zeta(12)$.

Next we consider a one-dimensional chain with two alternating species of atoms A and B, with pairwise interactions. We assume that the interaction potential between A atoms is V_{AA}, the interaction potential between B atoms is V_{BB}, and the interaction potential between A and B atoms is V_{AB}. The dynamic equations are:

$$\begin{aligned} m_A \partial_t^2 y_i^A &= V'_{AB}(y_i^B - y_i^A) + V'_{AA}(y_{i+1}^A - y_i^A) \\ &\qquad - V'_{AB}(y_i^A - y_{i-1}^B) - V'_{AA}(y_i^A - y_{i-1}^A), \\ m_B \partial_t^2 y_i^B &= V'_{AB}(y_{i+1}^A - y_i^B) + V'_{BB}(y_{i+1}^B - y_i^B) \\ &\qquad - V'_{AB}(y_i^B - y_i^A) - V'_{BB}(y_i^B - y_{i-1}^B). \end{aligned}$$

Denote the shift of a B atom from its left neighboring A atom by p. Let $y_i^A = i\varepsilon + \widetilde{y}_i^A$ and $y_i^B = i\varepsilon + p + \widetilde{y}_i^B$, where ε is the equilibrium bond length. Linearizing the above equation, and using the Euler-Lagrange equation for optimizing with respect to the shift p, we obtain

$$\begin{aligned} m_A \partial_t^2 \widetilde{y}_i^A &= V''_{AB}(p)(\widetilde{y}_i^B - \widetilde{y}_i^A) - V''_{AB}(\varepsilon - p)(\widetilde{y}_i^A - \widetilde{y}_{i-1}^B) \\ &\quad + V''_{AA}(\varepsilon)(\widetilde{y}_{i+1}^A - 2\widetilde{y}_i^A + \widetilde{y}_{i-1}^A), \\ m_B \partial_t^2 \widetilde{y}_i^B &= V''_{AB}(\varepsilon - p)(\widetilde{y}_{i+1}^A - \widetilde{y}_i^B) - V''_{AB}(p)(\widetilde{y}_i^B - \widetilde{y}_i^A) \\ &\quad + V''_{BB}(\varepsilon)(\widetilde{y}_{i+1}^B - 2\widetilde{y}_i^B + \widetilde{y}_{i-1}^B). \end{aligned}$$

To make clear the dependence of the phonon spectrum on the mass, we let

$$\alpha_A = \frac{m_{\mathrm{har}}}{m_A} \quad \text{and} \quad \alpha_B = \frac{m_{\mathrm{har}}}{m_B},$$

where m_{har} is the harmonic mean of m_A and m_B. Obviously, α_A and α_B are independent of the mass unit, and $\alpha_A + \alpha_B = 2$.

Let $\widetilde{y}_i^A = \varepsilon_A e^{i(ki\varepsilon - \omega\, t)}$ and $\widetilde{y}_i^B = \varepsilon_B e^{i(ki\varepsilon - \omega\, t)}$, we get

$$\begin{pmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{pmatrix} \begin{pmatrix} \varepsilon_A \\ \varepsilon_B \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix},$$

where

$$
\begin{aligned}
D_{11} &= \omega^2 - \frac{\alpha_A}{m_{\text{har}}}\big(4V''_{AA}(\varepsilon)\sin^2\frac{k\varepsilon}{2} + V''_{AB}(p) + V''_{AB}(\varepsilon-p)\big),\\
D_{12} &= \frac{\alpha_A}{m_{\text{har}}}\big(V''_{AB}(\varepsilon-p)e^{-ik\varepsilon} + V''_{AB}(p)\big),\\
D_{21} &= \frac{\alpha_B}{m_{\text{har}}}\big(V''_{AB}(\varepsilon-p)e^{ik\varepsilon} + V''_{AB}(p)\big),\\
D_{22} &= \omega^2 - \frac{\alpha_B}{m_{\text{har}}}\big(4V''_{BB}(\varepsilon)\sin^2\frac{k\varepsilon}{2} + V''_{AB}(p) + V''_{AB}(\varepsilon-p)\big).
\end{aligned}
$$

It is seen that

$$
\begin{aligned}
\omega_a^2(k) + \omega_o^2(k) &= \frac{4}{m_{\text{har}}}[\alpha_A V''_{AA}(\varepsilon) + \alpha_B V''_{BB}(\varepsilon)]\sin^2\frac{k\varepsilon}{2} + \frac{2}{m_{\text{har}}}[V''_{AB}(p) + V''_{AB}(\varepsilon-p)],\\
\omega_a^2(k)\omega_o^2(k) &= \frac{4\alpha_A\alpha_B}{m_{\text{har}}^2}\Big([V''_{AA}(\varepsilon) + V''_{BB}(\varepsilon)][V''_{AB}(p) + V''_{AB}(\varepsilon-p)] + V''_{AB}(p)V''_{AB}(\varepsilon-p)\\
&\qquad + 4V''_{AA}(\varepsilon)V''_{BB}(\varepsilon)\sin^2\frac{k\varepsilon}{2}\Big)\sin^2\frac{k\varepsilon}{2}.
\end{aligned}
$$

We have, for any $k \in \mathbb{R}$,

$$
\varepsilon\omega_o(k) \geq \varLambda_2, \tag{4.3}
$$

where

$$
\varLambda_2 = \frac{1}{\sqrt{m_{\text{har}}}}\big(V''_{AB}(p) + V''_{AB}(\varepsilon-p)\big)^{1/2}\varepsilon.
$$

Next using the obvious facts

$$
\begin{aligned}
\omega_a^2(k)\omega_o^2(k) &\geq \frac{4\alpha_A\alpha_B}{m_{\text{har}}^2}\Big([V''_{AA}(\varepsilon) + V''_{BB}(\varepsilon)][V''_{AB}(p) + V''_{AB}(\varepsilon-p)]\\
&\qquad + V''_{AB}(p)V''_{AB}(\varepsilon-p)\Big)\sin^2\frac{k\varepsilon}{2},\\
\omega_a^2(k) + \omega_o^2(k) &\leq \frac{8}{m_{\text{har}}}[V''_{AA}(\varepsilon) + V''_{BB}(\varepsilon)] + \frac{2}{m_{\text{har}}}[V''_{AB}(p) + V''_{AB}(\varepsilon-p)],
\end{aligned}
$$

we obtain

$$
\begin{aligned}
\omega_a^2(k) &\geq \frac{\omega_a^2(k)\omega_o^2(k)}{\omega_a^2(k) + \omega_o^2(k)}\\
&\geq \frac{2\alpha_A\alpha_B}{m_{\text{har}}}\frac{V''_{AA}(\varepsilon) + V''_{BB}(\varepsilon) + \dfrac{V''_{AB}(p)V''_{AB}(\varepsilon-p)}{V''_{AB}(p) + V''_{AB}(\varepsilon-p)}}{1 + \dfrac{4(V''_{AA}(\varepsilon) + V''_{BB}(\varepsilon))}{V''_{AB}(p) + V''_{AB}(\varepsilon-p)}}\sin^2\frac{k\varepsilon}{2}.
\end{aligned}
$$

Using the basic inequality:

$$
\frac{\sin x}{x} \geq \frac{2}{\pi} \quad \text{for all } |\,x\,| \leq \frac{\pi}{2},
$$

we obtain, for k in the first Brillouin zone, i.e. $|\,k\varepsilon\,| \leq \pi/2$,

$$
\omega_a(k) \geq \varLambda_1|\,k\,|, \tag{4.4}
$$

where

$$
\varLambda_1 = \frac{\sqrt{2\alpha_A\alpha_B}/\pi}{\sqrt{m_{\text{har}}}}\left(\frac{V''_{AA}(\varepsilon) + V''_{BB}(\varepsilon) + \dfrac{V''_{AB}(p)V''_{AB}(\varepsilon-p)}{V''_{AB}(p) + V''_{AB}(\varepsilon-p)}}{1 + \dfrac{4(V''_{AA}(\varepsilon) + V''_{BB}(\varepsilon))}{V''_{AB}(p) + V''_{AB}(\varepsilon-p)}}\right)^{1/2}\varepsilon.
$$

In view of (4.4) and (4.3), we have verified that $0 \in \mathscr{O}_2(\Lambda_1', \Lambda_2')$ for any $0 < \Lambda_1' < \Lambda_1$ and $0 < \Lambda_2' < \Lambda_2$.

4.2. **Stability region.** The set $\mathscr{O}_1$ consists all the deformations at which the elasticity stiffness tensor is uniformly elliptic, while the set $\widetilde{\mathscr{O}}_1$ consists all the deformations at which the elasticity stiffness tensor is positive definite. The following example may help us to appreciate the difference between the stability regions $\mathscr{O}_1$ and $\widetilde{\mathscr{O}}_1$. Let

$$W(\mathsf{A}) = \frac{\mu}{2}|\,\mathsf{A} + \mathsf{A}^T\,|^2 + \lambda(\operatorname{tr}\mathsf{A})^2.$$

A straightforward calculation gives that

$$\mu > 0 \text{ and } \lambda + 2\mu > 0 \Longleftrightarrow \mathbf{0} \in \mathscr{O}_1(\Lambda) \quad \text{with} \quad 0 < \Lambda < \min(\lambda + 2\mu, \mu).$$

$$\mu > 0 \text{ and } d\lambda + 2\mu > 0 \Longleftrightarrow \mathbf{0} \in \widetilde{\mathscr{O}}_1(\Lambda) \quad \text{with} \quad 0 < \Lambda < \min(d\lambda + 2\mu, \mu).$$

However, it is easy to see that for any fixed μ, we may choose λ such that $2\mu + d\lambda < 0 < 2\mu + \lambda$, namely, $\mathbf{0} \in \mathscr{O}_1(\Lambda)$ for any $0 < \Lambda < \min(\lambda + 2\mu, \mu)$, while $\mathbf{0} \notin \widetilde{\mathscr{O}}_1(\Lambda)$ for any $\Lambda > 0$ in this case.

Next we consider the triangular lattice with the Lennard-Jones potential, and we assume that the displacement field depends only on y. In this case,

$$\mathsf{A} = \begin{pmatrix} 0 & \mu \\ 0 & \lambda \end{pmatrix}.$$

This special form of A helps us to visualize the stability region. The contours of the sets $\mathscr{O}_1(0)$ and $\mathscr{O}_2(0)$ are drawn in Fig. 1. The intersection of the two interior is the stability region.

The computation of the phonon spectrum of the homogeneously strained crystal is standard, we refer to [31] for details. The contour of $\mathscr{O}_2(0)$ is the set of the critical values of (λ, μ) at which the smallest eigenvalue of the phonon spectrum vanishes.

Given the above special form of A, using (2.2), we get that W_{CB} is a function of λ and μ. The contour of $\mathscr{O}_1(0)$ is the set of the critical values of (λ, μ) at which the smallest eigenvalue of the Hessian matrix of W_{CB}, i.e.

$$\begin{pmatrix} \dfrac{\partial^2 W_{\mathrm{CB}}}{\partial \lambda^2} & \dfrac{\partial^2 W_{\mathrm{CB}}}{\partial \lambda \partial \mu} \\ \dfrac{\partial^2 W_{\mathrm{CB}}}{\partial \lambda \partial \mu} & \dfrac{\partial^2 W_{\mathrm{CB}}}{\partial \mu^2} \end{pmatrix}$$

vanishes.

5. Proof of the Main Results

5.1. **Proof of Theorem 3.1.** The proof of Theorem 3.1 is essentially the same as that of [9]. We only need to prove the maximality of T_1^*. The first condition (3.8) characterizing the blow-up time follows from the energy estimates, while the second condition (3.9) comes from the simple observation that the *strong ellipticity* of $D^2_{\mathsf{A}} W_{\mathrm{CB}}$ is needed in order to guarantee existence of strong solutions.

For any integer $s > d/2 + 1$ and $T > 0$, we define

$$X_T = C^0\big([0, T); H^{s+1}\big) \cap C^1\big([0, T); H^s\big),$$

and for any given $\boldsymbol{v} \in X_T$, we linearize Problem 3.2 at $\boldsymbol{v}$ to obtain a linear problem:

$$\begin{cases} m\partial_t^2 \boldsymbol{w} - D^2_{\mathsf{A}} W_{\mathrm{CB}}(\nabla \boldsymbol{v}) D^2 \boldsymbol{w} = \mathbf{0} & \text{in } \mathbb{R}^d, \\ \boldsymbol{w}|_{t=0} = \boldsymbol{u}^0, \quad \partial_t \boldsymbol{w}|_{t=0} = \boldsymbol{u}^1. \end{cases} \tag{5.1}$$

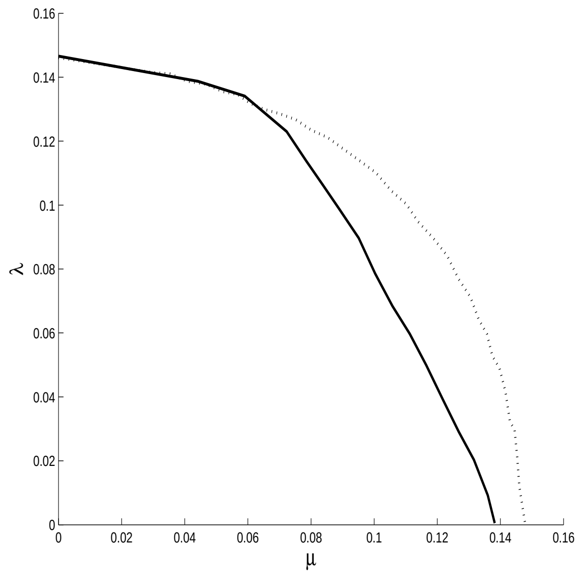

FIGURE 1. Dotted line: boundary of the region $\mathscr{O}_1(0)$ of the continuum model; Solid line: boundary of the region $\mathscr{O}_2(0)$ of the atomistic model.

It is convenient to write out the above linearized problem for each component: for $\alpha = 1, \dots, d$,

$$
\begin{cases} m\partial_t^2 \boldsymbol{w}^\alpha - \mathsf{C}_{\alpha\, i\beta\, j}(\nabla \boldsymbol{v})\partial_{ij}\boldsymbol{w}^\beta = \boldsymbol{0} & \text{in } \mathbb{R}^d, \\ \boldsymbol{w}^\alpha|_{t=0} = (\boldsymbol{u}^0)^\alpha, \quad \partial_t \boldsymbol{w}^\alpha|_{t=0} = (\boldsymbol{u}^1)^\alpha. \end{cases} \tag{5.2}
$$

Next, given $\boldsymbol{w}$, a solution of (5.1), for any $r = 0, \dots, s$ and $0 \le t \le T$, we define the energy integral

$$
E_r(t) = \int_{\mathbb{R}^d} \left[m |\, D^r \partial_t \boldsymbol{w}\, |^2 + D^r \partial_i \boldsymbol{w}^\alpha \mathsf{C}_{i\alpha\, j\beta}(\nabla \boldsymbol{v}) D^r \partial_j \boldsymbol{w}^\beta \right] \mathrm{d}\boldsymbol{x}. \tag{5.3}
$$

For $\ell = 2, \dots, s$, define

$$
M_{\boldsymbol{v}} = \sup_{2 \le \ell \le s} \max_{t \in [0,T]} |\, D_{\mathsf{A}}^\ell W_{\mathrm{CB}}(\nabla \boldsymbol{v}(\cdot, t))\, |.
$$

By $\nabla \boldsymbol{v} \in \mathring{\mathscr{O}}_1(\varLambda)$ with $\varLambda > 0$, for any $\boldsymbol{z} \in H^1(\mathbb{R}^d; \mathbb{R}^d)$, it follows from Gårding inequality [21] that

$$
\int_{\mathbb{R}^d} \partial_i \boldsymbol{z}^\alpha \mathsf{C}_{i\alpha\, j\beta}(\nabla \boldsymbol{v}) \partial_j \boldsymbol{z}^\beta \,\mathrm{d}\boldsymbol{x} + \kappa \int_{\mathbb{R}^d} \boldsymbol{z}^2 \,\mathrm{d}\boldsymbol{x} \ge \varLambda_0 \int_{\mathbb{R}^d} |\, \nabla \boldsymbol{z}\, |^2 \,\mathrm{d}\boldsymbol{x}, \tag{5.4}
$$

where $\varLambda_0$ depends on $\varLambda$ and d, while κ depends on $M_{\boldsymbol{v}}, \varLambda$ and d. On the other hand, given (5.4), we conclude that $\nabla \boldsymbol{v} \in \mathring{\mathscr{O}}_1(\varLambda')$ for certain $\varLambda' > 0$.

In the following proof, we shall frequently use the Gagliardo-Nirenberg inequality [19]: for any $f \in H^s(\mathbb{R}^d)$, there exists a constant C_s such that

$$
\sum_{r=0}^{s} \|D^r f\|_{L^2}^2 \le C_s \sum_{r=0}^{s} \|D^s f\|_{L^2}^{2r/s} \|f\|_{L^2}^{2(1-r/s)}, \tag{5.5}
$$

and the Sobolev imbedding inequality: there exists a constant c_* such that

$$
\|\psi\|_{L^\infty} \le c_* \|\psi\|_{H^{s-1}} \quad \text{for all } \psi \in H^{s-1}. \tag{5.6}
$$

Lemma 5.1. *Given T, we assume that $\boldsymbol{v} \in X_T$ with $s > d/2 + 1$ and $\nabla \boldsymbol{v} \in \mathring{\mathscr{O}}_1(\varLambda)$ for certain $\varLambda > 0$. Then we have*

$$\|\boldsymbol{w}\|_{H^{s+1}} + \|\partial_t \boldsymbol{w}\|_{H^s} \le c e^{K_1 t/(2\widetilde{\lambda})}(1 + c_1 t^{1/2})(\|\boldsymbol{u}^0\|_{H^{s+1}} + \|\boldsymbol{u}^1\|_{H^s}), \quad 0 < t \le T, \tag{5.7}$$

where c is a positive constant that continuously depends on $T, \varLambda, m, M_{\boldsymbol{v}}$ and d, and c_1 is a positive constant that continuously depends on $T, K_1, \varLambda, m$ and d. Here

$$K_1 = M_{\boldsymbol{v}} c_* [2\sqrt{s C_s}(c_*^{s-1} C_s \|\nabla \boldsymbol{v}\|_{H^s}^s + 1) + \|\partial \boldsymbol{v}\|_{H^s}], \tag{5.8}$$

where C_s and c_* are constants in the right-hand side of (5.5) *and* (5.6)*, respectively.* $\widetilde{\lambda} = \min(\varLambda_0, m)$ *where $\varLambda_0$ is the constant in the right-hand side of* (5.4).

Proof. By definition, $\mathsf{C}_{\alpha\, i\beta\, j} = \mathsf{C}_{\beta\, j\alpha\, i}$ for $i, j, \alpha, \beta = 1, \dots, d$, we have the following energy integral:

$$\begin{aligned} \frac{1}{2}\frac{d}{dt} E_r(t) &= \int_{\mathbb{R}^d} \left[m D^r \partial_t \boldsymbol{w} \cdot D^r \partial_t^2 \boldsymbol{w} + D^r \partial_i \partial_t \boldsymbol{w}^\alpha \mathsf{C}_{\alpha\, i\beta\, j} D^r\, \partial_j \boldsymbol{w}^\beta \right] \mathrm{d}\boldsymbol{x} \\ &\quad + \frac{1}{2} \int_{\mathbb{R}^d} D^r \partial_i \boldsymbol{w}^\alpha \partial_t \mathsf{C}_{\alpha\, i\beta\, j} D^r \partial_j \boldsymbol{w}^\beta \,\mathrm{d}\boldsymbol{x}. \end{aligned} \tag{5.9}$$

Using (5.1), we get

$$\begin{aligned} \int_{\mathbb{R}^d} m D^r \partial_t \boldsymbol{w}^\alpha \cdot D^r \partial_t^2 \boldsymbol{w}^\alpha &= \int_{\mathbb{R}^d} D^r \partial_t \boldsymbol{w}^\alpha D^r [\mathsf{C}_{\alpha\, i\beta\, j} \partial_{ij} \boldsymbol{w}^\beta] \,\mathrm{d}\boldsymbol{x} \\ &= \int_{\mathbb{R}^d} [D^r \partial_t \boldsymbol{w}^\alpha (D^r \mathsf{C}_{\alpha\, i\beta\, j}) \partial_{ij} \boldsymbol{w}^\beta + \mathsf{C}_{\alpha\, i\beta\, j} D^r \partial_{ij} \boldsymbol{w}^\beta] \,\mathrm{d}\boldsymbol{x}. \end{aligned}$$

Integrating by parts gives

$$\begin{aligned} \int_{\mathbb{R}^d} D^r \partial_t \boldsymbol{w}^\alpha \mathsf{C}_{\alpha\, i\beta\, j} D^r \partial_{ij} \boldsymbol{w}^\beta \,\mathrm{d}\boldsymbol{x} &= - \int_{\mathbb{R}^d} D^r \partial_t \boldsymbol{w}^\alpha \partial_i \mathsf{C}_{\alpha\, i\beta\, j} D^r \partial_j \boldsymbol{w}^\beta \,\mathrm{d}\boldsymbol{x} \\ &\quad - \int_{\mathbb{R}^d} D^r \partial_i \partial_t \boldsymbol{w}^\alpha \mathsf{C}_{\alpha\, i\beta\, j} D^r \partial_j \boldsymbol{w}^\beta \,\mathrm{d}\boldsymbol{x}. \end{aligned}$$

Substituting the above two equations into (5.9), we obtain

$$\begin{aligned} \frac{1}{2}\frac{d}{dt} E_r(t) &= \int_{\mathbb{R}^d} D^r \partial_t \boldsymbol{w}^\alpha \left(D^r \mathsf{C}_{\alpha\, i\beta\, j} \partial_{ij} \boldsymbol{w}^\beta - \partial_i \mathsf{C}_{\alpha\, i\beta\, j} D^r \partial_j \boldsymbol{w}^\beta \right) \mathrm{d}\boldsymbol{x} \\ &\quad + \frac{1}{2} \int_{\mathbb{R}^d} D^r \partial_i \boldsymbol{w}^\alpha \partial_t \mathsf{C}_{\alpha\, i\beta\, j} D^r \partial_j \boldsymbol{w}^\beta \,\mathrm{d}\boldsymbol{x}. \end{aligned}$$

By the Cauchy-Schwartz inequality, we get

$$\begin{aligned} \frac{1}{2}\frac{d}{dt} E_r(t) &\le \|D^r \mathsf{C}\|_{L^2} \|D^r \partial_t \boldsymbol{w}\|_{L^2} \|D^2 \boldsymbol{w}\|_{L^\infty} + \|\nabla \mathsf{C}\|_{L^\infty} \|D^r \partial_t \boldsymbol{w}\|_{L^2} \|D^{r+1} \boldsymbol{w}\|_{L^2} \\ &\quad + \frac{1}{2} \|\partial_t \mathsf{C}\|_{L^\infty} \|D^{r+1} \boldsymbol{w}\|_{L^2}^2. \end{aligned}$$

Adding up for all $r = 0, \dots, s$, we obtain

$$\begin{aligned} \frac{1}{2}\frac{d}{dt} \sum_{r=0}^s E_r(t) &\le \|D^2 \boldsymbol{w}\|_{L^\infty} \sum_{r=0}^s \|D^r \mathsf{C}\|_{L^2} \|D^r \partial_t \boldsymbol{w}\|_{L^2} \\ &\quad + \|\partial \mathsf{C}\|_{L^\infty} \sum_{r=0}^s \|D^r \partial \boldsymbol{w}\|_{L^2} \|D^{r+1} \boldsymbol{w}\|_{L^2}. \end{aligned}$$

Using (5.5), we have

$$\begin{aligned}\sum_{r=0}^{s}\|D^rC\|_{L^2}^2&\le C_s\sum_{r=0}^{s}\|D^s\mathsf{C}\|_{L^2}^{2r/s}\|\mathsf{C}\|_{L^2}^{2(1-r/s)}\\&\le 2C_s\sum_{r=0}^{s}\frac{r^2}{s^2}\|D^s\mathsf{C}\|_{L^2}^2+2C_s\sum_{r=0}^{s}(1-r/s)^2\|\mathsf{C}\|_{L^2}^2\\&\le 4sC_s(\|D^s\mathsf{C}\|_{L^2}^2+\|\mathsf{C}\|_{L^2}^2).\end{aligned}\tag{5.10}$$

Using the fact that H^{s-1} is a Banach algebra for $s>d/2+1$, and by Moser type of calculus inequality [19, Inequality C in pp. 43], we get

$$\begin{aligned}\|D^s\mathsf{C}(\nabla\boldsymbol{v})\|_{L^2}&\le C_sM_{\boldsymbol{v},s}\|\nabla\boldsymbol{v}\|_{L^\infty}^{s-1}\|D^{s+1}\boldsymbol{v}||_{L^2}\le C_sM_{\boldsymbol{v}}c_*^{s-1}\|\nabla\boldsymbol{v}\|_{H^{s-1}}^{s-1}\|\nabla\boldsymbol{v}\|_{H^s}\\&\le C_sc_*^{s-1}M_{\boldsymbol{v}}\|\nabla\boldsymbol{v}\|_{H^s}^s,\end{aligned}$$

where c_* is the constant in (5.6). Similarly, we have

$$\begin{aligned}\|\partial\mathsf{C}(\nabla\boldsymbol{v})\|_{L^\infty}&\le c_*M_{\boldsymbol{v}}\|\partial\boldsymbol{v}\|_{H^s},\\\|D^2\boldsymbol{w}\|_{L^\infty}&\le c_*\|D^2\boldsymbol{w}\|_{H^{s-1}}\le c_*\|\nabla\boldsymbol{w}\|_{H^s}.\end{aligned}$$

Therefore, we have

$$\frac{d}{dt}\sum_{r=0}^{s}E_r(t)\le K_1\|\partial\boldsymbol{w}\|_{H^s}^2.\tag{5.11}$$

Using (5.4), we have, for $r=0,\dots,s$,

$$E_r(t)+\kappa\int_{\mathbb{R}^d}|\,D^r\boldsymbol{w}\,|^2\,\mathrm{d}\boldsymbol{x}\ge\Lambda_0\int_{\mathbb{R}^d}|\,D^{r+1}\boldsymbol{w}\,|^2\,\mathrm{d}\boldsymbol{x}+m\int_{\mathbb{R}^d}|\,D^r\partial_t\boldsymbol{w}\,|^2\,\mathrm{d}\boldsymbol{x}.$$

Using the trivial bound

$$\|D^r\boldsymbol{w}\|_{L^2}\le\|D^r\boldsymbol{u}^0\|_{L^2}+\int_0^t\|\partial_\tau D^r\boldsymbol{w}(\cdot,\tau)\|_{L^2}\mathrm{d}\tau,\tag{5.12}$$

Combining the above two inequalities, and summing up for all $r=0,\dots,s$, we get

$$\widetilde{\lambda}\|\partial\boldsymbol{w}\|_{H^s}^2\le\sum_{r=0}^{s}E_r(t)+2\kappa\|\boldsymbol{u}^0\|_{H^s}^2+2\kappa t\int_0^t\|\partial_\tau\boldsymbol{w}\|_{H^s}^2\mathrm{d}\tau.\tag{5.13}$$

Using (5.11), we obtain

$$\frac{\widetilde{\lambda}}{K_1}\frac{d}{dt}\sum_{r=0}^{s}E_r(t)\le\sum_{r=0}^{s}E_r(t)+2\kappa\|\boldsymbol{u}^0\|_{H^s}^2+2\kappa t\int_0^t\|\partial_\tau\boldsymbol{w}\|_{H^s}^2\mathrm{d}\tau.$$

By Grownwall's inequality and using (5.13), we get

$$\begin{aligned}\widetilde{\lambda}\|\partial\boldsymbol{w}\|_{H^s}^2&\le(2\kappa+M_{\boldsymbol{v}}+m)\frac{K_1}{\widetilde{\lambda}}e^{K_1t/\widetilde{\lambda}}(\|\boldsymbol{u}^0\|_{H^{s+1}}^2+\|\boldsymbol{u}^1\|_{H^s}^2)\\&\quad+2\kappa(e^{K_1t/\widetilde{\lambda}}-1-K_1t/\widetilde{\lambda})\int_0^t\|\partial_\tau\boldsymbol{w}\|_{H^s}^2\mathrm{d}\tau,\end{aligned}\tag{5.14}$$

which implies

$$\begin{aligned}m\widetilde{\lambda}\|\partial_t\boldsymbol{w}\|_{H^s}^2&\le(2\kappa+M_{\boldsymbol{v}}+m)\frac{K_1}{\widetilde{\lambda}}e^{K_1t/\widetilde{\lambda}}(\|\boldsymbol{u}^0\|_{H^{s+1}}^2+\|\boldsymbol{u}^1\|_{H^s}^2)\\&\quad+2\kappa(e^{K_1t/\widetilde{\lambda}}-1-K_1t/\widetilde{\lambda})\int_0^t\|\partial_\tau\boldsymbol{w}\|_{H^s}^2\mathrm{d}\tau,\end{aligned}$$

Using Grownwall's inequality again, we get a bound on $\int_0^t \|\partial_\tau \boldsymbol{w}\|_{H^s}^2 \mathrm{d}\tau$, which together with (5.14) gives (5.7). $\square$

Proof of Theorem 3.1 Given $K, T > 0$ to be determined later, define

$$C(K,T) = \{\boldsymbol{w} \in X_T \mid \|\boldsymbol{w}(\cdot,t)\|_{H^{s+1}} + \|\partial_t \boldsymbol{w}(\cdot,t)\|_{H^s} \le K,\\ \boldsymbol{w}|_{t=0} = \boldsymbol{u}^0,\ \partial_t \boldsymbol{w}|_{t=0} = \boldsymbol{u}^1\}.$$

For sufficiently large K and sufficiently small T, the set $C(K,T)$ is not empty. Over $C(K,T)$ we define the metric

$$\varrho(\boldsymbol{v},\boldsymbol{w}) = \sup_{t\in[0,T]} \big[\|\boldsymbol{v}(\cdot,t) - \boldsymbol{w}(\cdot,t)\|_{H^1} + \|\partial_t \boldsymbol{v}(\cdot,t) - \partial_t \boldsymbol{w}(\cdot,t)\|_{L^2}\big].$$

It is well-known that $(C(K,T),\varrho)$ is a complete metric space (see [9]).

Given $\boldsymbol{v} \in C(K,T)$, define $\mathscr{T}(\boldsymbol{v}) = \boldsymbol{w}$, where $\boldsymbol{w}$ satisfies (5.1). For fixed $K, T > 0$, it is clear that c_1 in the right-hand side of (5.7) is uniformly bounded for any $\boldsymbol{v} \in C(K,T)$. Moreover, using the imbedding theorem and note that $s > d/2+1$, we get, for any $\boldsymbol{v} \in C(K,T)$,

$$\|\nabla \boldsymbol{v}(\cdot,t) - \nabla \boldsymbol{u}^0\|_{L^\infty} \le t\|\partial_t \nabla \boldsymbol{v}(\cdot,t)\|_{L^\infty} \le c_*\, t\|\partial_t \nabla \boldsymbol{v}(\cdot,t)\|_{H^{s-1}} \le c_* K t, \tag{5.15}$$

where we have used $\boldsymbol{v}|_{t=0} = \boldsymbol{u}^0$. Now, we choose K_0 such that

$$K_0 \ge 8c(m,\Lambda,M_{\boldsymbol{u}^0})(\|\boldsymbol{u}^0\|_{H^{s+1}} + \|\boldsymbol{u}^1\|_{H^s}),$$

and then by (5.15), we select $T_0 \in (0,1]$ such that for any $T \in (0,T_0]$, and for all $\boldsymbol{v} \in C(K_0,T)$, we have

$$c(m,\Lambda,M_{\boldsymbol{v}}) \le 2c(m,\Lambda,M_{\boldsymbol{u}^0}), \tag{5.16}$$

$$e^{K_1 t/(2\widetilde{\lambda})}(1 + c_1 t^{1/2}) \le 4. \tag{5.17}$$

Next let $T_1 = \Lambda_0/(4c_* K_0 M_{\boldsymbol{u}^0})$, for $t \in (0,T_1]$, we have

$$\|\nabla \boldsymbol{v}(\cdot,t) - \nabla \boldsymbol{u}^0\|_{L^\infty} \le \Lambda_0/(4M_{\boldsymbol{u}^0}).$$

Since $\nabla \boldsymbol{u}^0 \in \mathscr{O}_1(\Lambda)$, as in (5.4), we have

$$\int_{\mathbb{R}^d} \partial_i \boldsymbol{v}^\alpha \mathsf{C}_{i\alpha\, j\beta}(\nabla \boldsymbol{u}^0)\partial_j \boldsymbol{v}^\beta \,\mathrm{d}\boldsymbol{x} + \kappa \int_{\mathbb{R}^d} \boldsymbol{v}^2 \,\mathrm{d}\boldsymbol{x} \ge \Lambda_0 \int_{\mathbb{R}^d} |\,\nabla \boldsymbol{v}\,|^2 \,\mathrm{d}\boldsymbol{x}.$$

Combining the above two inequalities, we obtain, for $0 \le t \le T_2 = \min(T_1,T_0)$ and $\boldsymbol{z} \in H^1(\mathbb{R}^d;\mathbb{R}^d)$,

$$\begin{aligned}
&\int_{\mathbb{R}^d} \nabla \boldsymbol{z} \cdot D_{\mathsf{A}}^2 W_{\mathrm{CB}}(\nabla \boldsymbol{v}) \nabla \boldsymbol{z} \,\mathrm{d}\boldsymbol{x} + \kappa \int_{\mathbb{R}^d} |\,\boldsymbol{z}\,|^2 \,\mathrm{d}\boldsymbol{x}\\
&\ge \int_{\mathbb{R}^d} \nabla \boldsymbol{z} \cdot D_{\mathsf{A}}^2 W_{\mathrm{CB}}(\nabla \boldsymbol{u}^0) \nabla \boldsymbol{z} \,\mathrm{d}\boldsymbol{x} + \kappa \int_{\mathbb{R}^d} \boldsymbol{z}^2 \,\mathrm{d}\boldsymbol{x}\\
&\quad - M_{\boldsymbol{v}} \|\nabla \boldsymbol{v}(\cdot,t) - \nabla \boldsymbol{u}^0)\|_{L^\infty} \int_{\mathbb{R}^d} |\,\nabla \boldsymbol{z}\,|^2 \,\mathrm{d}\boldsymbol{x}\\
&\ge (\Lambda_0 - 2c_* K_0 t M_{\boldsymbol{u}^0}) \int_{\mathbb{R}^d} |\,\nabla \boldsymbol{z}\,|^2 \,\mathrm{d}\boldsymbol{x}\\
&\ge \frac{\Lambda_0}{2} \int_{\mathbb{R}^d} |\,\nabla \boldsymbol{z}\,|^2 \,\mathrm{d}\boldsymbol{x}.
\end{aligned} \tag{5.18}$$

By [21], we have $\nabla \boldsymbol{v} \in \mathring{\mathscr{O}}_1(\Lambda')$, where Λ' is positive and depends on Λ_0. Then the linear problem (5.1) has a unique solution $\mathscr{T}(\boldsymbol{v})$. This together with the priori estimate (5.7), (5.16) and (5.17) leads to the conclusion that with the above choice of K_0 and T_2, the mapping $\mathscr{T}$ leaves the set $C(K_0,T_2)$ invariant for every $t\in(0,T_2]$.

Next we prove that the mapping $\mathscr{T}$ is contractive for sufficiently small T. Given $\boldsymbol{v}_1,\boldsymbol{v}_2\in C(K_0,T_2)$, let $\boldsymbol{U}=\mathscr{T}(\boldsymbol{v}_1)-\mathscr{T}(\boldsymbol{v}_2)$, and a simple computation shows that $\boldsymbol{U}$ satisfies

$$\begin{cases} m\partial_t^2\boldsymbol{U}-D^2_{\mathsf{A}}W_{\mathrm{CB}}(\nabla\boldsymbol{v}_1)D^2\boldsymbol{U}=\boldsymbol{f} & \text{in }\mathbb{R}^d,\\ \boldsymbol{U}|_{t=0}=\boldsymbol{0},\quad \partial_t\boldsymbol{U}|_{t=0}=\boldsymbol{0} \end{cases} \tag{5.19}$$

with $\boldsymbol{f}=\bigl[D^2_{\mathsf{A}}W_{\mathrm{CB}}(\nabla\boldsymbol{v}_1)-D^2_{\mathsf{A}}W_{\mathrm{CB}}(\nabla\boldsymbol{v}_2)\bigr]D^2\mathscr{T}(\boldsymbol{v}_2)$.

By definition we have

$$\varrho^2(\mathscr{T}(\boldsymbol{v}_1),\mathscr{T}(\boldsymbol{v}_2))\le\Bigl(\frac{2}{\varLambda_0}+\frac{1}{m}\Bigr)E_0(t)+2t(\kappa+1)\int_0^t\|\partial_\tau\boldsymbol{U}(\cdot,\tau)\|_{L^2}^2\mathrm{d}\tau. \tag{5.20}$$

Proceeding along the same line that leads to (5.11), we get

$$\frac{d}{dt}E_0(t)\le cE_0(t)+2\kappa ct\int_0^t\|\partial_\tau\boldsymbol{U}(\cdot,\tau)\|_{L^2}^2\mathrm{d}\tau+\frac{2}{m}\max_{t\in[0,T_2]}\|\boldsymbol{f}(\cdot,t)\|_{L^2}^2,$$

where c depend on $\varLambda_0,m,M_{\boldsymbol{u}^0},T_2$ and K_0. By Grownwall's inequality, we get

$$E_0(t)\le\frac{4\kappa}{c}(e^{ct}-1)\Bigl(\int_0^t\|\partial_\tau\boldsymbol{U}(\cdot,\tau)\|_{L^2}^2\mathrm{d}\tau+\frac{1}{2\kappa m}\max_{t\in[0,T_2]}\|\boldsymbol{f}(\cdot,t)\|_{L^2}^2\Bigr),$$

$$\int_0^t\|\partial_\tau\boldsymbol{U}(\cdot,\tau)\|_{L^2}^2\mathrm{d}\tau\le\frac{2}{\kappa m}(e^{c_1t}-1)\max_{t\in[0,T_2]}\|\boldsymbol{f}(\cdot,t)\|_{L^2}^2,$$

where $c_1=4\kappa(e^{cT_2}-1)/(cm)$. A straightforward calculation leads to

$$\max_{t\in[0,T_2]}\|\boldsymbol{f}(\cdot,t)\|_{L^2}^2\le c_*M_{\boldsymbol{u}^0}K_0\varrho^2(\boldsymbol{v}_1,\boldsymbol{v}_2).$$

Substituting the above three inequalities into (5.20), we obtain

$$\varrho(\mathscr{T}(\boldsymbol{v}_1),\mathscr{T}(\boldsymbol{v}_2))\le C(e^{ct}-1)^{1/2}\varrho(\boldsymbol{v}_1,\boldsymbol{v}_2),$$

where C depends on $T_2,c_*,M_{\boldsymbol{u}^0},\kappa,m,K_0$ and $\varLambda_0$. If we choose T_3 such that $C(e^{cT_3}-1)^{1/2}<1$, we conclude that for sufficiently small $t\in(0,T_3]$, the mapping $\mathscr{T}$ is contractive. By the fixed point principle, the fixed point is the unique solution of (3.2).

Let $T_1^*:=\min(T_2,T_3)$. To prove the maximality of T_1^*, we repeat the steps that lead to (5.7) and obtain the following estimate for the solution of (3.2):

$$\begin{aligned}\frac12\frac{d}{dt}E_s(t)\le&\bigl(C_sM\|D^2\boldsymbol{u}\|_{L^\infty}\|\nabla\boldsymbol{u}\|_{L^\infty}^{s-1}+M\|D^2\boldsymbol{u}\|_{L^\infty}+\|\partial_t\nabla\boldsymbol{u}\|_{L^\infty}\bigr)\\&\times(\|D^s\partial_t\boldsymbol{u}\|_{L^2}^2+\|D^{s+1}\boldsymbol{u}\|_{L^2}^2).\end{aligned}$$

It follows from

$$\|\nabla\boldsymbol{u}(\cdot,t)\|_{L^\infty}\le\|\nabla\boldsymbol{u}^0\|_{L^\infty}+t\|\partial_t\nabla\boldsymbol{u}(\cdot,t)\|_{L^\infty}$$

that

$$\frac{d}{dt}E_s(t)\le C(\|\partial\nabla\boldsymbol{u}\|_{L^\infty}^s+\|\partial\nabla\boldsymbol{u}\|_{L^\infty})\|\partial\boldsymbol{u}\|_{H^s}^2,$$

where C depends on $s,M_{\boldsymbol{u}^0},c_*,m,\varLambda,\kappa,K_2$ and T_1^*. Similar to Lemma 5.1, we may obtain a bound for $\|\partial\boldsymbol{u}\|_{H^s}$ similar to (5.7) except that the factor K_1t is replaced by

$$\int_0^t(\|\partial\nabla\boldsymbol{u}(\cdot,\tau)\|_{L^\infty}^s+\|\partial\nabla\boldsymbol{u}(\cdot,\tau)\|_{L^\infty})\mathrm{d}\tau.$$

This leads to the conclusion that

$$\|D^s\partial\boldsymbol{u}(\cdot,t)\|_{L^2}\to\infty\quad\text{as }t\to T_1^*$$

cannot occur unless either (3.8) or (3.9) holds. This completes the proof. □

Remark 5.2. *Theorem 3.1 can also be proved by converting* (3.2) *into a first-order system, and proceeded along the same line as* [27] *and* [19, §2]*. Another way to prove Theorem 3.1 is to use semigroups, as was done by Hughes, Kato and Marsden* [14] *in order to establish the existence of the local smooth solution of the initial value problem* (3.2)*. However, neither Schochet* [27] *nor Hughes, Kato and Marsden* [14] *discussed the characterization of the blow-up time (cf.* (3.8) *and* (3.9)*).*

5.2. **Proof of Theorem 3.2.** Since we only consider the case when L is a simple lattice, we drop some of the subscripts and write the atomistic model (3.1) as: for $i = 1, \dots, N$,

$$\begin{cases} m\partial_t^2 \boldsymbol{y}_i(t) + \mathscr{L}_\varepsilon(\boldsymbol{y}_i(t)) = \boldsymbol{0}, \\ \boldsymbol{y}_i(0) = \boldsymbol{x}_i + \boldsymbol{u}^0(\boldsymbol{x}_i), \quad \partial_t \boldsymbol{y}_i(0) = \boldsymbol{u}^1(\boldsymbol{x}_i) \end{cases} \tag{5.21}$$

with $\mathscr{L}_\varepsilon(\boldsymbol{y}_i) = \frac{\partial V}{\partial \boldsymbol{y}_i}$.

First, proceeding along the same line as in [11, §5.1], we carry out the asymptotic analysis of (5.21) to derive formally the continuum equations (3.2). We make the following ansatz:

$$\boldsymbol{y}_i(t) = \boldsymbol{x}_i + \boldsymbol{u}(\boldsymbol{x}_i, t) \quad \text{for } i = 1, \dots, N.$$

Substituting this ansatz into (5.21), we obtain

$$m\partial_t^2 \boldsymbol{y}_i(t) + \mathscr{L}_\varepsilon(\boldsymbol{y}_i(t)) = m\partial_t^2 \boldsymbol{u}(\boldsymbol{x}_i, t) + \mathscr{L}_0(\boldsymbol{u}) + \varepsilon \mathscr{L}_1(\boldsymbol{u}) + \varepsilon^2 \mathscr{L}_2(\boldsymbol{u}) + \mathcal{O}(\varepsilon^3). \tag{5.22}$$

By [11, Lemma 5.4], $\mathscr{L}_0$ is the variational operator of W_{CB}, $\mathscr{L}_1$, and $\mathscr{L}_2$ are in divergence form. Next let

$$\boldsymbol{u} = \boldsymbol{u}_0 + \varepsilon \boldsymbol{u}_1 + \varepsilon^2 \boldsymbol{u}_2.$$

Substituting it into (5.22), and collecting the equations of the same order, we obtain

$$\begin{cases} m\partial_t^2 \boldsymbol{u}_0 + \mathscr{L}_0(\boldsymbol{u}_0) = \boldsymbol{0}, \\ \boldsymbol{u}_0|_{t=0} = \boldsymbol{u}^0, \quad \partial_t \boldsymbol{u}_1|_{t=0} = \boldsymbol{u}^1(\boldsymbol{x}), \end{cases} \tag{5.23}$$

and

$$\begin{cases} m\partial_t^2 \boldsymbol{u}_1 + \mathscr{L}_{\mathrm{lin}}(\boldsymbol{u}_0)\boldsymbol{u}_1 = -\mathscr{L}_1(\boldsymbol{u}_0), \\ \boldsymbol{u}_1|_{t=0} = \boldsymbol{0}, \quad \partial_t \boldsymbol{u}_1|_{t=0} = \boldsymbol{0}, \end{cases} \tag{5.24}$$

and

$$\begin{cases} m\partial_t^2 \boldsymbol{u}_2 + \mathscr{L}_{\mathrm{lin}}(\boldsymbol{u}_0)\boldsymbol{u}_2 = -\mathscr{L}_2(\boldsymbol{u}_0) \\ \qquad\qquad - \dfrac{\delta \mathscr{L}_1}{\delta \mathsf{A}} \boldsymbol{u}_1 - \dfrac{1}{2}\Big(\dfrac{\delta^2 \mathscr{L}_0}{\delta \mathsf{A}^2} \boldsymbol{u}_1\Big)\boldsymbol{u}_1, \\ \boldsymbol{u}_2|_{t=0} = \boldsymbol{0}, \quad \partial_t \boldsymbol{u}_2|_{t=0} = \boldsymbol{0}, \end{cases} \tag{5.25}$$

where $\mathscr{L}_{\mathrm{lin}}$ is the linearized operator of $\mathscr{L}_0$ at $\boldsymbol{u}_0$.

The existence of $\boldsymbol{u}_0$ follows from Theorem 3.1, while the existence of $\boldsymbol{u}_1$ and $\boldsymbol{u}_2$ is standard [28].

Lemma 5.3. *Under the same assumptions of Theorem 3.1,* $\boldsymbol{u}_0 = \boldsymbol{u}_{CB}$*. Moreover, if* $s > d/2+6$*, then there exist* $\boldsymbol{u}_1, \boldsymbol{u}_2 \in X_{T_1^*}$ *that satisfy* (5.24) *and* (5.25)*, respectively, where* T_1^* *is the same as that in Theorem 3.1.*

As a direct consequence of the above lemma and Theorem 3.1, we get

Lemma 5.4. *Define*

$$\widetilde{\boldsymbol{y}}(t) = \boldsymbol{x} + \boldsymbol{u}_{CB}(\boldsymbol{x},t) + \varepsilon \boldsymbol{u}_1(\boldsymbol{x},t) + \varepsilon^2 \boldsymbol{u}_2(\boldsymbol{x},t).$$

Under the same assumptions of Theorem 3.1 except that $s > d/2+6$, we have

$$|\, r(\widetilde{\boldsymbol{y}}(t)) \,| \le C\varepsilon^3, \qquad \text{for} \quad 0 \le t \le T_1^*, \tag{5.26}$$

where $r(\widetilde{\boldsymbol{y}}(t)) = \{r^i(\widetilde{\boldsymbol{y}}(t))\}_{i=1}^N = m\partial_t^2 \widetilde{\boldsymbol{y}}_i(t) + \mathscr{L}_\varepsilon(\widetilde{\boldsymbol{y}}_i(t))$.

We state a characterization of the $d-$norm, which is key to the results concerning the atomistic model. The proof of this characterization depends on the exploitation of the symmetry properties of the phonon spectra and the dynamical matrix [20].

Lemma 5.5. *If $\mathbf{0} \in \overset{\circ}{\mathscr{O}}_2(\Lambda_1)$, then*

$$\|\, \boldsymbol{z} \,\|_d \simeq \varepsilon^{d/2-1} \left(\sum_{i=1}^N \sum_{|\, \boldsymbol{x}_{ij} \,| = \varepsilon} |\, \boldsymbol{z}_i - \boldsymbol{z}_j \,|^2 \right)^{1/2}. \tag{5.27}$$

If $\nabla \boldsymbol{u} \in \overset{\circ}{\mathscr{O}}_2(\Lambda_1)$, then there exists a constant κ that depends on Λ_1 and d but independent of ε and t such that

$$\boldsymbol{z} \cdot \mathsf{H}\big(\boldsymbol{x} + \boldsymbol{u}(\boldsymbol{x},t)\big) \cdot \boldsymbol{z} \ge \kappa \varepsilon^{-1} \left(\sum_{i=1}^N \sum_{|\, \boldsymbol{x}_{ij} \,| = \varepsilon} |\, \boldsymbol{z}_i - \boldsymbol{z}_j \,|^2 \right)^{1/2}. \tag{5.28}$$

The characterization (5.27) is a special case of [11, Lemma 6.2 and Lemma 6.3], while the inequality (5.28) can be proved using arguments along the same line as that of [11, Lemma 6.2 and Lemma 6.3].

The next lemma is a perturbation result for $d-$norm. We define, for any $\boldsymbol{z} \in \mathbb{R}^{N\times d}$, a discrete $W^{1,\infty}-$norm by

$$|\, \boldsymbol{z} \,|_{1,\infty} := \varepsilon^{-1} \max_{1\le i\le N} |\, D\boldsymbol{z}_i \,|. \tag{5.29}$$

Lemma 5.6. [11, Lemma 6.6] *If there exists a constant κ such that*

$$\varepsilon^d \boldsymbol{z}^T \mathsf{H}(\boldsymbol{y}_1) \boldsymbol{z} \ge \kappa \|\boldsymbol{z}\|_d^2 \qquad \text{for all} \quad \boldsymbol{z} \in \mathbb{R}^{N\times d}. \tag{5.30}$$

Then there exists a constant δ such that for any $\boldsymbol{y}_2$ satisfying $|\, \boldsymbol{y}_1 - \boldsymbol{y}_2 \,|_{1,\infty} \le \delta$, we have

$$\varepsilon^d \boldsymbol{z}^T \mathsf{H}(\boldsymbol{y}_2) \boldsymbol{z} \ge \frac{\kappa}{2} \|\boldsymbol{z}\|_d^2 \qquad \text{for all} \quad \boldsymbol{z} \in \mathbb{R}^{N\times d} \tag{5.31}$$

for sufficiently small ε.

Now we are ready to prove Theorem 3.2.

Proof of Theorem 3.2 Given $\alpha \in (1, 3-d/2)$ with $d = 1,2,3$, define

$$\begin{aligned} B_T := \{\, \boldsymbol{y}(t) \in \mathbb{R}^{N\times d} \;\; |\; \varepsilon^{d/2} \|\, \partial_t(\boldsymbol{y} - \widetilde{\boldsymbol{y}})(t) \,\|_{\ell_2} + \|\, (\boldsymbol{y} - \widetilde{\boldsymbol{y}})(t) \,\|_d < \varepsilon^{\alpha + d/2} \quad 0 < t < T, \\ \boldsymbol{y}|_{t=0} = \boldsymbol{x} + \boldsymbol{u}^0(\boldsymbol{x}), \quad \partial_t \boldsymbol{y}|_{t=0} = \boldsymbol{u}^1(\boldsymbol{x}) \}. \end{aligned}$$

Define a mapping $F : B_T \to B_T$ as follows: for any $\boldsymbol{y} \in B_T$, let $F(\boldsymbol{y})$ be the solution of system

$$\begin{cases} m\partial_t^2 \big(F(\boldsymbol{y}) - \widetilde{\boldsymbol{y}}\big) + \displaystyle\int_0^1 (1-s) \mathsf{H}(\boldsymbol{y}^s(t)) \mathrm{d}s \cdot (F(\boldsymbol{y}) - \widetilde{\boldsymbol{y}}) = -r(\widetilde{\boldsymbol{y}}(t)), \\ F(\boldsymbol{y})|_{t=0} = \boldsymbol{x} + \boldsymbol{u}^0(\boldsymbol{x}), \quad \partial_t F(\boldsymbol{y})|_{t=0} = \boldsymbol{u}^1(\boldsymbol{x}), \end{cases} \tag{5.32}$$

where $\boldsymbol{y}^s(t) = s\boldsymbol{y}(t) + (1-s)\widetilde{\boldsymbol{y}}(t)$. Denote $\boldsymbol{z} = F(\boldsymbol{y}) - \widetilde{\boldsymbol{y}}, \mathcal{H}(t) = \int_0^1 (1-s)\mathsf{H}(\boldsymbol{y}^s)\mathrm{d}s$ and

$$E_d(t) = m\|\,\partial_t \boldsymbol{z}\,\|_{\ell_2}^2 + \boldsymbol{z}\cdot\mathcal{H}(t)\cdot\boldsymbol{z}.$$

We write (5.32) as

$$m\partial_t^2\boldsymbol{z} + \mathcal{H}(t)\cdot\boldsymbol{z} = -r(\widetilde{\boldsymbol{y}}) \tag{5.33}$$

with the initial conditions

$$\boldsymbol{z}|_{t=0} = \boldsymbol{0}, \qquad \partial_t\boldsymbol{z}|_{t=0} = \boldsymbol{0},$$

which implies $E_d(0) = 0$.

Multiplying both sides of (5.33) with $\partial_t\boldsymbol{z}$, and summing by parts, we get

$$\frac{1}{2}\frac{\partial}{\partial t}\big(m\|\,\partial_t\boldsymbol{z}\,\|_{\ell_2}^2 + \boldsymbol{z}\cdot\mathcal{H}(t)\cdot\boldsymbol{z}\big) = \frac{1}{2}\boldsymbol{z}\cdot\partial_t\mathcal{H}(t)\cdot\boldsymbol{z} - r(\widetilde{\boldsymbol{y}})\cdot\partial_t\boldsymbol{z}. \tag{5.34}$$

By the translation invariance of $\partial_t\mathcal{H}$ and using (5.27), we can easily bound

$$\begin{aligned}|\,\boldsymbol{z}\cdot\partial_t\mathcal{H}(t)\cdot\boldsymbol{z}\,| &\le C\varepsilon^{-2}|\,\partial_t\boldsymbol{y}^s\,|_{1,\infty}\sum_{i=1}^N\sum_{|\,\boldsymbol{x}_{ij}\,|=\varepsilon}|\,\boldsymbol{z}_i - \boldsymbol{z}_j\,|^2\\ &\le C|\,\partial_t\boldsymbol{y}^s\,|_{1,\infty}(\varepsilon^{-d}\|\,\boldsymbol{z}\,\|_d^2).\end{aligned}$$

Using the fact that $\|\,\partial_t(\boldsymbol{y}-\widetilde{\boldsymbol{y}})(t)\,\|_{\ell_2} < \varepsilon^\alpha$, we have

$$|\,\partial_t(\boldsymbol{y}-\widetilde{\boldsymbol{y}})(t)\,|_{1,\infty} \le \varepsilon^{-1}\|\,\partial_t(\boldsymbol{y}-\widetilde{\boldsymbol{y}})(t)\,\|_{\ell_2} \le \varepsilon^{\alpha-1} \le C$$

since $\alpha > 1$. This inequality together with

$$|\,\partial_t\widetilde{\boldsymbol{y}}(t)\,|_{1,\infty} \le C(\|\partial_t\boldsymbol{u}_0\|_{1,\infty} + \varepsilon\|\partial_t\boldsymbol{u}_1\|_{1,\infty} + \varepsilon^2\|\partial_t\boldsymbol{u}_2\|_{1,\infty})$$

leads to

$$|\,\partial_t\boldsymbol{y}^s(t)\,|_{1,\infty} \le |\,\partial_t(\boldsymbol{y}-\widetilde{\boldsymbol{y}})(t)\,|_{1,\infty} + |\,\partial_t\widetilde{\boldsymbol{y}}(t)\,|_{1,\infty} \le C.$$

Combining the above two inequalities, we obtain

$$|\,\boldsymbol{z}\cdot\partial_t\mathcal{H}(t)\cdot\boldsymbol{z}\,| \le C\varepsilon^{-d}\|\,\boldsymbol{z}\,\|_d^2. \tag{5.35}$$

Since $\nabla\boldsymbol{u}^0 \in \mathring{\mathscr{O}}_2(\Lambda_1)$, by (5.28), there exists κ such that

$$\boldsymbol{z}\cdot\mathsf{H}\big(\boldsymbol{x}+\boldsymbol{u}^0(\boldsymbol{x})\big)\cdot\boldsymbol{z} \ge \kappa\varepsilon^{-d}\|\,\boldsymbol{z}\,\|_d^2.$$

Note that

$$|\,\boldsymbol{y}_{\mathrm{CB}}(t) - \boldsymbol{x} - \boldsymbol{u}^0(\boldsymbol{x})\,|_{1,\infty} \le t|\,\partial_t\boldsymbol{u}_{\mathrm{CB}}(\boldsymbol{x},t)\,|_{1,\infty} \le c_* t\|\partial_t\boldsymbol{u}_{\mathrm{CB}}\|_{H^s} \le c_* K_0 t.$$

For δ in Lemma 5.6, there exists $T_4 = \delta/(3c_*K_0)$ such that for any $0 < t < T_4$, we have

$$|\,\boldsymbol{y}_{\mathrm{CB}}(t) - \boldsymbol{x} - \boldsymbol{u}^0(\boldsymbol{x})\,|_{1,\infty} < \delta/3.$$

Next, for any $0 < t < T_1^*$, we have, for sufficiently small ε,

$$|\,(\widetilde{\boldsymbol{y}} - \boldsymbol{y}_{\mathrm{CB}})(t)\,|_{1,\infty} \le C\varepsilon(\|\nabla\boldsymbol{u}_1\|_{L^\infty} + \varepsilon\|\nabla\boldsymbol{u}_2\|_{L^\infty}) \le C\varepsilon < \delta/3,$$

and

$$|\,(\boldsymbol{y}-\widetilde{\boldsymbol{y}})(t)\,|_{1,\infty} \le C\varepsilon^{-d/2}\|\,(\boldsymbol{y}-\widetilde{\boldsymbol{y}})(t)\,\|_d \le C\varepsilon^\alpha < \delta/3.$$

Therefore,

$$\begin{aligned}|\,\boldsymbol{y}^s(t) - \boldsymbol{x} - \boldsymbol{u}^0(\boldsymbol{x})\,|_{1,\infty} &\le |\,(\boldsymbol{y}^s - \boldsymbol{y}_{\mathrm{CB}})(t)\,|_{1\,\infty} + |\,\boldsymbol{y}_{\mathrm{CB}}(t) - \boldsymbol{x} - \boldsymbol{u}^0(\boldsymbol{x})\,|_{1,\infty}\\ &\le s|\,(\boldsymbol{y}-\widetilde{\boldsymbol{y}})(t)\,|_{1,\infty} + |\,(\widetilde{\boldsymbol{y}} - \boldsymbol{y}_{\mathrm{CB}})(t)\,|_{1,\infty} + |\,\boldsymbol{y}_{\mathrm{CB}}(t) - \boldsymbol{x} - \boldsymbol{u}^0(\boldsymbol{x})\,|_{1,\infty}\\ &< \delta.\end{aligned}$$

By Lemma 5.6, we have

$$\boldsymbol{z}\cdot\mathcal{H}(t)\cdot\boldsymbol{z}=\boldsymbol{z}\cdot\int_0^1(1-s)\mathsf{H}(\boldsymbol{y}^s)\,ds\cdot\boldsymbol{z}\geq(\kappa/2)\varepsilon^{-d}\|\,\boldsymbol{z}\,\|_d^2,$$

which together with (5.35) leads to

$$|\,\boldsymbol{z}\cdot\partial_t\mathcal{H}\cdot\boldsymbol{z}\,|\leq C_1\boldsymbol{z}\cdot\mathcal{H}(t)\cdot\boldsymbol{z}.$$

Using Lemma 5.4, we get

$$|\,r(\widetilde{\boldsymbol{y}}(t))\cdot\partial_t\boldsymbol{z}\,|\leq C\varepsilon^{3-d/2}\|\,\partial_t\boldsymbol{z}\,\|_{\ell_2}.$$

Substituting the above two estimates into (5.34), we obtain

$$\frac{d}{dt}E_d(t)\leq CE_d(t)+C\varepsilon^{6-d}. \tag{5.36}$$

It follows from Grownwall's inequality that

$$E_d(t)\leq Ce^{Ct}\varepsilon^{6-d}\qquad\text{for any } 0<t<T_2^*=\min(T_1^*,T_4).$$

Therefore, for any $0<t<T_2^*$,

$$\varepsilon^{d/2}\|\,\partial_t(\boldsymbol{y}-\widetilde{\boldsymbol{y}})(t)\,\|_{\ell_2}+\|\,(\boldsymbol{y}-\widetilde{\boldsymbol{y}})(t)\,\|_d\leq Ce^{Ct}\varepsilon^3<\varepsilon^{\alpha+d/2}$$

for sufficiently small ε. We thus conclude $F(\boldsymbol{y})\in B_{T_2^*}$. The existence of $\boldsymbol{y}$ follows from fixed point principle. Moreover, we conclude that $\boldsymbol{y}$ satisfies (3.1).

Repeating the procedure that led to (5.36), we conclude that the solution $\boldsymbol{y}$ is locally unique. Let $T^*=T_2^*$, we obtain, for $0\leq t<T^*$,

$$\|\,(\boldsymbol{y}-\boldsymbol{y}_{\mathrm{CB}})(t)\,\|_d\leq\|\,(\boldsymbol{y}-\widetilde{\boldsymbol{y}})(t)\,\|_d+\|\,(\widetilde{\boldsymbol{y}}-\boldsymbol{y}_{\mathrm{CB}})(t)\,\|_d\leq\varepsilon^{\alpha+d/2}+C\varepsilon\leq C\varepsilon,$$

since $\alpha+d/2>1$ for $d=1,2,3$. This gives (3.11).

The maximality of T^* is obviously characterized by (3.10). □

Remark 5.7. *We only consider the initial value problems for both the continuum model and the atomistic model. The extension of Theorem 3.1 to the initial-boundary value problem is straightforward by* [9]*. However, the extension of Theorem 3.2 is much more involved since the surface wave effects has to be taken into account* [22]*. From a technical point of view, the auxiliary higher-order approximation* $\widetilde{\boldsymbol{y}}$ *is required to approximate the boundary condition to the higher-order. We believe that the construction in* [10] *is useful to that end.*

References

[1] Adams, R. A., Fournier, J.J.F. Sobolev Spaces, 2nd edition, Academic Press, 2003

[2] Ashcroft. N.W., Mermin, N.D. Solid State Physics, Saunders College Publishing, 1976

[3] Blanc, X., Le Bris, C., Lions, P.-L. From Molecular Models to Continuum Mechanics. *Arch. Ration. Mech. Anal.*, 2002, 164: 341–381

[4] Born, M. Dynamik der Kristallgitter, B. G. Teubner, Leipzig-Berlin, 1915

[5] Born, M., Huang, K. Dynamical Theory of Crystal Lattices, Oxford University Press, 1954

[6] Braides, A., Dal Maso, G., Garroni, A. Variational Formulation of Softening Phenomena in Fracture Mechanics: the One-dimensional Case. *Arch. Ration. Mech. Anal.,* 1999, 146: 23–58

[7] Cauchy, A.-L. Sur l'equilibre et le Muvement d'un Systéme de Points Materiels Sollicités par Forces d'attratction ou de Réulsion Mutuelle. *Ex. de Math.,* 1827, 3: 227–287

[8] Conti, S., Dolzmann, G., Kirchheim, B., Müller, S. Sufficient Conditions for the Validity of the Cauchy-Born Rule Close to $SO(n)$. *J. Eur. Math. Soc.,* 2006, 8: 515–530

[9] Dafermos, C.M., Hrusa, W.J. Energy Methods for Quasilinear Hyperbolic Initial-boundary Value Problems. Applications to Elastodynamics. *Arch. Ration. Mech. Anal.,* 1985, 87: 267–292

[10] E, W., Liu, J.G. Projection Method. I. Convergence and Numerical Boundary Layers. *SIAM J. Numer. Anal.,* 1995, 32: 1017–1057

[11] E, W., Ming, P.-B. Cauchy-Born Rule and the Stability of Crystalline Solids: Static Problems. *Arch. Ration. Mech. Anal.,* to appear

[12] Ericksen, J.L. The Cauchy and Born Hypotheses for Crystals. In: Phase Transformations and Material Instabilities in Solids. ed. by M.E. Gurtin, Academic Press, 1984, 61–77

[13] Friesecke, G., Theil, F. Validity and Failure of the Cauchy-Born Hypothesis in a Two Dimensional Mass-spring Lattice. *J. Nonlinear Sci.,* 2002, 12: 445–478

[14] Hughes, T.J.R., Kato, T., Marsden, J. Well-posed Quasi-linear Second-order Hyperbolic Systems with Applications to Nonlinear Elastodynamics and General Relativity. *Arch. Ration. Mech. Anal.,* 1977, 63: 273–294

[15] Keating, P.N. Effect of Invariance Requirements on the Elastic Strain Energy of Crystals with Application to the Diamond Structure. *Phys. Rev.,* 1965, 145: 637–645

[16] Lennard-Jones, J.E., Devonshire, A.F. Critical and Cooperative Phenomena. III. A Theory of Melting and the Structure of Liquids. *Proc. Roy. Soc. Lond. A.,* 1939, 169: 317–338

[17] Liu, F., Ming, P.-B. Crystal Stability and Instability. In preparation

[18] Love, A.E.H. A Treatise on the Mathematical Theory of Elasticity, 4th ed, Cambridge University Press, 1927

[19] Majda, A. Compressible Fluid Flow and Systems of Conservation Laws in Several Space Variables. Springer-Verlag, New York, Inc., 1984

[20] Maradudin, A.A., Vosko, S.H. Symmetry Properties of the Normal Vibrations of a Crystal. *Rev. Mod. Phy.,* 1968, 40: 1–37

[21] Morrey, C.B. Multiple Integrals in the Calculus of Variations. Springer-Verlag, New York, 1966

[22] Musgrave, M.J.P. Crystal Acoustics: Introduction to the Study of Elastic Waves and Vibrations in Crystals. Holden-Day, Inc., San Francisco, 1970

[23] Parry, G.P. On Phase Transitions Involving Internal Strain. *Int. J. Solids Structures,* 1981, 17: 361–378

[24] Pitteri, M. On $\nu+1-$Lattices. *J. of Elasticity,* 1985, 15: 3–25

[25] Pitteri, M., Zanzotto, G. Continuum Models for Phase Transitions and Twinning in Crystals. Chapman & Hall/CRC Press LLC, 2003

[26] Ruelle, D. Statistical Mechanics: Rigorous Results. Imperial College Press, 3rd ed, 1998

[27] Schochet, S. The Incompressible Limit in Nonlinear Elasticity. *Comm. Math. Phys.,* 1985, 102: 207–215

[28] Shatah, J., Struwe, M. Geometric Wave Equations. American Mathematical Society, Providence, R.I. 2000

[29] Stakgold, I. The Cauchy Relations in a Molecular Theory of Elasticity. *Quart. Appl. Math.,* 1950, 8: 169–186

[30] Strang, G. Accurate Partial Difference Methods. II: Non-linear Problems. *Numer. Math.,* 1964, 6: 37–46

[31] Wallace, D.C. Thermodynamics of Crystals. John Wiley & Sons Inc., New York, 1972

[32] Weiner, J.H. Statistical Mechanics of Elasticity. A Wiley-Interscience Publication, 1983

[33] Xuan, Y., E, W. Instability of Crystalline Solids under Stress. In preparation.

[34] Zanzotto, G. On the Material Symmetry Group of Elastic Crystals and the Born Rule. *Arch. Ration. Mech. Anal.,* 1992, 121: 1–36

[35] Zanzotto, G. The Cauchy and Born Hypothesis, Nonlinear Elasticity and Mechanical Twinning in Crystals. *Acta Cryst.,* 1996, A52: 839–849

Department of Mathematics and PACM, Princeton University

E-mail address: weinan@Princeton.EDU

LSEC, Institute of Computational Mathematics and Scientific/Engineering Computing, AMSS, Chinese Academy of Sciences, No. 55. Zhong-Guan-Cun East Road, Beijing, 100080, China

E-mail address: mpb@lsec.cc.ac.cn