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ARTICLE TYPE

Existence of weak solutions and numerical simulations for a new phase-field model with periodic boundary conditions†

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Summary

This article is concerned with an initial-boundary value problem (IBVP) for a new phase-field model describing the evolution of structural phase transition in elastically deformable solid materials. The model consists of an elliptic-parabolic system in which the displacement field and the order parameter both satisfy periodic boundary conditions. We prove the existence of global solutions to this IBVP by applying the method of continuation of local solutions and perform numerical simulations to investigate the microstructure evolution of MnNi alloys by using this new phase-field model.

KEYWORDS:
existence of weak solutions, elliptic-parabolic system, phase transition, phase-field simulations

1 | INTRODUCTION

Martensitic transformation is a diffusionless, solid-to-solid phase transformation commonly observed in various metals and alloys. Materials undergoing this phase transformation often lead to significant changes in material properties, which can be beneficial or harmful as well[1]. Transformation is mainly dominated by chemical energy, interfacial energy, elastic strain energy and applied external energy. The elastic strain energy stems from the lattice misfit between parent and product phases is the resistance of martensitic transformation and determines the evolution direction of microstructure in phase transition. The martensite phase grows and shrinks elastically during cooling and heating is called thermoelastic martensite, it refers to the interface between martensite and austenite phases can move reversibly, crystal undergoing a thermoelastic martensitic transformation often exhibit shape memory effect[2,3], which has been widely used in temperature automatic regulator, automatic positioner, artificial satellite antenna and so on.

The physical and mechanical properties of materials on the macroscopic scale highly depend on their microstructure. Because the positions of the sharp interfaces change with time in some microstructure evolution, so it is a typical free-moving boundary value problem, which is difficult to solve mathematically. However, the phase-field method employs a set of conserved or non-conserved field variables, these are continuous functions of space and time, hence the interfacial regions in a phase-field model are diffuse, separating the adjoining phases and domains, then the total free energy may include chemical energy, interfacial energy, elastic strain energy and applied external energy are dependent continuously on the field variables.

During the last few decades, the phase-field approach has emerged as one of the most powerful approaches for predicting morphological and microstructure evolution in materials at the mesoscale, including solidification[4], phase transition in thin

†This is an example for title footnote.
[0]**Abbreviations:** ANA, anti-nuclear antibodies; APC, antigen-presenting cells; IRF, interferon regulatory factor

films[5] and martensitic transformation in metallic materials[6]. It has been demonstrated that the microstructure predicted by phase-field method agrees well with experimental results. Phase-field method avoids the difficulty of describing the sharp interface, and has the unique advantage in simulating arbitrary structure and complex microstructure evolution in materials.

There are two famous phase-field models for the evolution of field variables: the Cahn-Hilliard nonlinear diffusion equation[7] used to describe the evolution of conserved field variables such as atomic concentration, and the time-dependent Ginzburg-Landau (Allen-Cahn) equation[8,9] used of representing the variation of the non-conserved field variables, for instance, orientation field in martensitic transformation. A large number of achievements have been made in theory[10,11,12,13,14] and numerical studies[1,2,3,4,5,6,15] of those two models.

In this study, we investigate a new phase-field model derived by Alber and Zhu[16] that is more suitable for structural transitions such as martensitic transformation in shape memory alloys. The new phase-field model differs from the well-known Allen-Cahn model by a nonlinear gradient term for the order parameter. We will study this elliptic-parabolic coupled system where the displacement field and the order parameter both satisfy periodic boundary conditions.

We first introduce the new phase-field model in three space dimensions. Let $\Omega \subset \mathbb{R}^3$ be an open set, it represents the material points of a solid body. The different phases are characterized by the order parameter $S(t,x) \in \mathbb{R}$, a value of $S(t,x)$ near to 0 indicates that the material is in the parent phase at the point $x \in \Omega$ at time t; a value near to 1 (or -1) indicates that the material is in the product phase. The other unknowns are the displacement $u(t,x) \in \mathbb{R}^3$ of the material point x at time t and the Cauchy stress tensor $\sigma(t,x) \in \mathcal{S}^3$, where $\mathcal{S}^3$ denotes the set of symmetric 3×3-matrices. Then the unknowns must satisfy the following quasi-static equations (we name it the Alber-Zhu model)

$$-\mathrm{div}_x \sigma(t,x) = b(t,x), \tag{1}$$

$$\sigma(t,x) = D(\varepsilon(\nabla_x u(t,x)) - \bar{\varepsilon} S(t,x)), \tag{2}$$

$$S_t(t,x) = -c(\psi_S(\varepsilon(\nabla_x u(t,x)), S(t,x)) - \nu \Delta_x S(t,x))|\nabla_x S(t,x)| \tag{3}$$

for $(t,x) \in (0,\infty) \times \Omega$. Here $D : \mathcal{S}^3 \to \mathcal{S}^3$ is a linear, symmetric, positive definite mapping, the elastic modulus of materials; $\nabla_x u(t,x)$ denotes the 3×3-matrix of the first order spatial derivatives of u, the deformation gradient; $\varepsilon(\nabla_x u) = \frac{1}{2}(\nabla_x u + (\nabla_x u)^{\mathrm{T}})$ is the strain tensor; $\bar{\varepsilon} \in \mathcal{S}^3$ is a given matrix, the misfit strain; $c > 0$ is a constant, the kinetic coefficient which characterizes the interface mobility and $\nu > 0$ represents the interfacial energy coefficient. The total free energy density of the system is

$$\psi^*(\varepsilon, S, \nabla_x S) = \psi(\varepsilon, S) + \frac{\nu}{2}|\nabla_x S|^2, \tag{4}$$

the second term on the right-hand side of (4) denotes the interfacial energy density caused by nonhomogeneous distribution of the order parameter, and

$$\psi(\varepsilon, S) = \frac{1}{2}(D(\varepsilon - \bar{\varepsilon}S)) \cdot (\varepsilon - \bar{\varepsilon}S) + \hat{\psi}(S), \tag{5}$$

here, the first term represents the elastic strain energy density caused by lattice mismatch between parent and product phases, the scalar product of two matrices is $A \cdot B = \sum a_{ij} b_{ij}$, $\hat{\psi}(S)$ is the chemical free energy density of the system. We choose $\hat{\psi}(S) \in C^\infty(\mathbb{R};\mathbb{R})$ is a polynomial with at least two minimum points and one maximum point between them

$$\hat{\psi}(S) = A_0 S^{2k+2} + \sum_{i=1}^{2k+2} A_i S^{2k+2-i}, \quad A_0 \text{ is a positive constant}, \tag{6}$$

where $k \in N^+$ and A_i $(i = 1 \ldots 2k+2)$ are the arbitrary constants. To simplify the writing in Section 3, we let

$$\psi^*(\varepsilon, S, \nabla_x S) = \psi_1^*(\varepsilon, S, \nabla_x S) + \psi_2^*(S), \tag{7}$$

here,

$$\psi_1^*(\varepsilon, S, \nabla_x S) = \frac{\nu}{2}|\nabla_x S|^2 + \frac{1}{2}(D(\varepsilon - \bar{\varepsilon}S)) \cdot (\varepsilon - \bar{\varepsilon}S) + A_0 S^{2k+2} \tag{8}$$

is a positive term, and

$$\psi_2^*(S) = \sum_{i=1}^{2k+2} A_i S^{2k+2-i}. \tag{9}$$

Given are the volume force $b : [0,\infty) \times \Omega \to \mathbb{R}^3$ and $S_0 : \Omega \to \mathbb{R}$. This completes the formulation of the new phase-field model.

Remark 1. When the gradient term $|\nabla_x S(t,x)|$ in (3) disappears, it becomes the classical Allen-Cahn equation.

In multidimensional space, $|\nabla_x S|\Delta_x S$ in (3) can't be written in divergence type, then it has some difficulties to prove the existence of weak solutions in this case, but $|S_x|S_{xx}$ can be written in the divergence form $\frac{1}{2}(S_x|S_x|)_x$ in one space dimension. We next simplify the model to a one-dimensional case and give the main results of this paper.

Let $\Omega = (a, d)$ is a bounded open interval with constants $a < d$ and write $Q_{T_e} := (0, T_e) \times \Omega$, T_e is a positive constant. If we denote the first column of matrix $\sigma(t, x)$ by $\sigma_1(t, x)$ and let $\varepsilon(u_x) = \frac{1}{2}(u_x, 0, 0) + (u_x, 0, 0)^{\mathrm{T}})$. Then, we consider the periodic boundary conditions, the unknown functions (u, σ, S) satisfy the following initial-boundary value problem (IBVP)

$$-\sigma_{1x} = b, \tag{10}$$

$$\sigma = D(\varepsilon(u_x) - \bar{\varepsilon}S), \tag{11}$$

$$S_t = -c(\hat{\psi}'(S) - \bar{\varepsilon}\cdot\sigma - \nu S_{xx})|S_x| \tag{12}$$

for $(t, x) \in (0, \infty) \times \Omega$. The periodic boundary and initial conditions are

$$u|_{x=a} = u|_{x=d}, \quad \frac{\partial u}{\partial x}|_{x=a} = \frac{\partial u}{\partial x}|_{x=d}, \tag{13}$$

$$S|_{x=a} = S|_{x=d}, \quad \frac{\partial S}{\partial x}|_{x=a} = \frac{\partial S}{\partial x}|_{x=d}, \tag{14}$$

$$S(0, x) = S_0(x), \quad x \in \Omega. \tag{15}$$

Next, we denote $H^m_{\mathrm{per}}(\Omega)$ $(W^{m,p}_{\mathrm{per}}(\Omega))$ the Sobolev spaces with periodic boundary conditions, X' denotes the dual space of X. Because of $\frac{1}{2}(y|y|)' = |y|$, (12) is equivalent to

$$S_t - \frac{c\nu}{2}(S_x|S_x|)_x - c(\sigma\cdot\bar{\varepsilon} - \hat{\psi}'(S))|S_x| = 0,$$

then the definition of weak solutions to IBVP (10)-(15) as follows.

Definition 1. Let $S_0 \in L^2(\Omega)$, $b \in L^\infty(0, T_e; L^2(\Omega))$. A function (u, σ, S) with

$$u \in L^\infty(0, T_e; H^2_{\mathrm{per}}(\Omega)), \quad \sigma \in L^\infty(0, T_e; H^1_{\mathrm{per}}(\Omega)), \tag{16}$$

$$S \in L^\infty(0, T_e; H^1_{\mathrm{per}}(\Omega)), \tag{17}$$

is a weak solution to IBVP (10)-(15) if (10), (11), (13) are satisfied weakly, and if for all $\varphi \in C_0^\infty(-\infty, T_e; C^\infty_{\mathrm{per}}(\Omega))$,

$$(S, \varphi_t)_{Q_{T_e}} - \frac{c\nu}{2}(S_x|S_x|, \varphi_x)_{Q_{T_e}} + c((\sigma\cdot\bar{\varepsilon} - \hat{\psi}'(S))|S_x|, \varphi)_{Q_{T_e}} + (S_0, \varphi(0))_\Omega = 0. \tag{18}$$

The main result of this article is

Theorem 1. For all $S_0 \in H^1_{\mathrm{per}}(\Omega)$ and $b \in L^2(Q_{T_e})$ with $b_t \in L^2(Q_{T_e})$, there exists a weak solution (u, σ, S) to IBVP (10)-(15), which in addition to (16)-(18) satisfies

$$S_t \in L^{\frac{4}{3}}(Q_{T_e}), \;\; \sigma_t \in L^{\frac{4}{3}}(Q_{T_e}), \tag{19}$$

$$S_x|S_x| \in L^{\frac{4}{3}}(0, T_e; W^{1,\frac{4}{3}}_{\mathrm{per}}(\Omega)), \quad S_x \in L^{\frac{8}{3}}(0, T_e; L^\infty(\Omega)), \tag{20}$$

$$|S_x|S_{xt} \in L^1(0, Te; (H^2_{\mathrm{per}}(\Omega))'). \tag{21}$$

Alber and Zhu proved the existence of weak solutions in one space dimension if u satisfies Dirichlet boundary condition, S satisfy Dirichlet boundary condition [16] and Neumann boundary condition [17], then they studied the global existence of viscosity solutions to this new phase-field model with u and S both satisfy Dirichlet boundary conditions [18]. They introduced a little parameter $\kappa > 0$ to regularize term $|S_x|$ in (12), then it can be approximated as a uniformly parabolic equation, when S is given, u satisfies Dirichlet boundary condition, u and σ can be expressed in terms of S, then (10)-(15) can be reduced to a single equation. However, we can't reduce (10)-(15) into a single equation when u and S both satisfy periodic boundary conditions, then the method in the above paper is not applicable. The theoretical analyses for this new phase-field model from various aspects we refer to [19,20,21,22,23]. The above results for this new phase-field model with elastic effect, however, do not consider the numerical simulations.

In our previous work [24], we omitted the effect of elasticity, that is, without equations (10) and (11), and proved the existence and large-time behavior of weak solutions with u and S both satisfy periodic boundary conditions, furthermore, chose MnNi alloys as the prototype materials to study the microstructure evolution of martensitic transformation by employing that model. We have validated that the martensite variants distribute randomly with the shape of little pieces and exhibit no directionality. However, due to the difference of lattice parameters between austenite and martensite phases, elastic stress will be generated during martensitic transformation, and the elastic strain energy is the most important factor for determining the evolution direction of martensite variants. In present study, we add elastic strain energy to the total free energy and discover that the different variants appear alternately and form a self-accommodation twinned substructure, furthermore, the martensite variants arrange along diagonal with plate-like shape. These results are consistent with the results obtained by applying the Allen-Cahn model when we use the identical material parameters, but it takes less time to achieve its equilibrium state in the Alber-Zhu system.

The main difficulties of theoretical proofs and numerical simulations come from the term $|S_x|$ in (12), because of this term, equation (12) is degenerate, and it is not differentiable with respect to S_x.

The remaining Section 2 and Section 3 are devoted to the proof of Theorem 1. We prove the existence of local solutions to IBVP (10)-(15) by using iteration method combining with Aubin-Lions lemma and weak compactness lemma in Section 2. Since the estimates in Section 2 only for a sufficiently small time t_0, so we drive uniform *a priori* estimates in Section 3 then that imply the global solutions exist for any time T_e. At last, we choose actual material parameters and perform a series of numerical simulations by employing this new phase-field model to demonstrate the microstructure evolution of martensitic transformation in MnNi alloys.

2 | EXISTENCE OF LOCAL SOLUTIONS

Assume that t_0 is a sufficiently small constant and $\|\hat{S}\|_{L^\infty(0,t_0;H^1_{\mathrm{per}}(\Omega))} \leq K$, K is related to the norm of initial value. We first replace S by $\hat{S}$ in (11), we have proved that, for a given $\hat{S}$, IBVP (10)-(15) has a solution global in time by Galerkin method[24]. Then we replace $\hat{S}$ by S^{n-1}, IBVP (10)-(15) becomes

$$-\sigma^n_{1x} = b, \tag{22}$$

$$\sigma^n = D(\varepsilon(u^n_x) - \bar{\varepsilon}S^{n-1}), \tag{23}$$

$$S^n_t = -c(\hat{\psi}'(S^n) - \bar{\varepsilon}\cdot\sigma^n - \nu S^n_{xx})|S^n_x| \tag{24}$$

for $(t,x) \in (0,\infty)\times\Omega$. The periodic boundary and initial conditions are

$$u^n|_{x=a} = u^n|_{x=d}, \quad \frac{\partial u^n}{\partial x}|_{x=a} = \frac{\partial u^n}{\partial x}|_{x=d}, \tag{25}$$

$$S^n|_{x=a} = S^n|_{x=d}, \quad \frac{\partial S^n}{\partial x}|_{x=a} = \frac{\partial S^n}{\partial x}|_{x=d}, \tag{26}$$

$$S^n(0,x) = S^n_0(x), \quad x \in \Omega. \tag{27}$$

We next perform uniform *a priori* estimates independent of n. We choose for every n a function $S^n_0 \in C^\infty_{\mathrm{per}}(\Omega)$ such that

$$\|S^n_0 - S_0\|_{H^1_{\mathrm{per}}(\Omega)} \to 0, \quad n \to \infty, \tag{28}$$

where $S_0 \in H^1_{\mathrm{per}}(\Omega)$ is the initial data given in Theorem 1. Then we get the following results.

Theorem 2. For all $b \in L^2(Q_{t_0})$ with $b_t \in L^2(Q_{t_0})$, there exists a local solution (u,σ,S) to IBVP (10)-(15) for $t \in [0,t_0]$ satisfies

$$S_t \in L^{\frac{3}{2}}(Q_{t_0}), \ \ \sigma_t \in L^{\frac{3}{2}}(Q_{t_0}), \tag{29}$$

$$S_x|S_x| \in L^{\frac{3}{2}}(0,t_0;W^{1,\frac{3}{2}}_{\mathrm{per}}(\Omega)), \quad S_x \in L^3(0,t_0;L^\infty(\Omega)), \tag{30}$$

$$|S_x|S_{xt} \in L^1(0,t_0;(H^2_{\mathrm{per}}(\Omega))'). \tag{31}$$

In what follows, the norm of $L^2(\Omega)$ is denoted by $\|\cdot\|$ and the letter C is a universal positive constant independent of n. In order to prove Theorem 2, we need the following conclusions.

Lemma 1. There holds for any $t \in [0, t_0]$

$$\frac{1}{2}\|S^n\|^2 + \frac{c\nu}{8}\int_0^{t_0} \|S_x^n\|^3_{L^3(\Omega)} d\tau + C\int_{Q_{t_0}} (S^n)^{2k+2}|S_x^n| d(\tau, x) \le C. \tag{32}$$

Proof. Multiplying (24) by S^n, applying the relationship $|S_x^n|S_{xx}^n = \frac{1}{2}(S_x^n|S_x^n|)_x$ and integrating the resulting equation with respect to x over Ω, we have

$$(S_t^n, S^n) + \frac{c\nu}{2}(S_x^n|S_x^n|, S_x^n) - c\bar{\varepsilon}(\sigma^n|S_x^n|, S^n) + c(\hat{\psi}'(S^n)|S_x^n|, S^n) = 0. \tag{33}$$

From the elliptic regularity theory for (22)-(23), thanks to the Sobolev embedding theorem, we obtain $\|\sigma^n\|_{L^\infty(Q_{t_0})} \le CK$. Using the definition of $\hat{\psi}(S)$ in (6), invoking the Young inequality and Hölder's inequality, that for all $t \in [0, t_0]$

$$\begin{aligned}
&\frac{1}{2}\frac{d}{dt}||S^n||^2 + \frac{c\nu}{2}\|S_x^n\|^3_{L^3(\Omega)} + 2c(k+1)A_0\int_\Omega (S^n)^{2k+2}|S_x^n| dx \\
&\le C\int_\Omega \sum_{i=1}^{2k+1} |A_i||S^n|^{2k+2-i}|S_x^n| dx + c|\bar{\varepsilon}|\int_\Omega |\sigma^n||S_x^n||S^n| dx \\
&:= C\int_\Omega \sum_{i=1}^{2k+1} |A_i||S^n|^{2k+2-i}|S_x^n| dx + I,
\end{aligned} \tag{34}$$

where

$$\begin{aligned}
I &\le c|\bar{\varepsilon}|\|\sigma^n\|_{L^\infty(\Omega)}\int_\Omega |S_x^n||S^n| dx \\
&\le C\int_\Omega K|S_x^n||S^n| dx \\
&\le C\|1\|_{L^3(\Omega)}\|K(S_x^n)^{\frac{1}{2}}\|_{L^6(\Omega)}\|(S_x^n)^{\frac{1}{2}}S^n\| \\
&\le CK^6\eta\|S_x^n\|^3_{L^3(\Omega)} + \eta C\int_\Omega (S^n)^2|S_x^n| dx + C_\eta.
\end{aligned} \tag{35}$$

Then (34), (35) and the Young inequality imply

$$\begin{aligned}
&\frac{1}{2}\frac{d}{dt}||S^n||^2 + \frac{c\nu}{2}\|S_x^n\|^3_{L^3(\Omega)} + 2c(k+1)A_0\int_\Omega (S^n)^{2k+2}|S_x^n| dx \\
&\le C\int_\Omega \sum_{i=1}^{2k+1} |A_i||S^n|^{2k+2-i}|S_x^n| dx + CK^6\eta\|S_x^n\|^3_{L^3(\Omega)} + \eta C\int_\Omega (S^n)^2|S_x^n| dx + C_\eta \\
&\le \mu C\int_\Omega (S^n)^{2k+2}|S_x^n| dx + C_\mu\int_\Omega (\xi|S_x^n|^3 + C_\xi) dx \\
&+ CK^6\eta\|S_x^n\|^3_{L^3(\Omega)} + \eta C\int_\Omega (S^n)^2|S_x^n| dx + C_\eta,
\end{aligned} \tag{36}$$

let μ and ξ be small enough, then

$$\begin{aligned}
&\frac{1}{2}\frac{d}{dt}||S^n||^2 + \frac{c\nu}{4}\|S_x^n\|^3_{L^3(\Omega)} + c(k+1)A_0\int_\Omega (S^n)^{2k+2}|S_x^n| dx \\
&\le \eta C\int_\Omega (S^n)^2|S_x^n| dx + CK^6\eta\|S_x^n\|^3_{L^3(\Omega)} + C_\eta,
\end{aligned} \tag{37}$$

let $\eta = \frac{c\nu}{8CK^6}$ be sufficiently small, so that $\frac{c\nu}{4} - CK^6\eta = \frac{c\nu}{8} > 0$, then from (37) we get

$$\frac{1}{2}\frac{d}{dt}||S^n||^2 + \frac{c\nu}{8}\|S^n_x\|^3_{L^3(\Omega)} + C\int\limits_{\Omega}(S^n)^{2k+2}|S^n_x|dx \le C_\eta. \tag{38}$$

Integrating (38) with respect to t from 0 to t_0, we assert that

$$\begin{aligned}&\frac{1}{2}\|S^n\|^2 + \frac{c\nu}{8}\int\limits_0^{t_0}\|S^n_x\|^3_{L^3(\Omega)}d\tau + C\int\limits_{Q_{t_0}}(S^n)^{2k+2}|S^n_x|d(\tau,x)\\ &\le \frac{1}{2}\|S^n(0)\|^2 + C_\eta t_0 \le C_{t_0} \le C.\end{aligned} \tag{39}$$

Although the constant C_η, which is related to K may be very large, but when we multiply a sufficiently small t_0, then the uniform boundedness can be guaranteed. Thus, the proof of Lemma 1 is completed. □

Lemma 2. There holds for any $t \in [0, t_0]$

$$\frac{1}{2}\|S^n_x\|^2 + \frac{c\nu}{2}\int\limits_{Q_{t_0}}|S^n_x|(S^n_{xx})^2d(\tau,x) + C\int\limits_{Q_{t_0}}(S^n)^{2k}|S^n_x|^3d(\tau,x) \le C. \tag{40}$$

Proof. Multiplying (24) by $-S^n_{xx}$ and integrating by parts with respect to x, where we take the boundary conditions into account, that for all $t \in [0, t_0]$

$$(S^n_t, -S^n_{xx}) - c\nu(|S^n_x|S^n_{xx}, -S^n_{xx}) - c\bar{\varepsilon}(\sigma^n|S^n_x|, -S^n_{xx}) + \frac{c}{2}((\hat{\psi}'(S^n))_x, S^n_x|S^n_x|) = 0,$$

that is

$$\frac{1}{2}\frac{d}{dt}||S^n_x||^2 + c\nu\int\limits_{\Omega}|S^n_x|(S^n_{xx})^2dx + c\bar{\varepsilon}\int\limits_{\Omega}\sigma^n|S^n_x|S^n_{xx}dx + \frac{c}{2}\int\limits_{\Omega}\hat{\psi}''(S^n)|S^n_x|^3dx = 0.$$

Using (6) and invoking the Young inequality and Hölder's inequality, we obtain

$$\begin{aligned}&\frac{1}{2}\frac{d}{dt}||S^n_x||^2 + c\nu\int\limits_{\Omega}|S^n_x|(S^n_{xx})^2dx + c(k+1)(2k+1)A_0\int\limits_{\Omega}(S^n)^{2k}|S^n_x|^3dx\\ &\le c|\bar{\varepsilon}|\int\limits_{\Omega}|\sigma^n||S^n_x||S^n_{xx}|dx + C\int\limits_{\Omega}\sum_{i=1}^{2k}|A_i||S^n|^{2k-i}|S^n_x|^3dx\\ &\le C\int\limits_{\Omega}K|S^n_x||S^n_{xx}|dx + C\int\limits_{\Omega}(\mu(S^n)^{2k} + C_\mu)|S^n_x|^3dx\\ &\le C\|(S^n_x)^{\frac{1}{2}}\|\|K(S^n_x)^{\frac{1}{2}}S^n_{xx}\| + C\int\limits_{\Omega}(\mu(S^n)^{2k} + C_\mu)|S^n_x|^3dx\\ &\le C_\eta + C\int\limits_{\Omega}(S^n_x)^2dx + CK^2\eta\int\limits_{\Omega}|S^n_x|(S^n_{xx})^2dx\\ &+ \mu C\int\limits_{\Omega}(S^n)^{2k}|S^n_x|^3dx + CC_\mu\int\limits_{\Omega}|S^n_x|^3dx,\end{aligned} \tag{41}$$

let $\eta = \frac{c\nu}{2CK^2}$, $\mu = \frac{c(k+1)(2k+1)A_0}{2C}$ be small enough, so that $c\nu - CK^2\eta = \frac{c\nu}{2} > 0$, $c(k+1)(2k+1)A_0 - \mu C = \frac{c(k+1)(2k+1)A_0}{2} > 0$, then (41) becomes

$$\frac{1}{2}\frac{d}{dt}||S^n_x||^2 + \frac{c\nu}{2}\int\limits_{\Omega}|S^n_x|(S^n_{xx})^2dx + C\int\limits_{\Omega}(S^n)^{2k}|S^n_x|^3dx \le C\|S^n_x\|^2 + C\|S^n_x\|^3_{L^3(\Omega)} + C_\eta. \tag{42}$$

Invoking (32) and the differential form of Gronwall's inequality, one can easily conclude (40). □

It follows from estimates (32) and (40) that $S^n \in L^\infty(0, t_0; H^1_{\text{per}}(\Omega))$. From the elliptic regularity theory for (22)-(23) and the Sobolev embedding theorem, we obtain

Lemma 3. There hold for any $t \in [0, t_0]$

$$\|u^n\|_{L^\infty(0,t_0;H^2_{\text{per}}(\Omega))} + \|\sigma^n\|_{L^\infty(0,t_0;H^1_{\text{per}}(\Omega))} \leq C, \tag{43}$$

$$\|S^n\|_{L^\infty(Q_{t_0})} + \|u^n\|_{L^\infty(Q_{t_0})} + \|\sigma^n\|_{L^\infty(Q_{t_0})} \leq C. \tag{44}$$

Lemma 4. There hold for any $t \in [0, t_0]$

$$\||S^n_x|S^n_{xx}\|_{L^{\frac{3}{2}}(Q_{t_0})} \leq C, \tag{45}$$

$$\|S^n_x|S^n_x|\|_{L^{\frac{3}{2}}(0,t_0;W^{1,\frac{3}{2}}_{\text{per}}(\Omega))} \leq C, \quad \|S^n_x\|_{L^3(0,t_0;L^\infty(\Omega))} \leq C. \tag{46}$$

Proof. By the interpolation technique and (40). For some $1 \leq p < 2$, $pq = 2$ and $\frac{1}{q} + \frac{1}{q'} = 1$ we yield that

$$\begin{aligned}
\int_{Q_{t_0}} (|S^n_x||S^n_{xx}|)^p d(\tau, x) &= \int_{Q_{t_0}} |S^n_x|^{\frac{p}{2}} |S^n_x|^{\frac{p}{2}} |S^n_{xx}|^p d(\tau, x) \\
&\leq (\int_{Q_{t_0}} |S^n_x|^{\frac{pq'}{2}} d(\tau, x))^{\frac{1}{q'}} (\int_{Q_{t_0}} |S^n_x|^{\frac{pq}{2}} |S^n_{xx}|^{pq} d(\tau, x))^{\frac{1}{q}} \\
&\leq (\int_{Q_{t_0}} |S^n_x|^{\frac{p}{2-p}} d(\tau, x))^{\frac{2-p}{2}} (\int_{Q_{t_0}} |S^n_x||S^n_{xx}|^2 d(\tau, x))^{\frac{p}{2}} \\
&\leq C(\int_{Q_{t_0}} |S^n_x|^{\frac{p}{2-p}} d(\tau, x))^{\frac{2-p}{2}}.
\end{aligned} \tag{47}$$

It follows from (32) that if p satisfies $\frac{p}{2-p} \leq 3$, i.e. $p \leq \frac{3}{2}$, then the right-hand side of (47) is bounded, when $p = \frac{3}{2}$, we obtain (45).

Next we are going to prove $S^n_x|S^n_x| \in L^{\frac{3}{2}}(Q_{t_0})$, then one can easily obtain that $S^n_x|S^n_x| \in L^{\frac{3}{2}}(0, t_0; W^{1,\frac{3}{2}}_{\text{per}}(\Omega))$. Applying the Poincaré inequality of the form: $\|f - \bar{f}\|_{L^p(\Omega)} \leq \|f_x\|_{L^p(\Omega)}$, where $\bar{f} := \frac{1}{|\Omega|} \int_\Omega f(x)dx$, and $|\Omega|$ denotes the measure of Ω, we choose $p = \frac{3}{2}$, $f = S^n_x|S^n_x|$, then obtain

$$\begin{aligned}
\int_0^{t_0} \|S^n_x|S^n_x|\|^{\frac{3}{2}}_{L^{\frac{3}{2}}(\Omega)} d\tau &\leq C \int_0^{t_0} \|(S^n_x|S^n_x|)_x\|^{\frac{3}{2}}_{L^{\frac{3}{2}}(\Omega)} d\tau + C \int_0^{t_0} \|\overline{S^n_x|S^n_x|}\|^{\frac{3}{2}}_{L^{\frac{3}{2}}(\Omega)} d\tau \\
&\leq C \int_0^{t_0} \|(S^n_x|S^n_x|)_x\|^{\frac{3}{2}}_{L^{\frac{3}{2}}(\Omega)} d\tau + \frac{C}{|\Omega|^{\frac{1}{2}}} \int_0^{t_0} d\tau \\
&\leq C \int_0^{t_0} \|(S^n_x|S^n_x|)_x\|^{\frac{3}{2}}_{L^{\frac{3}{2}}(\Omega)} d\tau + C,
\end{aligned} \tag{48}$$

which implies, by (45), that

$$S^n_x|S^n_x| \in L^{\frac{3}{2}}(0, t_0; W^{1,\frac{3}{2}}_{\text{per}}(\Omega)). \tag{49}$$

The Sobolev embedding theorem implies that $S^n_x|S^n_x| \in L^{\frac{3}{2}}(0, t_0; L^\infty(\Omega))$, that is $S^n_x \in L^3(0, t_0; L^\infty(\Omega))$. □

Lemma 5. There hold for any $t \in [0, t_0]$

$$\|S^n_t\|_{L^{\frac{3}{2}}(Q_{t_0})} + \|\sigma^n_t\|_{L^{\frac{3}{2}}(Q_{t_0})} \leq C, \tag{50}$$

$$\||S^n_x|S^n_{xt}\|_{L^1(0,t_0;(H^2_{\text{per}}(\Omega))')} \leq C. \tag{51}$$

Proof. We know

$$S^n_t = c(\nu S^n_{xx} + \bar{\varepsilon} \cdot \sigma^n - \hat{\psi}'(S^n))|S^n_x|. \tag{52}$$

It follows from (44) that

$$\max_{\overline{Q}_{t_0}} |c(\bar{\varepsilon}\cdot\sigma^n - \hat{\psi}'(S^n))| \le C, \tag{53}$$

which implies that $\|\psi_S\|_{L^\infty(Q_{t_0})} \le C$. It thus follows from (32), (40), (45) and (53) that $S_t^n \in L^{\frac{3}{2}}(Q_{t_0})$, then we differentiate (22) formally with respect to t and use $b_t \in L^2(Q_{t_0})$, we have $\sigma_t^n \in L^{\frac{3}{2}}(Q_{t_0})$.

To prove (51) we show that there is a constant C, which is independent of n, such that

$$(|S_x^n|S_{xt}^n, \varphi)_{Q_{t_0}} \le C\|\varphi\|_{L^\infty(0,t_0;H^2_{\mathrm{per}}(\Omega))} \tag{54}$$

for all $\varphi \in L^\infty(0,t_0;H^2_{\mathrm{per}}(\Omega))$.
Integrating by parts to get

$$\begin{aligned}(|S_x^n|S_{xt}^n, \varphi)_{Q_{t_0}} &= (-(|S_x^n|\varphi)_x, S_t^n)_{Q_{t_0}} \\ &= (S_t^n, -\frac{S_x^n}{|S_x^n|}S_{xx}^n\varphi)_{Q_{t_0}} + (S_t^n, -|S_x^n|\varphi_x)_{Q_{t_0}} := I_1 + I_2.\end{aligned} \tag{55}$$

Applying estimates (32), (40), (52), (53) and the Young inequality, we obtain

$$\begin{aligned}|I_1| &= |(S_t^n, -\frac{S_x^n}{|S_x^n|}S_{xx}^n\varphi)_{Q_{t_0}}| \\ &= |(c\bar{\varepsilon}\cdot\sigma^n - c\hat{\psi}'(S^n) + c\nu S_{xx}^n, -S_x^n S_{xx}^n\varphi)_{Q_{t_0}}| \\ &\le \|\varphi\|_{L^\infty(Q_{t_0})}\int_{Q_{t_0}} |c\bar{\varepsilon}\cdot\sigma^n - c\hat{\psi}'(S^n)||S_x^n||S_{xx}^n| + c\nu|S_x^n|(S_{xx}^n)^2 d(\tau,x) \\ &\le C\|\varphi\|_{L^\infty(Q_{t_0})}\int_{Q_{t_0}} |S_x^n||S_{xx}^n| + |S_x^n|(S_{xx}^n)^2 d(\tau,x) \\ &\le C\|\varphi\|_{L^\infty(Q_{t_0})}(\mu\int_{Q_{t_0}} |S_x^n|^2 d(\tau,x) + \mu\int_{Q_{t_0}} |S_x^n|(S_{xx}^n)^2 d(\tau,x) + C_\mu) \\ &\le C\|\varphi\|_{L^\infty(0,t_0;H^2_{\mathrm{per}}(\Omega))}.\end{aligned} \tag{56}$$

And estimates (32), (40), (52), (53) and Hölder's inequality imply

$$\begin{aligned}|I_2| &= |(S_t^n, -|S_x^n|\varphi_x)_{Q_{t_0}}| \\ &= |((c\bar{\varepsilon}\cdot\sigma^n - c\hat{\psi}'(S^n))|S_x^n| + c\nu|S_x^n|S_{xx}^n, -|S_x^n|\varphi_x)_{Q_{t_0}}| \\ &\le C\|\varphi_x\|_{L^\infty(Q_{t_0})}\int_{Q_{t_0}} |S_x^n|^2 + |S_x^n|^2|S_{xx}^n| d(\tau,x) \\ &\le C\|\varphi_x\|_{L^\infty(Q_{t_0})}\int_0^{t_0}(\int_\Omega |S_x^n|^2 dx + \||S_x^n|^{\frac{1}{2}}\|_{L^\infty(\Omega)}\||S_x^n|^{\frac{1}{2}}S_{xx}^n\|\|S_x^n\|)d\tau \\ &\le C\|\varphi_x\|_{L^\infty(Q_{t_0})}\int_0^{t_0} \||S_x^n|^{\frac{1}{2}}\|_{L^\infty(\Omega)}\||S_x^n|^{\frac{1}{2}}S_{xx}^n\| d\tau \\ &\le C\|\varphi_x\|_{L^\infty(Q_{t_0})}(\int_0^{t_0} \||S_x^n|^{\frac{1}{2}}\|^2_{L^\infty(\Omega)} d\tau)^{\frac{1}{2}}(\int_0^{t_0} \||S_x^n|^{\frac{1}{2}}S_{xx}^n\|^2 d\tau)^{\frac{1}{2}} \\ &\le C\|\varphi\|_{L^\infty(0,t_0;H^2_{\mathrm{per}}(\Omega))},\end{aligned} \tag{57}$$

here, we also used (46). Then estimates (55)-(57) yield the desired estimate (51). □

Next we study the convergence of S^n as $n \to \infty$ by the *a priori* estimates established in the previous part. We shall show that there is a subsequence, which converges to a weak solution to IBVP (10)-(15) for $t \in [0, t_0]$.

It follows from (32), (40) and (50) that

$$\|S^n\|_{W^{1,\frac{3}{2}}_{\mathrm{per}}(Q_{t_0})} \le C. \tag{58}$$

Hence, we can select a subsequence of S^n, not relabeled, satisfies

$$\|S^n - S\|_{L^{\frac{3}{2}}(Q_{t_0})} \to 0, \quad S^n_x \rightharpoonup S_x, \quad S^n_t \rightharpoonup S_t, \tag{59}$$

where the weak convergence is in $L^{\frac{3}{2}}(Q_{t_0})$.

Theorem 3. (Aubin-Lions)[26] Let B_0, B, B_1 be Banach spaces which satisfy that B_0, B_1 are reflexive and that $B_0 \hookrightarrow\hookrightarrow B \hookrightarrow B_1$, here $\hookrightarrow\hookrightarrow$ denotes the compact embedding. For $0 \le p_0, p_1 \le \infty$, define

$$W = \{f | f \in L^{p_0}(0, t_0; B_0),\ f' = \frac{df}{dt} \in L^{p_1}(0, t_0; B_1)\}.$$

(i) if $1 \le p_0 < \infty$, $p_1 = 1$, then the embedding of W into $L^{p_0}(0, t_0; B)$ is compact.

(ii) if $p_0 = \infty$, $1 < p_1 \le \infty$, then the embedding of W into $C([0, t_0]; B)$ is compact.

Lemma 6. (Weak compactness lemma)[27] Let $(0, t_0) \times \Omega$ be an open set in $\mathbb{R}^+ \times \mathbb{R}^n$. Suppose functions g_n, g are in $L^q((0, t_0) \times \Omega)$ for any given $1 < q < \infty$, which satisfy

$$||g_n||_{L^q((0,t_0)\times\Omega)} \le C, \quad g_n \to g\ a.e.\ in\ (0, t_0) \times \Omega.$$

Then g_n converges to g weakly in $L^q((0, t_0) \times \Omega)$.

Lemma 7. There exists a subsequence of S^n_x, not relabeled, satisfies

$$S^n_x \to S_x,\ a.e.\ in\ Q_{t_0}, \quad \sigma^n \to \sigma,\ a.e.\ in\ Q_{t_0}, \tag{60}$$

$$S^n_x|S^n_x| \rightharpoonup S_x|S_x|, \quad weakly\ in\ L^{\frac{3}{2}}(Q_{t_0}), \tag{61}$$

$$S^n_x|S^n_x| \to S_x|S_x|, \quad strongly\ in\ L^{\frac{3}{2}}(0, t_0; L^2(\Omega)), \tag{62}$$

as $n \to \infty$.

Proof. We choose $p_0 = \frac{3}{2}$ and

$$B_0 = W^{1,\frac{3}{2}}_{\mathrm{per}}(\Omega), \quad B = L^2(\Omega), \quad B_1 = (H^2_{\mathrm{per}}(\Omega))'.$$

These spaces satisfy the assumptions of Theorem 3. Since estimates (49) and (51) imply that the sequence $S^n_x|S^n_x|$ is uniformly bounded in $L^{p_0}(0, t_0; B_0)$ and $(S^n_x|S^n_x|)_t$ is uniformly bounded in $L^1(0, t_0; B_1)$, then there is a subsequence, still denoted by $S^n_x|S^n_x|$, which converges strongly in $L^{p_0}(0, t_0; B) = L^{\frac{3}{2}}(0, t_0; L^2(\Omega))$ to a limit function $G \in L^{\frac{3}{2}}(0, t_0; L^2(\Omega))$. Consequently, we can select another subsequence, denoted in the same way, converges pointwise almost everywhere in Q_{T_e}. Letting $f(S^m_x) = S^m_x|S^m_x|$, using the mapping $y \mapsto f(y) := y|y|$ that has a continuous inverse $f^{-1} : \mathbb{R} \to \mathbb{R}$, we deduce that the sequence $S^m_x \to f^{-1}(S^m_x)$ converges pointwise almost everywhere to $f^{-1}(G)$ in Q_{T_e}. Applying the uniqueness of the weak limit, we infer that $S^m_x \to S_x$ converges pointwise almost everywhere in Q_{T_e}. From this we also obtain that the sequence $|S^m_x| \to |S_x|$ and $S^m_x|S^m_x| \to S_x|S_x|$ converges pointwise almost everywhere in Q_{T_e}.

Note that the estimate $S^n_x|S^n_x| \in L^{\frac{3}{2}}(0, t_0; W^{1,\frac{3}{2}}_{\mathrm{per}}(\Omega))$ and the Sobolev embedding theorem imply that $W^{1,\frac{3}{2}}_{\mathrm{per}}(\Omega) \subset L^{\frac{3}{2}}(\Omega)$, we can also obtain that $||S^n_x|S^n_x|||_{L^{\frac{3}{2}}(Q_{t_0})} \le C$, using Lemma 6, $S^n_x|S^n_x|$ converges to $S_x|S_x|$ weakly in $L^{\frac{3}{2}}(Q_{t_0})$, that is, $G = S_x|S_x|$. Hence, (62) follows.

Similarly, we choose $p_0 = \infty$, $p_1 = \frac{3}{2}$ and

$$B_0 = H^1(\Omega), \quad B = L^2(\Omega), \quad B_1 = L^{\frac{3}{2}}(\Omega).$$

It thus follows from (43), (50) and Theorem 3 that there exist a subsequence of σ^n, not relabeled, and a function $\sigma \in C([0, t_0]; L^2(\Omega))$, such that σ^n converges strongly to σ in $C([0, t_0]; L^2(\Omega))$, and converges pointwise almost everywhere in Q_{t_0}. Hence, (60) follows. ☐

We now prove that (u, σ, S) is a weak solution to IBVP (10)-(15) for $t \in [0, t_0]$. If we multiply (24) by a test function $\varphi \in C_0^\infty(-\infty, t_0; C_{\mathrm{per}}^\infty(\Omega))$, and integrate the resulting equation over Q_{t_0}, we obtain

$$(S^n, \varphi_t)_{Q_{t_0}} - \frac{cv}{2}(S_x^n|S_x^n|, \varphi_x)_{Q_{t_0}} + c((\bar{\varepsilon} \cdot \sigma^n - \hat{\psi}'(S^n))|S_x^n|, \varphi)_{Q_{t_0}} + (S_0^n, \varphi(0))_\Omega = 0. \tag{63}$$

For $t \in [0, t_0]$, (18) follows from this relation if we show that

$$(S^n, \varphi_t)_{Q_{t_0}} \to (S, \varphi_t)_{Q_{t_0}}, \tag{64}$$

$$(S_x^n|S_x^n|, \varphi_x)_{Q_{t_0}} \to (S_x|S_x|, \varphi_x)_{Q_{t_0}}, \tag{65}$$

$$((\bar{\varepsilon} \cdot \sigma^n - \hat{\psi}'(S^n))|S_x^n|, \varphi)_{Q_{t_0}} \to ((\sigma \cdot \bar{\varepsilon} - \hat{\psi}'(S))|S_x|, \varphi)_{Q_{t_0}}, \tag{66}$$

$$(S_0^n, \varphi(0))_\Omega \to (S_0, \varphi(0))_\Omega, \tag{67}$$

for $n \to \infty$.

Now, (64) is a consequence of (59) and (65) is obtained from Lemma 7, to verify (66) we note that (40), (53) and (60) imply

$$\|(\bar{\varepsilon} \cdot \sigma^n - \hat{\psi}'(S^n))|S_x^n|\|_{L^2(Q_{t_0})} \le C, \tag{68}$$

$$(\bar{\varepsilon} \cdot \sigma^n - \hat{\psi}'(S^n))|S_x^n| \to (\sigma \cdot \bar{\varepsilon} - \hat{\psi}'(S))|S_x|, \quad \text{almost everywhere in } Q_{t_0}. \tag{69}$$

Then by Lemma 6

$$(\bar{\varepsilon} \cdot \sigma^n - \hat{\psi}'(S^n))|S_x^n| \rightharpoonup (\sigma \cdot \bar{\varepsilon} - \hat{\psi}'(S))|S_x|, \qquad \text{weakly in } L^2(Q_{t_0}), \tag{70}$$

and (67) follows from (28). We thus complete the proof that (u, σ, S) is a weak solution to IBVP (10)-(15) for $t \in [0, t_0]$.

3 | UNIFORM *A PRIORI* ESTIMATES

This section is devoted to derive some uniform *a priori* estimates for a arbitrarily positive constant T_e.

Theorem 4. There hold for any $t \in [0, T_e]$

$$\|S\|_{L^\infty(0,T_e;H^1_{\mathrm{per}}(\Omega))} \le C, \tag{71}$$

$$\|u\|_{L^\infty(0,T_e;H^2_{\mathrm{per}}(\Omega))} + \|\sigma\|_{L^\infty(0,T_e;H^1_{\mathrm{per}}(\Omega))} \le C, \tag{72}$$

$$\int_{Q_{T_e}} (\psi_S - vS_{xx})^2 |S_x| d(\tau, x) \le C, \tag{73}$$

$$\int_{Q_{T_e}} |S_x| S_{xx}^2 d(\tau, x) \le C. \tag{74}$$

Proof. Differentiating the energy ψ^* in (4), and according to the symmetry of σ, we get

$$\begin{aligned}
&\frac{d}{dt}\int_\Omega \psi^*(\varepsilon, S, S_x)(t, x) dx \\
&= \int_\Omega \nabla_\varepsilon \psi \cdot \varepsilon_t + \psi_S S_t + vS_x S_{xt} dx \\
&= \int_\Omega \sigma \cdot u_{xt} + \psi_S S_t - vS_{xx} S_t dx \\
&= \int_\Omega (\psi_S - vS_{xx}) S_t + b \cdot u_t dx \\
&= -c \int_\Omega (\psi_S - vS_{xx})^2 |S_x| dx + \int_\Omega b \cdot u_t dx.
\end{aligned} \tag{75}$$

Integrating (75) with respect to t from 0 to T_e obtains

$$\begin{aligned}
&\int_\Omega \psi^*(\varepsilon, S, S_x)(t,x)dx + c\int_{Q_{T_e}} (\psi_S - \nu S_{xx})^2|S_x|d(\tau,x)\\
&= \int_\Omega \psi^*(\varepsilon, S, S_x)(0,x)dx + \int_{Q_{T_e}} b\cdot u_t d(\tau,x)\\
&= \int_\Omega \psi^*(\varepsilon, S, S_x)(0,x)dx + \int_\Omega bu dx - \int_\Omega b(0,x)\cdot u(0,x)dx - \int_{Q_{T_e}} b_t\cdot u d(\tau,x),
\end{aligned} \tag{76}$$

then, we obtain, by (7)-(9)

$$\begin{aligned}
&\int_\Omega \psi_1^*(\varepsilon, S, S_x)(t,x)dx + c\int_{Q_{T_e}} (\psi_S - \nu S_{xx})^2|S_x|d(\tau,x)\\
&\le |\int_\Omega \psi_2^*(S)(t,x)dx| + |\int_\Omega \psi^*(\varepsilon, S, S_x)(0,x)dx| + |\int_\Omega b\cdot u dx|\\
&+ |\int_\Omega b(0,x)\cdot u(0,x)dx| + |\int_{Q_{T_e}} b_t\cdot u d(\tau,x)|.
\end{aligned} \tag{77}$$

From $S_0 \in H^1_{\text{per}}(\Omega)$ and the elliptic regularity theory for elliptic system (10)-(11), we obtain

$$\|u_0\|_{H^2_{\text{per}}(\Omega)} \le C, \tag{78}$$

noting $b \in L^2(Q_{T_e})$ with $b_t \in L^2(Q_{T_e})$ and the Sobolev embedding theorem, there is a constant C such that

$$\|b(t)\| \le C, \tag{79}$$

for all $t \in [0, T_e]$. Then we use Hölder's inequality get that

$$|\int_\Omega b(0,x)u(0,x)dx| \le \|b(0)\|\|u(0)\| \le C. \tag{80}$$

It follows from the definition of ψ^* in (4) and the assumption for S_0 together with estimate (78) that

$$|\int_\Omega \psi^*(\varepsilon, S, S_x)(0,x)dx| \le C. \tag{81}$$

Next we let $b = (\int_a^x bdy)_x$ and $\int_a^d bdy = 0$. Invoking the definition of $\varepsilon(u_x)$, we find, owing to (79)

$$\begin{aligned}
&|\int_\Omega bu dx| = |\int_\Omega (\int_a^x bdy)u_x dx| \le \|\int_a^x bdy\|\|u_x\| \le \xi\|\varepsilon\|^2 + C_\xi,\\
&|\int_{Q_{T_e}} b_t u d(\tau,x)| = |\int_0^{T_e}\int_\Omega (\int_a^x bdy)_t u_x dx d\tau|\\
&\le \|(\int_a^x bdy)_t\|_{L^2(Q_{T_e})}\|u_x\|_{L^2(Q_{T_e})}\\
&\le C\int_0^{T_e} \|\varepsilon\|^2 d\tau,
\end{aligned} \tag{82}$$

we also used $b \in L^2(Q_{T_e})$ with $b_t \in L^2(Q_{T_e})$, then $(\int_a^x bdy)_t \in L^2(Q_{T_e})$.

Thanks to the Young inequality

$$\begin{aligned}|\int_\Omega \psi_2^*(S)(t,x)dx| &\le \int_\Omega \sum_{i=1}^{2k+2} |A_i||S^n|^{2k+2-i}dx\\ &\le C\int_\Omega (\mu S^{2k+2}+C_\mu)dx\\ &\le \mu C\int_\Omega S^{2k+2}dx + C. \end{aligned} \tag{83}$$

Let μ and ξ be sufficiently small, by (76)-(83) and (8) we arrive at

$$\int_\Omega \psi_1^*(\varepsilon,S,S_x)(t,x)dx + c\int_{Q_{T_e}}(\psi_S-\nu S_{xx})^2|S_x|d(\tau,x) \le C\int_0^{T_e}\|\varepsilon\|^2 d\tau + C. \tag{84}$$

For the term $\|\varepsilon\|^2$, we use (8) find that

$$\begin{aligned}\|\varepsilon\|^2 &\le 2\|\bar{\varepsilon}S\|^2 + 2\|\varepsilon-\bar{\varepsilon}S\|^2\\ &\le CA_0\int_\Omega S^{2k+2}+\frac{1}{2}D(\varepsilon-\bar{\varepsilon}S)\cdot(\varepsilon-\bar{\varepsilon}S)dx\\ &\le C\int_\Omega \psi_1^*(\varepsilon,S,S_x)(t,x)dx. \end{aligned} \tag{85}$$

Then from (84) and (85), we obtain

$$\begin{aligned}&\int_\Omega \psi_1^*(\varepsilon,S,S_x)(t,x)dx + c\int_{Q_{T_e}}(\psi_S-\nu S_{xx})^2|S_x|d(\tau,x)\\ &\le C(1+\int_0^{T_e}\int_\Omega \psi_1^*(\varepsilon,S,S_x)(t,x)dxd\tau). \end{aligned} \tag{86}$$

Applying the Gronwall inequality in the integral form we conclude that there exists a constant C such that for every $t\in[0,T_e]$

$$\int_0^{T_e}\int_\Omega \psi_1^*(\varepsilon,S,S_x)(t,x)dxd\tau \le C. \tag{87}$$

From (8) we conclude that

$$|S|^2+\frac{\nu}{2}|S_x|^2 \le C(\psi_1^*(\varepsilon,S,S_x)+1)\le C, \tag{88}$$

then we arrive at (71) and (73). From (88) and apply elliptic regularity theory for system (10)-(11) again, then u and σ satisfy (72). To prove (74), we use inequality $(a+b)^2\le 2a^2+2b^2$ to get

$$\begin{aligned}\nu^2\int_{Q_{T_e}}|S_x|S_{xx}^2 d(\tau,x) &\le 2\int_{Q_{T_e}}(\psi_S-\nu S_{xx})^2|S_x|d(\tau,x) + 2\int_{Q_{T_e}}|S_x||\psi_S|^2 d(\tau,x)\\ &\le C + 2\|\psi_S\|^2_{L^\infty(Q_{T_e})}\int_{Q_{T_e}}|S_x|d(\tau,x)\\ &\le C + C\int_{Q_{T_e}}|S_x|^2 d(\tau,x)\\ &\le C. \end{aligned}$$

□

Repeating the steps in Section 2, we have estimates (19)-(21). The framework of the proof is presented as follows.

(i) It follows from (71), (73) and Lemma 4 that

$$\| |S_x| S_{xx} \|_{L^{\frac{4}{3}}(Q_{T_e})} \leq C, \tag{89}$$

$$\| S_x |S_x| \|_{L^{\frac{4}{3}}(0,T_e;W^{1,\frac{4}{3}}_{\text{per}}(\Omega))} \leq C, \quad \| S_x \|_{L^{\frac{8}{3}}(0,T_e;L^\infty(\Omega))} \leq C. \tag{90}$$

(ii) Similar to Lemma 5, we have

$$\| S_t \|_{L^{\frac{4}{3}}(Q_{T_e})} + \| \sigma_t \|_{L^{\frac{4}{3}}(Q_{T_e})} \leq C, \tag{91}$$

$$\| |S_x| S_{xt} \|_{L^1(0,T_e;H^2_{\text{per}}(\Omega)')} \leq C. \tag{92}$$

Remark 2. We do not have the estimate for $\|S_x\|_{L^3(Q_{T_e})}$ in this section, we just have $\|S_x\|_{L^2(Q_{T_e})} \leq C$, therefore, the value of p in Lemma 4 is no longer equal to $\frac{3}{2}$ but equal to $\frac{4}{3}$.

Therefore, we complete the proof of the existence of solutions global in time.

4 | PHASE-FIELD SIMULATIONS

We are going to perform a series of numerical simulations for the Alber-Zhu model in two-dimensional space, and compare the results by applying the Allen-Cahn system. We choose the Mn-12.6at.%Ni alloys as the prototype materials, which are subjected to a martensitic transformation from cubic structure to tetragonal structure. Different phase-field simulations are performed as follows.

(i) The phase transformation is triggered by random nucleation of the order parameter. We investigate the microstructure evolution of martensitic transformation in the Allen-Cahn and the Alber-Zhu systems.

(ii) The periodic function as initial value. We are concerned about the characters of martensitic transformation in the Alber-Zhu system.

4.1 | Simulation parameters

The following material parameters are used[28]: the thermodynamic equilibrium temperature T_0=465K; the latent heat $Q = 5 \times 10^7 \text{J/m}^3$; the interfacial energy coefficient $\nu = 1.25 \times 10^{-10}\text{J/m}$; the misfit strain

$$\bar{\varepsilon} = \begin{pmatrix} 0.03 & 0 \\ 0 & -0.03 \end{pmatrix}.$$

The similar elastic constants for different phases are taken into account, Young's modulus $E = 1.11 \times 10^{11}$Pa and Poisson's ratio $\kappa = 0.15$. Parameters are divided by Q to obtain their dimensionless form. Then the dimensionless elastic modulus of material

$$D = \begin{pmatrix} 2322.98 & 409.938 & 0 \\ 409.938 & 2322.98 & 0 \\ 0 & 0 & 956.522 \end{pmatrix},$$

the reduced mobility coefficient is assume as $c^* = 1$, and the dimensionless interfacial energy coefficient ν^* is chosen as 3.66×10^{-5}, therefore, the length scale of the computational grid increment $l = 0.26\mu$m. We use a square computational domain, and a simulation cell have number of grid points $N_x = N_y = 128$.

In this study, we neglect inertia effects and do not consider the volume forces, which imply $b = 0$, and choose $\hat{\psi}(S)$ is a six-order Landau polynomial as follows

$$\hat{\psi}(S) = \frac{A_1}{2} S^2 - \frac{A_2}{4} S^4 + \frac{A_3}{6} S^6,$$

where the coefficients A_1, A_2 and A_3 are positive constants and can be expressed as: $A_1 = 32\Delta G^\star$, $A_2 = 4A_1 - 12\Delta G_m(T)$ and $A_3 = 3A_1 - 12\Delta G_m(T)$. $\Delta G^\star$ is the energy barrier which is shown as $\Delta G^\star = Q(2.867 \times 10^{-4} T - 0.1223)$ and $\Delta G_m(T)$ is the driving force of martensitic transformation, which is expressed by $\Delta G_m(T) = \frac{Q(T-T_0)}{T_0}$. This study we choose T=427K, then the dimensionless chemical energy parameters $A_1^* = 0.0039$, $A_2^* = 0.9961$, $A_3^* = 0.9923$ and reduced barrier $\Delta G^* = 1.21 \times 10^{-4}$.

4.2 | The initial value is random nucleation of the order parameter

The phase-field simulation can reveal the process of minimizing Gibbs free energy. In two-dimensional martensitic transformation of MnNi alloys, there are two kinds of martensite variants (variant1 and variant2), we use one order parameter S represent the change in crystal structure. As can be seen from Figure 1, there are two wells at $S = 1$ and $S = -1$ correspond to stable martensite variant1 and variant2, respectively, and the value $S = 0$ corresponds to metastable austenite phase. The system transform from metastable austenite phase to stable martensite phase has to overcome the energy barrier ΔG^* that can be seen in the figure (the area within the rectangular region marked in the figure is magnified and presented in the bottom), we can change the value of A_1^*, A_2^* and A_3^* by adjusting the temperature T, thus change the value of the energy barrier.

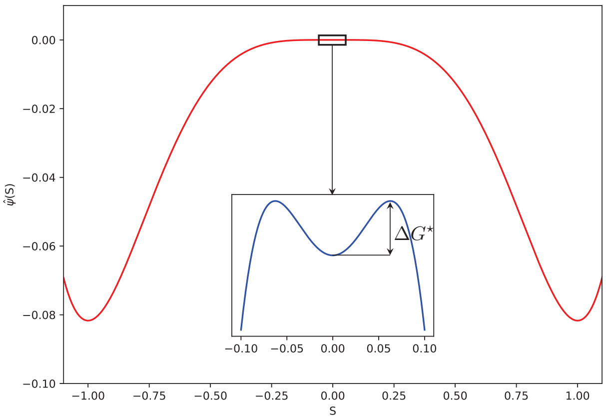


FIGURE 1 Diagram of variation of chemical free energy $\hat{\psi}(S)$ with respect to order parameter S.

The temporal microstructure of the martensite phase in MnNi alloys for the Allen-Cahn and the Alber-Zhu systems are presented in Figure 2. The simulation domain is a square plate 33.28μm × 33.28μm in dimension, the periodic boundary conditions are used for both order parameter S and displacement field u. Where the white regions represent the austenite phase, the red and blue regions represent martensite variant1 and variant2, respectively, and other regions represent the phase interfaces.

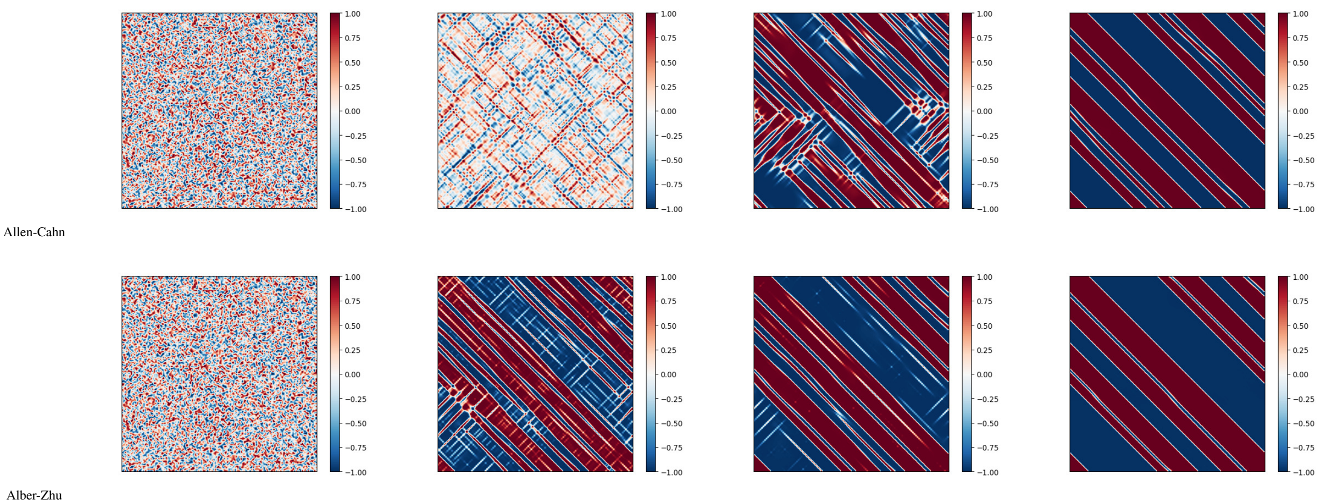
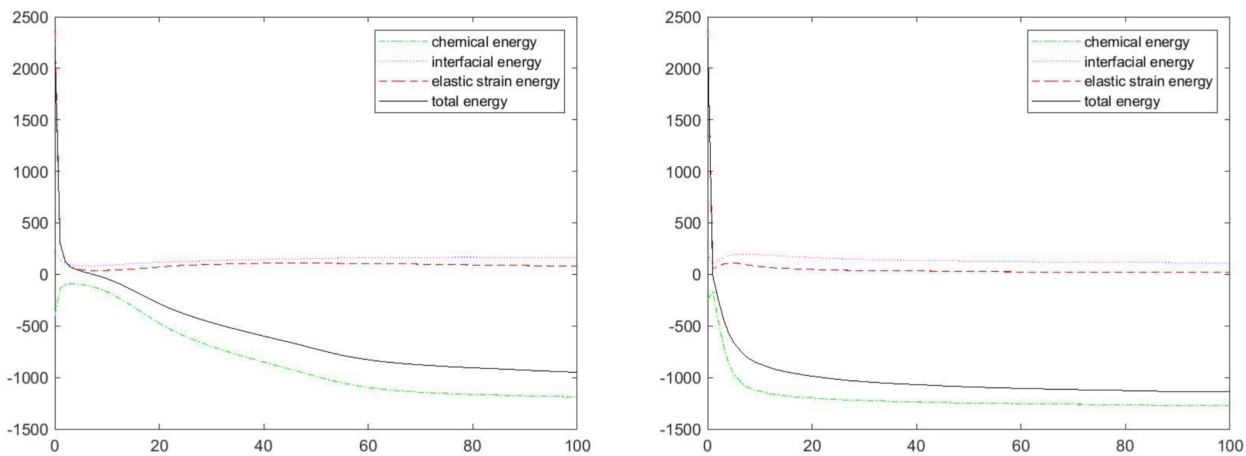


FIGURE 2 Evolution of martensite phase during the martensitic transformation in the Allen-Cahn and the Alber-Zhu systems at dimensionless time t^*=0, 10, 60, 800.

A random distribution of the order parameter is given as the initial value to trigger the nucleation of martensite phase for both the Allen-Cahn and the Alber-Zhu systems. In order to minimize the elastic strain energy so as to minimize the total free energy, variant1 and variant2 generally interact with each other and generate self-accommodation twinning domains, the formation of twinning domains are realized by the alternate appearance of variant1 and variant2. The final plate-like martensite phase and the growth of martensite phase along the diagonal have been conformed by the theory of martensite transformation[29] and crystallographic theory[30]. It can be clearly seen from Figure 2 that the martensite variant1 and variant2 have formed in the Alber-Zhu system at $t^* = 10$, however, the martensite in the Allen-Cahn system is still at nucleation stage. This indicates that the nucleation of martensitic transformation in the Alber-Zhu system takes place in a shorter time than that in the Allen-Cahn system.

The change of various energies with respect to chemical free energy, interfacial energy, elastic strain energy and total energy in the Allen-Cahn and the Alber-Zhu systems are shown in Figure 3. These free energies show the similar tendency, at the early stage of evolution, the order parameter $S \to 0$ to minimize the total free energy by minimizing the elastic strain energy, while the chemical energy increases, when the chemical energy increases to a certain extent, the systems tend to reduce the chemical energy, this means $S \to -1$ or $S \to 1$, so the martensite phase begins to grow up. The interfacial energy decreases dramatically at the early stage, then increases slowly due to the growth of martensite phase, finally, it reduces to its equilibrium value. The total free energy decreases throughout the evolution process. But one can easily see that those free energies of the Alber-Zhu system change faster than that of the Allen-Cahn system and approach their equilibrium values within a shorter time. It means that the Alber-Zhu system can approach its equilibrium state within a shorter time than that for the Allen-Cahn system.



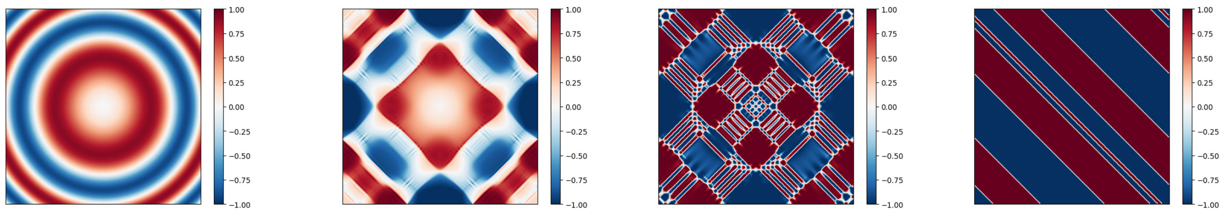
Allen-Cahn Alber-Zhu

FIGURE 3 The change of chemical free energy, interfacial energy, elastic strain energy and total energy with dimensionless time t^* in the Allen-Cahn and the Alber-Zhu systems.

4.3 | The periodic function as initial value

Next, we attempt to study the effect of initial value on martensitic transformation in the Alber-Zhu system. Here we choose a periodic function as the initial value, which is expressed by $S(r) = 0.9\sin((\frac{r-r_0}{L})^2 * 8\pi)$, where r_0 is the center point of simulation region, r is the position of the point and L is the width of simulation region. The values of the order parameter at each node are uniquely determined by that function, which is different from the random distribution of the order parameter.

As can be seen from Figure 4, at the beginning of phase transition, in order to minimize the elastic strain energy, the value of the order parameter tends to 0 which means the decay of martensite nuclei. The direction of reduction is dominated by elastic strain energy, which is similar to the random nucleation of the order parameter. In the local region, the martensite variants originally distributed along [110] and $[\bar{1}10]$ directions keep the same direction during the decayed process, while the order



$t^* = 0$ $t^* = 2$ $t^* = 200$ $t^* = 1200$

FIGURE 4 Evolution of martensite phase during the martensitic transformation in the Alber-Zhu system.

parameter in other regions gradually tend to 0 along those two directions. Then, due to the chemical free energy of the system decreases, the value of the order parameter tends to 1 or -1, and martensite nucleates again at the junction of some variant along [110] and $[\bar{1}10]$ directions, and grows along those two directions. Before the dimensionless time $t^* = 1200$, there are two kinds of polytwinned martensite plates with (110) and $(\bar{1}10)$ twin planes, in the following evolution, the polytwinned plate with $(\bar{1}10)$ twin plane disappears gradually, there only exists one kind of polytwinned plate with (110) twin plane at last.

In our past work, we chose the same initial function, but did not consider the elastic effect. We have come to the conclusion that the martensite phase distributes along the initial path in an annulus at last. However, when we introduce the elastic strain energy, the final microstructure is no longer an annulus, but forms the plate-like martensite phase, which distributes along the diagonal, and generates self-accommodation twinning domains. It is similar to the random distribution of the order parameter as initial value. This again indicates that the elastic strain energy plays a dominant role in the evolution direction of the system.

5 | CONCLUSIONS

(i) We prove the the existence of global solutions of the Alber-Zhu model with periodic boundary conditions, and perform the numerical simulations by applying this model. The numerical results imply that there show the same microstructure with the identical material parameters under the Allen-Cahn and the Alber-Zhu systems, but it takes less time to achieve its equilibrium state in the Alber-Zhu system.

(ii) The elastic strain energy has the important influence on the evolution direction of microstructure, in order to minimize the elastic strain energy of the system, self-accommodation twinning domains along the diagonal are finally generated for both random nucleation of the order parameter and periodic function as initial value.

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