SIAM J. NUMER. ANAL.
Vol. 53, No. 1, pp. 184–205

ERROR ANALYSIS OF A MIXED FINITE ELEMENT METHOD FOR THE MOLECULAR BEAM EPITAXY MODEL*

ZHONGHUA QIAO†, TAO TANG‡, AND HEHU XIE§

Abstract. This paper investigates the error analysis of a mixed finite element method with Crank–Nicolson time-stepping for simulating the molecular beam epitaxy (MBE) model. The fourth-order differential equation of the MBE model is replaced by a system of equations consisting of one nonlinear parabolic equation and an elliptic equation. Then a mixed finite element method requiring only continuous elements is proposed to approximate the resulting system. It is proved that the semidiscrete and fully discrete versions of the numerical schemes satisfy the nonlinearity energy stability property, which is important in the numerical implementation. Moreover, detailed analysis is provided to obtain the convergence rate. Numerical experiments are carried out to validate the theoretical results.

Key words. molecular beam epitaxy, error analysis, mixed finite element, Crank–Nicolson, unconditionally energy stable

AMS subject classifications. 35Q99, 65N30, 65M12, 65M70

DOI. 10.1137/120902410

1. Introduction.

This paper is concerned with the continuum model for the evolution of the molecular beam epitaxy (MBE) growth with an isotropic symmetry current, with the following initial value problem [16, 25]:

$$\begin{cases} \frac{\partial \phi}{\partial t} = -\varepsilon \Delta^2 \phi - \nabla \cdot [(1-|\nabla\phi|^2)\nabla\phi] & \text{in } \Omega \times (0,T), \\ \phi(\mathbf{x},0) = \phi_0(\mathbf{x}) & \text{in } \Omega, \end{cases} \tag{1.1}$$

subject to the periodic boundary condition. Here $\phi = \phi(\mathbf{x}, t)$ is a scaled height function of a thin film in a co-moving frame and ε is a positive constant; $\Omega = (0, L)^2$ with $L > 0$. The nonlinear second-order term models the Ehrlich–Schwoebel effect, and the fourth-order term models surface diffusion. Problem (1.1) is the gradient flow with respect to the $L^2(\Omega)$ inner product of the energy functional [20, 22]

$$E_0(\phi(\cdot,t)) = \frac{\varepsilon}{2}\|\Delta\phi\|_0^2 + \frac{1}{4}\|1-|\nabla\phi|^2\|_0^2, \tag{1.2}$$

*Received by the editors December 12, 2012; accepted for publication (in revised form) November 6, 2014; published electronically January 8, 2015. The research of the first and third authors was partially supported by the AMSS-PolyU Joint Research Institute.
http://www.siam.org/journals/sinum/53-1/90241.html
†Department of Applied Mathematics, The Hong Kong Polytechnic University, Hong Kong, China (zqiao@polyu.edu.hk). The research of this author was partially supported by Hong Kong RGC grant PolyU 2021/12P and by Hong Kong Polytechnic University grants A-PL61 and 1-ZV9Y.
‡Institute of Theoretical and Computational Studies and Department of Mathematics, Hong Kong Baptist University, Hong Kong, China (ttang@math.hkbu.edu.hk). This author's work was supported by Hong Kong Research Grants Council CERG grants and by Hong Kong Baptist University FRG grants.
§LSEC, ICMSEC, NCMIS, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing 100190, China (hhxie@lsec.cc.ac.cn). The research of this author was supported in part by the National Science Foundation of China through NSFC (11371026, 91330202, 11001259, 11031006, and 2011CB309703), by the National Center for Mathematics and Interdisciplinary Science, and by the President Foundation of AMSS-CAS.

where the energy on the right-hand side is the standard 2-norm in space. The growth equation (1.1) is the gradient flow in the sense that

$$E_0(\phi(\cdot,t)) \leq E_0(\phi(\cdot,s)) \quad \forall\, t > s \geq 0. \tag{1.3}$$

This type of energy definition (1.2) often appears in other areas of material modeling such as in structural phase transitions in solids [3, 21], in the theory of liquid crystals [2], and in the buckling-driven delimitation of thin films [15, 18].

In recent years, several models describing the dynamics of MBE growth have been developed, including atomistic models, continuum models, and hybrid models; see, e.g., [5, 9, 24]. Many numerical methods for approximating the solutions of these models have also been proposed. For example, semi-implicit time-stepping methods were proposed in [27, 30] to solve the thin-film epitaxy model (1.1), where the unconditional energy stability was proved based on the convex splitting of the energy functional. Besides application to the energy functional (1.2), the convex splitting method has been used to solve the phase field crystal equation [31], the Cahn–Hilliard–Brinkman system [10], and the thin-film epitaxy model without slope selection [6]. In [32], an implicit-explicit approach for solving MBE growth models was presented where the nonlinear terms are treated explicitly. By adding some linear terms consistent with the truncation errors in time, a gradient stability of type (1.3) is established for the corresponding schemes. Similar techniques are used for the Cahn–Hilliard equation in [33]. Recently, two semi-implicit schemes have been proposed in [26]: one handles the diffusion term explicitly using the known previous data, and the other uses the Crank–Nicolson (CN) approximation. For both schemes, the energy decay (1.3) is preserved without introducing any artificial terms (compared with [17, 32]). The CN-type implicit scheme uses a special treatment of the nonlinear term which has also been used in [11] for a full discretization of one-dimensional Cahn–Hilliard equations. In [26], an adaptive time-stepping technique is developed based on the energy variation which is an important physical quantity in MBE growth models. It is noted that the adaptive time-stepping method has been studied for many important problems, including solving initial value problems in [28], coupled flow and deformation models [24], and hyperbolic conservation laws [29].

As for discretizing MBE growth models in space, the spectral discretization method is analyzed in [23, 27, 32], and the finite difference method is discussed in [26]. Further, [7] proposes using the mixed finite element method and a backward Euler semi-implicit scheme with convex-concave decomposition of the nonlinear term. It is noted that the MBE model (1.1) has three important features, namely high nonlinearity, small parameters ($0 < \epsilon \ll 1$), and high-order derivatives. In practice, the biharmonic terms cannot be approximated in standard ways such as central differencing, which may yield more strict conditions for time steps. To handle this, splitting the biharmonic operators into two Laplacians has been used; see, e.g., [7, 12]. This is similar to the well-known Navier–Stokes equations in terms of the streamfunction or in terms of streamfunction-vorticity formulations; the latter seems more useful in numerics. Furthermore, the biharmonic term makes the application of conforming finite element methods become complicated since we need to use C^1 elements. The mixed finite element method gives a way to use the normal C^0 elements, which can be implemented by many software packages.

In this work, we will also use the operator splitting method to handle the biharmonic operator in (1.1). We will then use the mixed finite element method in space and a CN time-stepping scheme in time. Our main interest in this work is to give the error analysis for the proposed numerical scheme. Corresponding convergence results will be obtained, which will be confirmed by numerical experiments.

2. Mixed finite element discretization in space and error estimate. In this section, we introduce a mixed finite element method for (1.1) and give the corresponding error estimate for the semidiscrete approximation.

We shall use the standard notation for Sobolev spaces $W^{s,p}(\Omega)$ and their associated norms and seminorms (see, e.g., [1, 8]). We denote $H^s(\Omega) = W^{s,2}(\Omega)$ and

$$H^1_{\mathrm{per}}(\Omega) = \big\{ v \in H^1(\Omega) \text{ with periodic boundary condition} \big\}.$$

The corresponding norms $\|v\|_s = \|v\|_{s,2,\Omega}$ and $\|v\|_0 = \|v\|_{0,2,\Omega}$ are defined as

$$\|v\|_s^2 = \sum_{|\alpha| \le s} \|D^\alpha v\|_0^2 \quad \text{and} \quad \|v\|_0^2 = \int_\Omega |v|^2 d\Omega.$$

To define the norm in Bochner spaces, let X be a Banach space with a norm $\|\cdot\|_X$ and seminorm $|\cdot|_X$. Then we define

$$C\big(0,T;X\big) = \left\{ v : [0,T] \to X, \quad \|v\|_{C(0,T;X)} = \sup_{t\in[0,T]} \|v(t)\|_X \right\},$$

$$L^2(0,T;X) = \left\{ v : (0,T) \to X, \quad \|v\|_{L^2(0,T;X)} = \left(\int_0^T \|v(t)\|_X^2 dt \right)^{1/2} < \infty \right\},$$

$$H^m(0,T;X) = \left\{ v \in L^2(0,T;X) : \frac{\partial^j v}{\partial t^j} \in L^2(0,T;X), \quad 1 \le j \le m \right\},$$

where the derivatives $\partial^j v/\partial t^j$ are considered in the sense of distributions on $(0,T)$. The norm in space $H^m(0,T;X)$ is defined by

$$\|v\|^2_{H^m(0,T;X)} = \int_0^T \sum_{j=0}^m \left\| \frac{\partial^j v}{\partial t^j} \right\|_X^2 dt.$$

The weak solution of (1.1) can be defined as follows [23]: Find $\phi \in L^\infty(0,T;H^2_{\mathrm{per}}(\Omega))$ and $\partial_t\phi \in L^2(0,T;H^{-2}_{\mathrm{per}}(\Omega))$ such that for any $\varphi \in H^2_{\mathrm{per}}(\Omega)$,

$$\left\{ \begin{array}{rcl} (\partial_t\phi,\varphi) + \varepsilon(\Delta\phi,\Delta\varphi) + (|1-|\nabla\phi|^2|\nabla\phi,\nabla\varphi) &=& 0 \quad \text{for } t\in(0,T), \\ (\phi(\mathbf{x},0),\varphi) - (\phi_0(\mathbf{x}),\varphi) &=& 0. \end{array} \right. \tag{2.1}$$

In [23], the stability of the weak solution for the MBE model is studied. Relevant work has been done for the Cahn–Hilliard and Allen–Cahn phase field equations; see, e.g., [13, 14]. Numerical stability is also studied in [13, 14, 23]. There are two kinds of stability properties: one is in the classical sense, i.e., continuous dependence of solutions on the initial conditions, and the other is the energy-type stability in the sense of (1.3). In this work, both kinds of stability will be considered for our numerical scheme.

To analyze the numerical stability, we first state the following known results for the continuum MBE models.

LEMMA 2.1 (energy identities [23]). *If $\phi(x,t)$ is a solution of the MBE model* (1.1)*, then the following energy identities hold:*

$$\frac{d}{dt}\|\phi\|_0^2 + 4E_0(\phi) + \|\nabla\phi\|_{0,4}^4 = |\Omega| \qquad a.e.\ t\in(0,T), \tag{2.2}$$

$$\frac{d}{dt}E_0(\phi) + \|\partial_t\phi\|_0^2 = 0 \quad a.e.\ t \in (0,T), \tag{2.3}$$

where $\|\cdot\|_0$ *is the standard* L^2*-norm on* Ω*,* $\|\cdot\|_{0,p}$ *is the standard* L^p*-norm, and the energy functional is defined in* (1.2).

2.1. The mixed weak form. The objective of this paper is to use a mixed finite element method to solve an MBE model problem. We also give the corresponding error estimates for the semidiscrete and fully discrete approximations.

For the aim of the mixed finite element discretization, we introduce a new function $w = -\Delta\phi$. Then the mixed form of (1.1) can be defined as

$$\begin{cases} \frac{\partial\phi}{\partial t} - \varepsilon\Delta w = -\nabla\cdot[(1-|\nabla\phi|^2)\nabla\phi] & \text{in } \Omega\times(0,T), \\ -\Delta\phi - w = 0 & \text{in } \Omega\times[0,T), \\ \phi(\mathbf{x},0) = \phi_0(\mathbf{x}) & \text{in } \Omega. \end{cases} \tag{2.4}$$

A weak solution to (2.4) is a pair (ϕ, w) solving the following problem.

Problem 1. Find $(\phi,w) \in L^\infty(0,T;H^1_{\text{per}}(\Omega)) \times L^2(0,T;H^1_{\text{per}}(\Omega))$, $\partial_t\phi \in L^2(0,T;H^{-1}_{\text{per}}(\Omega))$, and $|\nabla\phi|^2\nabla\phi \in L^2(0,T;(L^2(\Omega))^2)$ such that for any $(\varphi, v) \in H^1_{\text{per}}(\Omega) \times H^1_{\text{per}}(\Omega)$,

$$\begin{cases} \left(\frac{\partial\phi}{\partial t},\varphi\right) + \varepsilon(\nabla w,\nabla\varphi) = \left((1-|\nabla\phi|^2)\nabla\phi,\nabla\varphi\right) & \text{for } t\in(0,T), \\ (\nabla\phi,\nabla v) - (w,v) = 0 & \text{for } t\in(0,T), \\ (\phi(\mathbf{x},0),\varphi) = (\phi_0(\mathbf{x}),\varphi), & \\ (\nabla\phi(\mathbf{x},0),\nabla v) - (w(\mathbf{x},0),v) = 0. & \end{cases} \tag{2.5}$$

With a derivative similar to that in [23, Theorem 3.2], we can give the following stability result.

LEMMA 2.2. *Let* ϕ_0*,* $\theta_0 \in H^1_{\text{per}}(\Omega)$*. Let* (ϕ,w)*,* (θ,u) *be the weak solution of* (2.5) *with* $\phi_0(\mathbf{x},0) = \phi_0$ *and* $\theta(\mathbf{x},0) = \theta_0$ *a.e.* Ω*. Then*

$$\|\phi-\theta\|_{L^\infty(0,T;L^2(\Omega))} + \varepsilon\|w-u\|_{L^2(0,T;L^2(\Omega))} \le C\|\phi_0-\theta_0\|_0, \tag{2.6}$$

where $C = C(T) > 0$ *is a constant.*

Remark 2.1. Then the existence and uniqueness of the weak solution to (2.5) can be deduced by a process similar to that in [23] with the addition of the semidiscrete solution in Theorem 2.5, the error estimate in Theorem 2.8, and Lemma 2.2.

Similarly to [23, Theorem 3.3], we have the following regularity result.

LEMMA 2.3. *Let* $\phi_0(\mathbf{x}) \in H^r_{\text{per}}(\Omega)$ *for some integer* $r \ge 2$*. Then the weak solution pair* $\phi : \Omega\times[0,T] \to \mathcal{R}$ *and* $w : \Omega\times[0,T]\to\mathcal{R}$ *of the initial boundary value problem* (2.4) *has the regularity* $\phi \in L^\infty(0,T;H^r(\Omega)) \cap L^2(0,T;H^{r+2}(\Omega))$*,* $\partial_t\phi \in L^2(0,T;H^{r-2}(\Omega))$*, and* $w \in L^2(0,T;H^r(\Omega))$*.*

For the mixed form of the MBE equation, the energy functional corresponding to (1.2) is defined as

$$E(\phi,w) = \frac{\varepsilon}{2}\|w\|_0^2 + \frac{1}{4}\|1-|\nabla\phi|^2\|_0^2. \tag{2.7}$$

Similarly, the following energy identities hold.

LEMMA 2.4. *If* $(\phi(x,t), w(x,t))$ *is a weak solution pair of the mixed MBE model* (2.4)*, then the following energy identities hold:*

$$\frac{d}{dt}\|\phi\|_0^2 + 4E(\phi,w) + \|\nabla\phi\|_{0,4}^4 = |\Omega| \quad a.e.\ t\in(0,T), \tag{2.8}$$

$$\frac{d}{dt}E(\phi, w) + \|\partial_t \phi\|_0^2 = 0 \qquad a.e.\ t \in (0, T). \tag{2.9}$$

Proof. Choosing $\varphi = \phi$ in the first equation of (2.5) and combining the result with the second equation of (2.5) leads to

$$\begin{aligned}
\left(\frac{\partial \phi}{\partial t}, \phi\right) &= -\varepsilon(\nabla w, \nabla \phi) + \big((1 - |\nabla \phi|^2)\nabla \phi, \nabla \phi\big) \\
&= -\varepsilon\big(w, w\big) + \big((1 - |\nabla \phi|^2)\nabla \phi, \nabla \phi\big) \\
&= -\varepsilon\|w\|_0^2 - \frac{1}{2}\|1 - |\nabla \phi|^2\|_0^2 - \frac{1}{2}\|\nabla \phi\|_{0,4}^4 + \frac{|\Omega|}{2} \\
&= -2E(\phi, w) - \frac{1}{2}\|\nabla \phi\|_{0,4}^4 + \frac{|\Omega|}{2}. \qquad (2.10)
\end{aligned}$$

Thus the desired result (2.8) can be obtained by combining (2.10) and the fact that

$$\left(\frac{\partial \phi}{\partial t}, \phi\right) = \frac{1}{2}\frac{d}{dt}\|\phi\|_0^2.$$

It follows from the second equation of (2.5) that

$$\left(\frac{\partial w}{\partial t}, w\right) = \left(\nabla \frac{\partial \phi}{\partial t}, \nabla w\right). \tag{2.11}$$

Using (2.11) and choosing $\varphi = \partial_t \phi$ in the first equation of (2.5) yields

$$\begin{aligned}
\left(\frac{\partial \phi}{\partial t}, \frac{\partial \phi}{\partial t}\right) &= -\varepsilon\left(\nabla w, \nabla \frac{\partial \phi}{\partial t}\right) + \left((1 - |\nabla \phi|^2)\nabla \phi, \nabla \frac{\partial \phi}{\partial t}\right) \\
&= -\varepsilon\left(\frac{\partial w}{\partial t}, w\right) + \left((1 - |\nabla \phi|^2)\nabla \phi, \nabla \frac{\partial \phi}{\partial t}\right) \\
&= -\frac{\varepsilon}{2}\frac{d\|w\|_0^2}{dt} + \frac{1}{2}\frac{d\|\nabla \phi\|_0^2}{dt} - \frac{1}{4}\frac{d\|\nabla \phi\|_0^4}{dt} \\
&= -\frac{d}{dt}\left(\frac{\varepsilon}{2}\|w\|_0^2 + \frac{1}{4}\|1 - |\nabla \phi|^2\|_0^2 - \frac{|\Omega|}{4}\right).
\end{aligned}$$

Consequently,

$$\frac{dE(\phi, w)}{dt} = -\left(\frac{\partial \phi}{\partial t}, \frac{\partial \phi}{\partial t}\right), \tag{2.12}$$

which is the desired result (2.9). $\square$

2.2. Mixed finite element discretization. In order to do the finite element discretization, we introduce the face-to-face partition $\mathcal{T}_h$ of the computational domain Ω into elements K (triangles or rectangles) such that

$$\bar{\Omega} = \bigcup_{K \in \mathcal{T}_h} K.$$

Here $h := \max_{K \in \mathcal{T}_h} h_K$ and $h_K = \text{diam}K$ denote the global and local mesh size, respectively. A family of partitions $\mathcal{T}_h$ is said to be *quasi-uniform* if it satisfies (see, e.g., [8])

$$\exists \sigma > 0 \text{ such that } h_K/\tau_K > \sigma \quad \forall K \in \mathcal{T}_h,$$

$$\exists \beta > 0 \text{ such that } \max\left\{h/h_K,\ K \in \mathcal{T}_h\right\} \le \beta.$$

Based on the partition $\mathcal{T}_h$, we build the finite element space V_h of piecewise polynomial functions

$$V_h := \left\{v_h \in H^1_{\mathrm{per}}(\Omega), v_h|_K \in \mathcal{P}_m \text{ or } \mathcal{Q}_m\ \forall K \in \mathcal{T}_h\right\}, \tag{2.13}$$

where $\mathcal{P}_m$ denotes the space of polynomials with degree not greater than m and $\mathcal{Q}_m$ denotes the space of polynomials with degree not greater than m in each variable.

Below we define the corresponding semidiscrete weak solution to (2.5).

Problem 2. Find $(\phi_h, w_h) \in L^\infty(0,T;V_h) \times L^2(0,T;V_h)$ and $\partial_t \phi_h \in L^2(0,T;V_h)$ such that for any $(\varphi_h, v_h) \in V_h \times V_h$,

$$\left\{\begin{aligned} \left(\tfrac{\partial \phi_h}{\partial t}, \varphi_h\right) + \varepsilon(\nabla w_h, \nabla \varphi_h) &= \left((1-|\nabla\phi_h|^2)\nabla\phi_h, \nabla\varphi_h\right) && \text{for } t \in (0,T),\\ (\nabla\phi_h, \nabla v_h) - (w_h, v_h) &= 0 && \text{for } t \in (0,T),\\ (\nabla\phi_h(\mathbf{x},0), \nabla\varphi_h) &= (\nabla\phi_0(\mathbf{x}), \nabla\varphi_h),\\ (\nabla\phi_h(\mathbf{x},0), \nabla v_h) &= (w_h(\mathbf{x},0), v_h). \end{aligned}\right. \tag{2.14}$$

THEOREM 2.5. *The semidiscrete scheme* (2.14) *has a unique solution.*

Proof. Let $N = \mathrm{dim} V_h$ and $\{\lambda_j, \psi_j\}_{1\le j\le N}$ be the eigenpair system of the following eigenvalue problem: Find $(\lambda, \psi) \in \mathcal{R} \times V_h$ such that $\|\psi\|_0 = 1$ and

$$(\nabla\psi, \nabla v) = \lambda(\psi, v) \quad \forall v \in V_h.$$

Then we have

$$(\nabla\psi_i, \nabla\psi_j) = \lambda_i \delta_{ij}, \quad (\psi_i, \psi_j) = \delta_{ij},$$

where δ_{ij} is the Kronecker delta function. Let

$$\phi_h(\mathbf{x},t) = \sum_{j=1}^N a_j(t)\psi_j(\mathbf{x}), \qquad w_h(\mathbf{x},t) = \sum_{j=1}^N b_j(t)\psi_j(\mathbf{x}).$$

From the second equation in (2.14), we have $b_j(t) = \lambda_j a_j(t)$ for $j = 1, \dots, N$. Then the first equation in (2.14) can be written in the following form:

$$\frac{\partial a_j(t)}{\partial t} + \varepsilon\lambda_j^2 a_j(t) = f_j(a_1(t), \dots, a_N(t)), \qquad j = 1, \dots, N, \tag{2.15}$$

where all $f_j : \mathcal{R}^N \mapsto \mathcal{R}$ $(1 \le j \le N)$ are smooth and locally Lipschitz. Set

$$a_j(0) = (\phi_0(\mathbf{x}), \psi_j(\mathbf{x})), \qquad j = 1, \dots, N. \tag{2.16}$$

From the theory of initial value problems for ordinary differential equations, we know that the initial value problem (2.15) and (2.16) has a unique smooth solution $(a_1(t), \dots, a_N(t))$ for $t \in [0,T]$. ∎

For the semidiscrete weak solution (ϕ_h, w_h), similar energy identities hold.

LEMMA 2.6. *If* $(\phi_h(\mathbf{x},t), w_h(\mathbf{x},t))$ *is a weak solution of the discrete problem* (2.14)*, then the following energy identities also hold:*

$$\frac{d}{dt}\|\phi_h\|_0^2 + 4E(\phi_h, w_h) + \|\nabla\phi_h\|_{0,4}^4 = |\Omega| \qquad a.e.\ t \in (0,T), \tag{2.17}$$

$$\frac{d}{dt}E(\phi_h, w_h) + \|\partial_t \phi_h\|_0^2 = 0 \qquad a.e.\ t \in (0,T). \tag{2.18}$$

Proof. The first desired result (2.17) can be proved in the same way as for (2.8). To prove (2.18), we begin by using the second equation of (2.14) to obtain

$$\left(\frac{\partial w_h}{\partial t}, w_h\right) = \left(\nabla \frac{\partial \phi_h}{\partial t}, \nabla w_h\right). \tag{2.19}$$

Using (2.19) and choosing $\varphi_h = \partial_t \phi_h$ in the first equation of (2.14) yields

$$\begin{aligned}\left(\frac{\partial \phi_h}{\partial t}, \frac{\partial \phi_h}{\partial t}\right) &= -\varepsilon\left(\nabla w_h, \nabla\frac{\partial \phi_h}{\partial t}\right) + \left((1-|\nabla\phi_h|^2)\nabla\phi_h, \nabla\frac{\partial \phi_h}{\partial t}\right)\\ &= -\varepsilon\left(\frac{\partial w_h}{\partial t}, w_h\right) + \left((1-|\nabla\phi_h|^2)\nabla\phi_h, \nabla\frac{\partial \phi_h}{\partial t}\right)\\ &= -\frac{\varepsilon}{2}\frac{d\|w_h\|_0^2}{dt} + \frac{1}{2}\frac{d\|\nabla\phi_h\|_0^2}{dt} - \frac{1}{4}\frac{d\||\nabla\phi_h|^2\|_0^2}{dt}\\ &= -\frac{d}{dt}\left(\frac{\varepsilon}{2}\|w_h\|_0^2 + \frac{1}{4}\|1-|\nabla\phi_h|^2\|_0^2 - \frac{|\Omega|}{4}\right).\end{aligned} \tag{2.20}$$

Consequently,

$$\frac{dE(\phi_h, w_h)}{dt} = -\left(\frac{\partial \phi_h}{\partial t}, \frac{\partial \phi_h}{\partial t}\right), \tag{2.21}$$

which is the desired result (2.18). ∎

2.3. Error estimate of semidiscrete form. Now we turn to analyzing the error estimate of the semidiscrete approximation (ϕ_h, w_h) defined in (2.14).

Based on the finite element space V_h, we define the Ritz-projection P_h by

$$(\nabla P_h u, \nabla v_h) = (\nabla u, \nabla v_h) \qquad \forall v_h \in V_h, \tag{2.22}$$

and the L^2-projection operator π_h by

$$(\pi_h u, v_h) = (u, v_h) \qquad \forall v_h \in V_h. \tag{2.23}$$

Let

$$\xi_\phi := \phi_h - P_h\phi, \quad \eta_\phi := P_h\phi - \phi, \quad \xi_w := w_h - P_h w, \tag{2.24}$$

$$\eta_w := P_h w - w, \quad \tilde{\xi}_w := w_h - \pi_h w, \quad \tilde{\eta}_w := \pi_h w - w, \tag{2.25}$$

which gives

$$\phi_h - \phi = \xi_\phi + \eta_\phi, \tag{2.26}$$

$$w_h - w = \xi_w + \eta_w, \tag{2.27}$$

$$w_h - w = \tilde{\xi}_w + \tilde{\eta}_w. \tag{2.28}$$

It follows from (2.14), (2.22), and (2.23) that

$$\begin{aligned}(\nabla(\phi_h - P_h\phi), \nabla v_h) &= (\nabla\phi_h, \nabla v_h) - (\nabla\phi, \nabla v_h)\\ &= (w_h - w, v_h) = (w_h - \pi_h w, v_h) \qquad \forall v_h \in V_h,\end{aligned}$$

which leads to

$$\|\nabla\xi_\phi\|_0^2 \le \|\tilde{\xi}_w\|_0\|\xi_\phi\|_0. \tag{2.29}$$

On the other hand, it follows from (2.5) and (2.14) that

$$\begin{aligned}(\nabla\xi_w, \nabla\xi_\phi) &= (\nabla\xi_w, \nabla(\phi_h - P_h\phi)) = (\nabla\xi_w, \nabla(\phi_h - \phi))\\ &= (\nabla\xi_w, \nabla\phi_h) - (\nabla\xi_w, \nabla\phi)\\ &= (\xi_w, w_h - w) = (\xi_w, w_h - \pi_h w)\\ &= (\xi_w, w_h - P_h w) + (\xi_w, P_h w - \pi_h w)\\ &= \|\xi_w\|_0^2 + (\xi_w, \eta_w - \tilde{\eta}_w). \end{aligned} \tag{2.30}$$

In our analysis, we also need the following inequality:

$$\begin{aligned}\|\tilde{\xi}_w\|_0^2 &\le 2\|\xi_w\|_0^2 + 2\|P_h w - \pi_h w\|_0^2\\ &\le 2\|\xi_w\|_0^2 + 4\|P_h w - w\|_0^2 + 4\|w - \pi_h w\|_0^2\\ &= 2\|\xi_w\|_0^2 + 4\|\eta_w\|_0^2 + 4\|\tilde{\eta}_w\|_0^2, \end{aligned} \tag{2.31}$$

where $\tilde{\xi}_w$ is defined by (2.25).

LEMMA 2.7. *Let (ϕ, w) be the solution of (2.4). The finite element approximation (ϕ_h, w_h) of (2.14) has the following error estimate:*

$$\begin{aligned}&\|\phi(\mathbf{x}, T) - \phi_h(\mathbf{x}, T)\|_0^2 + \int_0^T \varepsilon\|w - w_h\|_0^2 dt\\ &\le C\left(\int_0^T \left(\|\nabla\eta_\phi\|_0^2 + \|\eta_w\|_0^2 + \|\tilde{\eta}_w\|_0^2 + \|\partial_t\eta_\phi\|_0^2\right)dt \right.\\ &\qquad \left. + \|\phi_0(\mathbf{x}) - \phi_h(\mathbf{x}, 0)\|_0^2\right), \end{aligned} \tag{2.32}$$

where the constant C is independent of the mesh size h but is dependent on ϕ and ε.

Proof. It follows from (2.5), (2.14), (2.22), (2.23), the regularity result in Lemma 2.3 (meaning $\phi \in L^\infty(0, T; W^{1,\infty}(\Omega))$), and the Cauchy–Schwarz inequality that

$$\begin{aligned}&(\partial_t\xi_\phi, \xi_\phi) + (|\nabla\phi_h|^2\nabla\phi_h, \nabla\xi_\phi) - (|\nabla P_h\phi|^2\nabla P_h\phi, \nabla\xi_\phi) + \varepsilon\big(\nabla\xi_w, \nabla\xi_\phi\big) - \|\nabla\xi_\phi\|_0^2\\ &\quad = (\partial_t\eta_\phi, \xi_\phi) + (|\nabla\phi|^2\nabla\phi, \nabla\xi_\phi) - \big(|\nabla P_h\phi|^2\nabla P_h\phi, \nabla\xi_\phi\big)\\ &\quad \le \big|(\partial_t\eta_\phi, \xi_\phi)\big| + \big|\big(|\nabla P_h\phi|^2 - |\nabla\phi|^2, \nabla P_h\phi\cdot\nabla\xi_\phi\big)\big| + \big|\big(|\nabla\phi|^2\nabla(P_h\phi - \phi), \nabla\xi_\phi\big)\big|\\ &\quad \le \|\partial_t\eta_\phi\|_0\|\xi_\phi\|_0 + C\|\nabla\eta_\phi\|_0\|\nabla\xi_\phi\|_0. \end{aligned} \tag{2.33}$$

Using the Cauchy–Schwarz inequality, we have the following estimate for the nonlinear term:

$$\begin{aligned}&\big(|\nabla\phi_h|^2\nabla\phi_h, \nabla(\phi_h - P_h\phi)\big) - \big(|\nabla P_h\phi|^2\nabla P_h\phi, \nabla(\phi_h - P_h\phi)\big)\\ &\quad = \|\nabla\phi_h\|_{0,4}^4 + \|\nabla P_h\phi\|_{0,4}^4 - \big(|\nabla\phi_h|^2\nabla\phi_h, \nabla P_h\phi\big) - \big(|\nabla P_h\phi|^2\nabla P_h\phi, \nabla\phi_h\big)\\ &\quad \ge \frac{1}{2}\|\nabla\phi_h\|_{0,4}^4 + \frac{1}{2}\|\nabla P_h\phi\|_{0,4}^4 - \big(|\nabla P_h\phi|^2, |\nabla\phi_h|^2\big) \ge 0. \end{aligned} \tag{2.34}$$

Combining (2.29), (2.31), and (2.33)–(2.34) leads to the following estimates:

$$
\begin{aligned}
&(\partial_t \xi_\phi, \xi_\phi) + \varepsilon\big(\nabla \xi_w, \nabla \xi_\phi\big) \\
&\qquad \le C\|\nabla \eta_\phi\|_0^2 + 2\|\nabla \xi_\phi\|_0^2 + \|\partial_t \eta_\phi\|_0 \|\xi_\phi\|_0 \\
&\qquad \le C\|\nabla \eta_\phi\|_0^2 + 2\|\xi_\phi\|_0 \|\tilde{\xi}_w\|_0 + \|\partial_t \eta_\phi\|_0 \|\xi_\phi\|_0 \\
&\qquad \le C\|\nabla \eta_\phi\|_0^2 + \frac{8}{\varepsilon}\|\xi_\phi\|_0^2 + \frac{\varepsilon}{8}\|\tilde{\xi}_w\|_0^2 + \|\partial_t \eta_\phi\|_0 \|\xi_\phi\|_0 \\
&\qquad \le C\|\nabla \eta_\phi\|_0^2 + \left(\frac{1}{2} + \frac{8}{\varepsilon}\right)\|\xi_\phi\|_0^2 + \frac{\varepsilon}{4}\|\xi_w\|_0^2 \\
&\qquad\quad + \frac{\varepsilon}{2}\left(\|\eta_w\|_0^2 + \|\tilde{\eta}_w\|_0^2\right) + \frac{1}{2}\|\partial_t \eta_\phi\|_0^2.
\end{aligned} \tag{2.35}
$$

It follows from (2.30) and (2.35) that

$$
\begin{aligned}
&(\partial_t \xi_\phi, \xi_\phi) + \frac{\varepsilon}{2}\|\xi_w\|_0^2 \\
&\quad \le C\Big(\|\nabla \eta_\phi\|_0^2 + \|\eta_w\|_0^2 + \|\tilde{\eta}_w\|_0^2\Big) + \left(\frac{1}{2} + \frac{4}{\varepsilon}\right)\|\xi_\phi\|_0^2 + \frac{1}{2}\|\partial_t \eta_\phi\|_0^2,
\end{aligned} \tag{2.36}
$$

which implies that

$$
\begin{aligned}
&\frac{1}{2}\frac{d}{dt}\|\xi_\phi\|_0^2 + \frac{\varepsilon}{2}\|\xi_w\|_0^2 \\
&\quad \le C\Big(\|\nabla \eta_\phi\|_0^2 + \|\eta_w\|_0^2 + \|\tilde{\eta}_w\|_0^2 + \|\partial_t \eta_\phi\|_0^2\Big) + C\|\xi_\phi\|_0^2.
\end{aligned} \tag{2.37}
$$

Using Gronwall's inequality gives

$$
\begin{aligned}
&\|\xi_\phi(\mathbf{x}, T)\|_0^2 + \int_0^T \varepsilon \|\xi_w\|_0^2 dt \\
&\quad \le C\left(\int_0^T \left(\|\nabla \eta_\phi\|_0^2 + \|\eta_w\|_0^2 + \|\tilde{\eta}_w\|_0^2 + \|\partial_t \eta_\phi\|_0^2|\right) dt + \|\xi_\phi(\mathbf{x}, 0)\|_0^2\right).
\end{aligned} \tag{2.38}
$$

We can arrive at the desired result, (2.32), by using the triangle inequality and (2.26)–(2.28). ∎

We close this section by providing the following error estimates for the semi-discrete approximations.

THEOREM 2.8. *Let (ϕ, w) be the solution of (2.4) and $\phi_0 \in H^{m+2}_{\text{per}}(\Omega)$. Then the finite element approximation (ϕ_h, w_h) of (2.14) has the following error estimate:*

$$
\begin{aligned}
&\|\phi(\mathbf{x}, T) - \phi_h(\mathbf{x}, T)\|_0^2 + \int_0^T \varepsilon \|w - w_h\|_0^2 dt \\
&\quad \le Ch^{2m}\left[\int_0^T \Big(\|\phi\|_{m+1}^2 + \|\partial_t \phi\|_m^2 + \|w\|_m^2\Big) dt + \|\phi_0\|_m^2\right],
\end{aligned} \tag{2.39}
$$

where the constant C is independent of the mesh size h.

Proof. We take $\phi_h(\mathbf{x}, 0) = P_h \phi_0$. Combining Lemmas 2.3 and 2.7 and the error estimates

$$
\begin{aligned}
\|\nabla \eta_\phi\|_0 \le Ch^m \|\phi\|_{m+1}, &\qquad \|\partial_t \eta_\phi\|_0 \le Ch^m \|\partial_t \phi\|_m, \\
\|\eta_w\|_0 \le Ch^m \|w\|_m, &\qquad \|\tilde{\eta}_w\|_0 \le Ch^m \|w\|_m, \\
\|\phi_0 - \phi_h(\mathbf{x}, 0)\|_0 \le Ch^m \|\phi_0\|_m, &
\end{aligned}
$$

we can obtain the desired result (2.39). ∎

Remark 2.2. Unlike the case with the normal error estimates for the parabolic equations, which give $(m+1)$th convergence order, the convergence rate obtained above is of mth order only. This is due to the difficulty arising from the second-order nonlinear term. This issue requires some future investigation.

3. Time discretization and energy properties. In this section, we use the Crank–Nicolson (CN) scheme to carry out the time discretization. Application of the CN scheme for MBE-type equations can be found in, e.g., [26, 27]. The use of the CN approximation leads to the following fully discretized scheme for (1.1).

Problem 3. Given $(\phi_h^n, w_h^n) \in V_h \times V_h$, find $(\phi_h^{n+1}, w_h^{n+1}) \in V_h \times V_h$ such that for any $(\varphi_h, v_h) \in V_h \times V_h$,

$$\left\{ \begin{array}{rcl} \left(\frac{\phi_h^{n+1}-\phi_h^n}{\Delta t}, \varphi_h\right) &=& -(\mu_h^{n+\frac{1}{2}}, \nabla\varphi_h), \\ (w_h^{n+1}, v_h) &=& (\nabla\phi_h^{n+1}, \nabla v_h), \end{array} \right. \tag{3.1}$$

with

$$\mu_h^{n+\frac{1}{2}} = \varepsilon\left(\frac{\nabla w_h^{n+1} + \nabla w_h^n}{2}\right) + \left(\frac{\left(|\nabla\phi_h^{n+1}|^2 + |\nabla\phi_h^n|^2\right)\left(\nabla\phi_h^{n+1} + \nabla\phi_h^n\right)}{4}\right) - \left(\frac{\nabla\phi_h^{n+1}}{2} + \frac{\nabla\phi_h^n}{2}\right).$$

To begin with, we will state the following discrete Volterra-type inequality which will be used in this section.

LEMMA 3.1 (see [4]). *Let k, B and a_μ, b_μ, c_μ, γ_μ, for integer $\mu \geq 0$, be nonnegative numbers such that*

$$a_n + k\sum_{\mu=0}^{n} b_\mu \leq k\sum_{\mu=0}^{n}\gamma_\mu a_\mu + k\sum_{\mu=0}^{n} c_\mu + B \quad \textit{for } n \geq 0. \tag{3.2}$$

Suppose that $k\gamma_\mu < 1$ for all μ, and set $\sigma_\mu = (1-k\gamma_\mu)^{-1}$. Then,

$$a_n + k\sum_{\mu=0}^{n} b_\mu \leq \exp\left(k\sum_{\mu=0}^{n}\gamma_\mu\sigma_\mu\right)\left\{k\sum_{\mu=0}^{n} c_\mu + B\right\} \quad \textit{for } n \geq 0. \tag{3.3}$$

LEMMA 3.2. *Let (ϕ_h^n, w_h^n) and (θ_h^n, u_h^n) be two solutions of (3.1) for the initial values $\phi(\mathbf{x},0) = \phi_0$ and $\theta(\mathbf{x},0) = \theta_0$, respectively. Then we have*

$$\|\phi_h^N - \theta_h^N\|_0^2 + \frac{\varepsilon}{2}\sum_{k=1}^{N-1}\|w_h^{k+1} + w_h^k - (u_h^{k+1} + u_h^k)\|_0^2 \leq C\|\phi_h^0 - \theta_h^0\|_0^2 \tag{3.4}$$

when the time step size Δt is small enough.

Proof. Set $f_h^k = \phi_h^k - \theta_h^k$ and $g_h^k = w_h^k - u_h^k$ $(k = 0, \ldots, N)$. We have

$$\left\{ \begin{array}{rcl} \left(\frac{f_h^{n+1}-f_h^n}{\Delta t}, f_h^{n+1} + f_h^n\right) &=& -(\nu_h^{n+\frac{1}{2}}, \nabla(f_h^{n+1} + f_h^n)), \\ (g_h^{n+1}, g_h^{n+1}) &=& -(\nabla f_h^{n+1}, \nabla g_h^{n+1}), \end{array} \right. \tag{3.5}$$

with

$$\nu_h^{n+\frac{1}{2}} = \varepsilon\left(\frac{\nabla g_h^{n+1} + \nabla g_h^n}{2}\right) + \left(\frac{\left(|\nabla\phi_h^{n+1}|^2 + |\nabla\phi_h^n|^2\right)\left(\nabla\phi_h^{n+1} + \nabla\phi_h^n\right)}{4}\right)$$

$$-\left(\frac{\big(|\nabla\theta_h^{n+1}|^2+|\nabla\theta_h^n|^2\big)\big(\nabla\theta_h^{n+1}+\nabla\theta_h^n\big)}{4}\right)-\left(\frac{\nabla f_h^{n+1}}{2}+\frac{\nabla f_h^n}{2}\right).$$

Similarly to (2.34), we assume the nonnegative estimate for the nonlinear terms in the left-hand side of (3.5),

$$\begin{aligned}&\left(\frac{\big(|\nabla\phi_h^{n+1}|^2+|\nabla\phi_h^n|^2\big)\big(\nabla\phi_h^{n+1}+\nabla\phi_h^n\big)}{4},\nabla(f_h^{n+1}+f_h^n)\right)\\ &-\left(\frac{\big(|\nabla\theta_h^{n+1}|^2+|\nabla\theta_h^n|^2\big)\big(\nabla\theta_h^{n+1}+\nabla\theta_h^n\big)}{4},\nabla(f_h^{n+1}+f_h^n)\right)\geq 0.\end{aligned}\tag{3.6}$$

Then the following estimates hold:

$$\begin{aligned}0&\geq\frac{\|f_h^{n+1}\|_0^2-\|f_h^n\|_0^2}{\Delta t}+\varepsilon\left(\frac{\nabla g_h^{n+1}+\nabla g_h^n}{2},\nabla(f_h^{n+1}+f_h^n)\right)\\ &\quad-\left(\frac{\nabla(f_h^{n+1}+f_h^n)}{2},\nabla(f_h^{n+1}+f_h^n)\right)\\ &=\frac{\|f_h^{n+1}\|_0^2-\|f_h^n\|_0^2}{\Delta t}+\frac{\varepsilon}{2}\big(g_h^{n+1}+g_h^n,g_h^{n+1}+g_h^n\big)-\frac{1}{2}\big(g_h^{n+1}+g_h^n,f_h^{n+1}+f_h^n\big)\\ &\geq\frac{\|f_h^{n+1}\|_0^2-\|f_h^n\|_0^2}{\Delta t}+\frac{\varepsilon}{2}\|g_h^{n+1}+g_h^n\|_0^2-\frac{\varepsilon}{4}\|g_h^{n+1}+g_h^n\|_0^2-\frac{1}{4\varepsilon}\|f_h^{n+1}+f_h^n\|_0^2\\ &=\frac{\|f_h^{n+1}\|_0^2-\|f_h^n\|_0^2}{\Delta t}+\frac{\varepsilon}{4}\|g_h^{n+1}+g_h^n\|_0^2-\frac{1}{4\varepsilon}\|f_h^{n+1}+f_h^n\|_0^2\\ &\geq\frac{\|f_h^{n+1}\|_0^2-\|f_h^n\|_0^2}{\Delta t}+\frac{\varepsilon}{4}\|g_h^{n+1}+g_h^n\|_0^2-\frac{1}{4\varepsilon}\big(\|f_h^{n+1}\|_0^2+\|f_h^n\|_0^2\big).\end{aligned}\tag{3.7}$$

From (3.7), we have

$$\|f_h^n\|_0^2+\frac{\varepsilon}{4}\sum_{k=0}^{n}\Delta t\|g_h^k+g_h^{k+1}\|_0^2\leq\frac{\Delta t}{2\varepsilon}\sum_{k=0}^{n}\|f_h^k\|_0^2+\|f_h^0\|_0^2.\tag{3.8}$$

The desired result (3.4) can be obtained by combining (3.8) and Lemma 3.1, provided that $\Delta t<2\varepsilon$. ◻

Below we will use the Brouwer fixed-point theorem to show the existence of the solution for the fully discrete scheme (3.1).

LEMMA 3.3 (see [19, p. 219]). *Let H be a finite-dimensional Hilbert space with the inner product $(\cdot,\cdot)$ and induced norm $\|\cdot\|_H$. Further, let L be a continuous mapping from H into itself and be such that $(L(\xi),\xi)>0$ for all $\xi\in H$ with $\|\xi\|=\alpha>0$. Then there exists an element $\xi^*\in H$ such that $L(\xi^*)=0$ and $\|\xi^*\|\leq\alpha$.*

THEOREM 3.4. *The fully discretized scheme* (3.1) *has a unique solution.*

Proof. Let $\xi=\frac{\phi_h^{n+1}+\phi_h^n}{2}$, $w=\frac{w_h^{n+1}+w_h^n}{2}$, and define $L(\xi)$ such that

$$\begin{aligned}(L(\xi),\varphi_h)&=(\xi,\varphi_h)-(\phi_h^n,\varphi_h)+\varepsilon\Delta t(\nabla w,\nabla\varphi_h)-\Delta t(\nabla\xi,\nabla\varphi_h)\\ &\quad+\Delta t\left(\frac{\big(|2\nabla\xi-\nabla\phi_h^n|^2+|\nabla\phi_h^n|^2\big)\nabla\xi}{2},\nabla\varphi_h\right)\qquad\forall\varphi_h\in V_h.\end{aligned}$$

From the Young and Hölder inequalities, we have the following estimates:

$$
\begin{aligned}
&(L(\xi),\xi)\\
&= (\xi,\xi) - (\phi_h^n,\xi) + \varepsilon\Delta t(\nabla w,\nabla\xi) + \Delta t\left(\frac{\left(|2\nabla\xi - \nabla\phi_h^n|^2 + |\nabla\phi_h^n|^2\right)\nabla\xi}{2},\nabla\xi\right)\\
&\qquad - \Delta t(\nabla\xi,\nabla\xi)\\
&= (\xi,\xi) - (\phi_h^n,\xi) + \varepsilon\Delta t(w,w) + \Delta t\left(\frac{4|\nabla\xi|^2 - 4\nabla\xi\cdot\nabla\phi_h^n + 2|\nabla\phi_h^n|^2}{2},|\nabla\xi|^2\right)\\
&\qquad - \Delta t(\nabla\xi,\nabla\xi)\\
&\geq \|\xi\|_0^2 - \frac{1}{2}\|\xi\|_0^2 - \frac{1}{2}\|\phi_h^n\|_0^2 + \varepsilon\Delta t(w,w) + \Delta t(|\nabla\phi_h^n|^2,|\nabla\xi|^2) + 2\Delta t\|\nabla\xi\|_{0,4}^4\\
&\qquad - 2\Delta t(|\nabla\xi|^3,|\nabla\phi_h^n|) - \Delta t\|\nabla\xi\|_0^2\\
&\geq \frac{1}{2}\|\xi\|_0^2 - \frac{1}{2}\|\phi_h^n\|_0^2 + \varepsilon\Delta t(w,w) + \Delta t(|\nabla\phi_h^n|^2,|\nabla\xi|^2) + 2\Delta t\|\nabla\xi\|_{0,4}^4\\
&\qquad - \frac{3\Delta t}{2}\|\nabla\xi\|_{0,4}^4 - \frac{\Delta t}{2}\|\nabla\phi_h^n\|_{0,4}^4 - \Delta t\|\nabla\xi\|_0^2\\
&= \frac{1}{2}\|\xi\|_0^2 - \frac{1}{2}\|\phi_h^n\|_0^2 + \varepsilon\Delta t(w,w) + \Delta t(|\nabla\phi_h^n|^2,|\nabla\xi|^2) + \frac{\Delta t}{2}\|\nabla\xi\|_{0,4}^4\\
&\qquad - \Delta t\|\nabla\xi\|_0^2 - \frac{\Delta t}{2}\|\nabla\phi_h^n\|_{0,4}^4\\
&= \frac{1}{2}\|\xi\|_0^2 - \frac{1}{2}\|\phi_h^n\|_0^2 + \varepsilon\Delta t\|w\|_0^2 + \Delta t(|\nabla\phi_h^n|^2,|\nabla\xi|^2) + \frac{\Delta t}{2}\||\nabla\xi|^2 - 1\|_0^2\\
&\qquad - \frac{\Delta t}{2}|\Omega| - \frac{\Delta t}{2}\|\nabla\phi_h^n\|_{0,4}^4\\
&\geq \frac{1}{2}\|\xi\|_0^2 - \frac{1}{2}\left(\|\phi_h^n\|_0^2 + \Delta t|\Omega| + \Delta t\|\nabla\phi_h^n\|_{0,4}^4\right).
\end{aligned}
$$

Take $\alpha = \|\phi_h^n\|_0^2 + \Delta t|\Omega| + \Delta t\|\nabla\phi_h^n\|_{0,4}^4$. If $\xi \in V_h$ and $\|\xi\|_0^2 = \alpha$, we have $(L(\xi),\xi) \geq 0$. By Lemma 3.3, there is at least one solution ξ satisfying $\|\xi\|_0^2 \leq \|\phi_h^n\|_0^2 + \Delta t|\Omega| + \Delta t\|\nabla\phi_h^n\|_{0,4}^4$. It means we have at least one solution ϕ_h^{n+1}. The uniqueness of the solution can be derived from Lemma 3.2. ∎

THEOREM 3.5. *The fully discrete scheme* (3.1) *is unconditionally energy-stable with respect to the initial energy. More precisely, for any time step size* $\Delta t > 0$ *there holds*

$$
E(\phi_h^{n+1}, w_h^{n+1}) \leq E(\phi_h^n, w_h^n), \tag{3.9}
$$

where the energy E *is defined by* (2.7) *and* (ϕ_h^n, w_h^n) *denotes the numerical solutions of* (3.1) *at* t_n. *Furthermore, we have the discrete form of the energy identity with the form* (2.18)*:*

$$
\frac{E(\phi_h^{n+1}, w_h^{n+1}) - E(\phi_h^n, w_h^n)}{\Delta t} + \left\|\frac{\phi_h^{n+1} - \phi_h^n}{\Delta t}\right\|_0^2 = 0. \tag{3.10}
$$

Proof. Choosing $\varphi_h = (\phi_h^{n+1} - \phi_h^n)/\Delta t$ in (3.1) leads to

$$
\begin{aligned}
&\left(\frac{\phi_h^{n+1} - \phi_h^n}{\Delta t}, \frac{\phi_h^{n+1} - \phi_h^n}{\Delta t}\right)\\
&= -\varepsilon\left(\frac{\nabla w_h^{n+1} + \nabla w_h^n}{2}, \frac{\nabla\phi_h^{n+1} - \nabla\phi_h^n}{\Delta t}\right)
\end{aligned}
$$

$$
\begin{aligned}
&-\left(\frac{(|\nabla\phi_h^{n+1}|^2+|\nabla\phi_h^n|^2)(\nabla\phi_h^{n+1}+\nabla\phi_h^n)}{4},\frac{\nabla\phi_h^{n+1}-\nabla\phi_h^n}{\Delta t}\right)\\
&+\left(\frac{\nabla\phi_h^{n+1}+\nabla\phi_h^n}{2},\frac{\nabla\phi_h^{n+1}-\nabla\phi_h^n}{\Delta t}\right)\\
=&-\varepsilon\left(\frac{w_h^{n+1}+w_h^n}{2},\frac{w_h^{n+1}-w_h^n}{\Delta t}\right)-\left(\frac{|\nabla\phi_h^{n+1}|^2+|\nabla\phi_h^n|^2}{4},\frac{|\nabla\phi_h^{n+1}|^2-|\nabla\phi_h^n|^2}{\Delta t}\right)\\
&+\frac{1}{2\Delta t}\Big(\big\|\nabla\phi_h^{n+1}\big\|_0^2-\big\|\nabla\phi_h^n\big\|_0^2\Big). \qquad (3.11)
\end{aligned}
$$

Similarly, from the energy definition (2.7) and (3.11), we have

$$
E(\phi_h^{n+1},w_h^{n+1})-E(\phi_h^n,w_h^n)=-\Delta t\left\|\frac{\phi_h^{n+1}-\phi_h^n}{\Delta t}\right\|_0^2.
$$

Thus we obtain the desired energy stable result (3.9) and the discrete energy identity (3.10). ◻

4. Error estimate of the fully discrete form. In this section, we derive the error estimate for the fully discrete solution of (3.1). Toward this aim, we now introduce some useful notation. Let

$$
\xi_\phi^n:=\phi_h^n-P_h\phi(\cdot,t_n),\quad \eta_\phi^n:=P_h\phi(\cdot,t_n)-\phi(\cdot,t_n), \tag{4.1}
$$

$$
\xi_w^n:=w_h^n-P_hw(\cdot,t_n),\quad \eta_w^n:=P_hw(\cdot,t_n)-w(\cdot,t_n), \tag{4.2}
$$

$$
\tilde\xi_w^n:=w_h^n-\pi_hw(\cdot,t_n),\quad \tilde\eta_w^n:=\pi_hw(\cdot,t_n)-w(\cdot,t_n). \tag{4.3}
$$

It can be easily verified that

$$
\phi_h^n-\phi(\cdot,t_n)=\xi_\phi^n+\eta_\phi^n, \tag{4.4}
$$

$$
w_h^n-w(\cdot,t_n)=\xi_w^n+\eta_w^n, \tag{4.5}
$$

$$
w_h^n-w(\cdot,t_n)=\tilde\xi_w^n+\tilde\eta_w^n. \tag{4.6}
$$

For simplicity, we set $\phi^n:=\phi(\mathbf{x},t_n)$, $w^n:=w(\mathbf{x},t_n)$, and

$$
\phi^{n+1/2}:=\phi\left(\mathbf{x},\frac{t_n+t_{n+1}}{2}\right),\quad w^{n+1/2}:=w\left(\mathbf{x},\frac{t_n+t_{n+1}}{2}\right).
$$

LEMMA 4.1. *Let (ϕ,w) be the solution of (2.5), and assume $\phi_0\in H^6_{\mathrm{per}}(\Omega)$, $\phi_h^0=P_h\phi_0$, and $T=N\Delta t$. If the time step size Δt is sufficiently small, then with the notation given in (4.1)–(4.3) the finite element approximation (ϕ_h^n,w_h^n) of (3.1) has the following error estimate:*

$$
\begin{aligned}
&\|\xi_\phi^N\|_0^2+\frac{\varepsilon}{4}\sum_{k=0}^{N-1}\Delta t\|\xi_w^{k+1}+\xi_w^k\|_0^2\\
\le\;& C\Delta t^4\int_0^T\|\phi_{ttt}\|_0^2ds+C\Delta t^4\int_0^T\|\nabla\phi_{tt}\|_0^2ds+C\varepsilon\Delta t^4\int_0^T\|\nabla w_{tt}\|_0^2ds\\
&+C\int_0^T\|\partial_t\eta_\phi\|_0^2ds+C\sum_{k=0}^{N-1}\Delta t\big\|\nabla(\eta_\phi^{k+1}+\eta_\phi^k)\big\|_0^2+C\sum_{k=0}^{N-1}\Delta t\|\eta_w^{k+1}+\eta_w^k\|_0^2\\
&+C\sum_{k=0}^{N-1}\Delta t\big\|\tilde\eta_w^{k+1}+\tilde\eta_w^k\big\|_0^2+\|\xi_\phi^0\|_0^2, \qquad (4.7)
\end{aligned}
$$

where the constant C is independent of the mesh size h and time step Δt but dependent on ϕ.

Proof. First, from the regularity results in [23, Theorem 3.3], we have $\phi_{ttt} \in L^2(0,T;L^2(\Omega))$ and $\phi \in L^\infty(0,T;W^{1,\infty}(\Omega))$ when $\phi_0 \in H^6_{\text{per}}(\Omega)$. From (2.14), (2.22), (2.23), and (3.1), we have

$$\begin{aligned}
&\left(\frac{\xi_\phi^{n+1}-\xi_\phi^n}{\Delta t}, \xi_\phi^{n+1}+\xi_\phi^n\right)\\
&\quad + \left(\frac{(|\nabla\phi_h^{n+1}|^2+|\nabla\phi_h^n|^2)(\nabla\phi_h^{n+1}+\nabla\phi_h^n)}{4}, \nabla(\xi_\phi^{n+1}+\xi_\phi^n)\right)\\
&\quad - \left(\frac{(|\nabla P_h\phi^{n+1}|^2+|\nabla P_h\phi^n|^2)(\nabla P_h\phi^{n+1}+\nabla P_h\phi^n)}{4}, \nabla(\xi_\phi^{n+1}+\xi_\phi^n)\right)\\
&\quad + \frac{\varepsilon}{2}\left(\nabla(\xi_w^{n+1}+\xi_w^n), \nabla(\xi_\phi^{n+1}+\xi_\phi^n)\right) - \frac{1}{2}\|\nabla(\xi_\phi^{n+1}+\xi_\phi^n)\|_0^2\\
&= \Upsilon_1+\Upsilon_2+\Upsilon_3+\Upsilon_4, \qquad (4.8)
\end{aligned}$$

where

$$\Upsilon_1 = \left(\partial_t\phi^{n+\frac12} - \frac{P_h\phi^{n+1}-P_h\phi^n}{\Delta t}, \xi_\phi^{n+1}+\xi_\phi^n\right), \qquad (4.9)$$

$$\begin{aligned}
\Upsilon_2 &= \left(|\nabla\phi^{n+\frac12}|^2\nabla\phi^{n+\frac12}, \nabla(\xi_\phi^{n+1}+\xi_\phi^n)\right)\\
&\quad - \left(\frac{(|\nabla P_h\phi^{n+1}|^2+|\nabla P_h\phi^n|^2)(\nabla P_h\phi^{n+1}+\nabla P_h\phi^n)}{4}, \nabla(\xi_\phi^{n+1}+\xi_\phi^n)\right), \qquad (4.10)
\end{aligned}$$

$$\Upsilon_3 = \varepsilon\left(\nabla w^{n+\frac12} - \frac{\nabla P_h w^{n+1}+\nabla P_h w^n}{2}, \nabla(\xi_\phi^{n+1}+\xi_\phi^n)\right), \qquad (4.11)$$

$$\Upsilon_4 = -\left(\nabla\phi^{n+\frac12} - \frac{\nabla P_h\phi^{n+1}+\nabla P_h\phi^n}{2}, \nabla(\xi_\phi^{n+1}+\xi_\phi^n)\right). \qquad (4.12)$$

We now estimate the terms Υ_1, Υ_2, Υ_3, and Υ_4. First we have the following estimate for Υ_1 by using a Taylor expansion, (2.22), and the Cauchy–Schwarz inequality:

$$\begin{aligned}
|\Upsilon_1| &\le \left|\left(\partial_t\phi^{n+\frac12} - \frac{\phi^{n+1}-\phi^n}{\Delta t}, \xi_\phi^{n+1}+\xi_\phi^n\right)\right|\\
&\quad + \left|\left(\frac{(\phi^{n+1}-P_h\phi^{n+1})-(\phi^n-P_h\phi^n)}{\Delta t}, \xi_\phi^{n+1}+\xi_\phi^n\right)\right|\\
&= \left|\left(\partial_t\phi^{n+\frac12} - \frac{\phi^{n+1}-\phi^n}{\Delta t}, \xi_\phi^{n+1}+\xi_\phi^n\right)\right| + \frac{1}{\Delta t}\left|\left(\int_{t_n}^{t_{n+1}}\partial_t\eta_\phi ds, \xi_\phi^{n+1}+\xi_\phi^n\right)\right|\\
&\le C\Delta t\int_{t_n}^{t_{n+1}}\|\phi_{ttt}\|_0 ds\|\xi_\phi^{n+1}+\xi_\phi^n\|_0 + \frac{1}{\Delta t}\left(\int_{t_n}^{t_{n+1}}\|\partial_t\eta_\phi\|_0 ds\right)\|\xi_\phi^{n+1}+\xi_\phi^n\|_0\\
&\le C\Delta t^3\int_{t_n}^{t_{n+1}}\|\phi_{ttt}\|_0^2 ds + \frac{C}{\Delta t}\int_{t_n}^{t_{n+1}}\|\partial_t\eta_\phi\|_0^2 ds + \|\xi_\phi^{n+1}\|_0^2 + \|\xi_\phi^n\|_0^2. \qquad (4.13)
\end{aligned}$$

The second step is to analyze the term Υ_2, which has the following decomposition:

$$\Upsilon_2 = \pi_1 + \pi_2, \qquad (4.14)$$

where

$$\pi_1 = \left(|\nabla\phi^{n+\frac{1}{2}}|^2\nabla\phi^{n+\frac{1}{2}}, \nabla(\xi_\phi^{n+1}+\xi_\phi^n)\right) - \left(\frac{(|\nabla\phi^{n+1}|^2+|\nabla\phi^n|^2)(\nabla\phi^{n+1}+\nabla\phi^n)}{4}, \nabla(\xi_\phi^{n+1}+\xi_\phi^n)\right),$$

$$\pi_2 = \left(\frac{(|\nabla\phi^{n+1}|^2+|\nabla\phi^n|^2)(\nabla\phi^{n+1}+\nabla\phi^n)}{4}, \nabla(\xi_\phi^{n+1}+\xi_\phi^n)\right) - \left(\frac{(|\nabla P_h\phi^{n+1}|^2+|\nabla P_h\phi^n|^2)(\nabla P_h\phi^{n+1}+\nabla P_h\phi^n)}{4}, \nabla(\xi_\phi^{n+1}+\xi_\phi^n)\right).$$

It follows from (2.29), (2.31), and regularity results in Lemma 2.3 that

$$\begin{aligned}
|\pi_1| &\le \left|\left(|\nabla\phi^{n+1/2}|^2\left(\nabla\phi^{n+1/2}-\frac{\nabla(\phi^{n+1}+\phi^n)}{2}\right), \nabla(\xi_\phi^{n+1}+\xi_\phi^n)\right)\right| \\
&\quad + \left|\left(\left(|\nabla\phi^{n+1/2}|^2 - \frac{|\nabla\phi^{n+1}|^2+|\nabla\phi^n|^2}{2}\right)\frac{\nabla(\phi^{n+1}+\phi^n)}{2}, \nabla(\xi_\phi^{n+1}+\xi_\phi^n)\right)\right| \\
&\le C\Delta t\left(\int_{t_n}^{t_{n+1}}\|\nabla\phi_{tt}\|_0 ds\right)\|\nabla(\xi_\phi^{n+1}+\xi_\phi^n)\|_0 \\
&\le C\Delta t^3\int_{t_n}^{t_{n+1}}\|\nabla\phi_{tt}\|_0^2 ds + \|\nabla(\xi_\phi^{n+1}+\xi_\phi^n)\|_0^2 \\
&\le C\Delta t^3\int_{t_n}^{t_{n+1}}\|\nabla\phi_{tt}\|_0^2 ds + \|\xi_\phi^{n+1}+\xi_\phi^n\|_0\|\tilde{\xi}_w^{n+1}+\tilde{\xi}_w^n\|_0 \\
&\le C\Delta t^3\int_{t_n}^{t_{n+1}}\|\nabla\phi_{tt}\|_0^2 ds + \frac{1}{4\delta_1}\|\xi_\phi^{n+1}+\xi_\phi^n\|_0^2 + \delta_1\|\tilde{\xi}_w^{n+1}+\tilde{\xi}_w^n\|_0^2 \\
&\le C\Delta t^3\int_{t_n}^{t_{n+1}}\|\nabla\phi_{tt}\|_0^2 ds + \frac{1}{4\delta_1}\|\xi_\phi^{n+1}+\xi_\phi^n\|_0^2 + 2\delta_1\|\xi_w^{n+1}+\xi_w^n\|_0^2 \\
&\quad + 4\delta_1\|\eta_w^{n+1}+\eta_w^n\|_0^2 + 4\delta_1\|\tilde{\eta}_w^{n+1}+\tilde{\eta}_w^n\|_0^2.
\end{aligned} \tag{4.15}$$

Similarly, using (2.33) yields

$$\begin{aligned}
|\pi_2| &\le C\|\nabla(\eta_\phi^{n+1}+\eta_\phi^n)\|_0\|\nabla(\xi_\phi^{n+1}+\xi_\phi^n)\|_0 \\
&\le C\|\nabla(\eta_\phi^{n+1}+\eta_\phi^n)\|_0^2 + \|\nabla(\xi_\phi^{n+1}+\xi_\phi^n)\|_0^2 \\
&\le C\|\nabla(\eta_\phi^{n+1}+\eta_\phi^n)\|_0^2 + \|\xi_\phi^{n+1}+\xi_\phi^n\|_0\|\tilde{\xi}_w^{n+1}+\tilde{\xi}_w^n\|_0 \\
&\le C\|\nabla(\eta_\phi^{n+1}+\eta_\phi^n)\|_0^2 + \frac{1}{4\delta_2}\|\xi_\phi^{n+1}+\xi_\phi^n\|_0^2 + \delta_2\|\tilde{\xi}_w^{n+1}+\tilde{\xi}_w^n\|_0^2 \\
&\le C\|\nabla(\eta_\phi^{n+1}+\eta_\phi^n)\|_0^2 + \frac{1}{4\delta_2}\|\xi_\phi^{n+1}+\xi_\phi^n\|_0^2 + 2\delta_2\|\xi_w^{n+1}+\xi_w^n\|_0^2 \\
&\quad + 4\delta_2\|\eta_w^{n+1}+\eta_w^n\|_0^2 + 4\delta_2\|\tilde{\eta}_w^{n+1}+\tilde{\eta}_w^n\|_0^2.
\end{aligned} \tag{4.16}$$

Combining (4.14)–(4.16) gives

$$\begin{aligned}
|\Upsilon_2| &\le C\Delta t^3\int_{t_n}^{t_{n+1}}\|\nabla\phi_{tt}\|_0^2 ds + C\|\nabla(\eta_\phi^{n+1}+\eta_\phi^n)\|_0^2 \\
&\quad + \left(\frac{1}{4\delta_1}+\frac{1}{4\delta_2}\right)\|\xi_\phi^{n+1}+\xi_\phi^n\|_0^2 + 2(\delta_1+\delta_2)\|\xi_w^{n+1}+\xi_w^n\|_0^2 \\
&\quad + 4(\delta_1+\delta_2)\|\eta_w^{n+1}+\eta_w^n\|_0^2 + 4(\delta_1+\delta_2)\|\tilde{\eta}_w^{n+1}+\tilde{\eta}_w^n\|_0^2.
\end{aligned} \tag{4.17}$$

From (2.22), (2.29), (2.31), and the Cauchy–Schwarz inequality, the following estimate holds:

$$\begin{aligned}
\left|\Upsilon_3\right| &\le \left|\varepsilon\left(\nabla w^{n+\frac12} - \frac{\nabla w^{n+1}+\nabla w^n}{2}, \nabla(\xi_\phi^{n+1}+\xi_\phi^n)\right)\right| \\
&\quad + \left|\varepsilon\left(\frac{\nabla w^{n+1}+\nabla w^n}{2} - \frac{\nabla P_h w^{n+1}+\nabla P_h w^n}{2}, \nabla(\xi_\phi^{n+1}+\xi_\phi^n)\right)\right| \\
&= \left|\varepsilon\left(\nabla w^{n+\frac12} - \frac{\nabla w^{n+1}+\nabla w^n}{2}, \nabla(\xi_\phi^{n+1}+\xi_\phi^n)\right)\right| \\
&\le C\varepsilon\Delta t\left(\int_{t_n}^{t_{n+1}} \|\nabla w_{tt}\|_0 ds\right)\|\nabla(\xi_\phi^{n+1}+\xi_\phi^n)\|_0 \\
&\le C\varepsilon\Delta t^3 \int_{t_n}^{t_{n+1}} \|\nabla w_{tt}\|_0^2 ds + \|\nabla(\xi_\phi^{n+1}+\xi_\phi^n)\|_0^2 \\
&\le C\varepsilon\Delta t^3 \int_{t_n}^{t_{n+1}} \|\nabla w_{tt}\|_0^2 ds + \|\xi_\phi^{n+1}+\xi_\phi^n\|_0\|\tilde\xi_w^{n+1}+\tilde\xi_w^n\|_0 \\
&\le C\varepsilon\Delta t^3 \int_{t_n}^{t_{n+1}} \|\nabla w_{tt}\|_0^2 ds + \frac{1}{4\delta_3}\|\xi_\phi^{n+1}+\xi_\phi^n\|_0^2 + 2\delta_3\|\xi_w^{n+1}+\xi_w^n\|_0^2 \\
&\quad + 4\delta_3\|\eta_w^{n+1}+\eta_w^n\|_0^2 + 4\delta_3\|\tilde\eta_w^{n+1}+\tilde\eta_w^n\|_0^2, \qquad (4.18)
\end{aligned}$$

where the constant C is independent of ε, h, and Δt. Similar arguments lead to

$$\begin{aligned}
\left|\Upsilon_4\right| &\le \left|\left(\nabla \phi^{n+\frac12} - \frac{\nabla \phi^{n+1}+\nabla \phi^n}{2}, \nabla(\xi_\phi^{n+1}+\xi_\phi^n)\right)\right| \\
&\quad + \left|\left(\frac{\nabla \phi^{n+1}+\nabla \phi^n}{2} - \frac{\nabla P_h \phi^{n+1}+\nabla P_h \phi^n}{2}, \nabla(\xi_\phi^{n+1}+\xi_\phi^n)\right)\right| \\
&= \left|\left(\nabla \phi^{n+\frac12} - \frac{\nabla \phi^{n+1}+\nabla \phi^n}{2}, \nabla(\xi_\phi^{n+1}+\xi_\phi^n)\right)\right| \\
&\le C\left(\Delta t\int_{t_n}^{t_{n+1}} \|\nabla \phi_{tt}\|_0 ds\right)\|\nabla(\xi_\phi^{n+1}+\xi_\phi^n)\|_0 \\
&\le C\Delta t^3 \int_{t_n}^{t_{n+1}} \|\nabla \phi_{tt}\|_0^2 ds + \|\nabla(\xi_\phi^{n+1}+\xi_\phi^n)\|_0^2 \\
&\le C\Delta t^3 \int_{t_n}^{t_{n+1}} \|\nabla \phi_{tt}\|_0^2 ds + \frac{1}{4\delta_4}\|\xi_\phi^{n+1}+\xi_\phi^n\|_0^2 + 2\delta_4\|\xi_w^{n+1}+\xi_w^n\|_0^2 \\
&\quad + 4\delta_4\|\eta_w^{n+1}+\eta_w^n\|_0^2 + 4\delta_4\|\tilde\eta_w^{n+1}+\tilde\eta_w^n\|_0^2. \qquad (4.19)
\end{aligned}$$

Similarly to (2.34), we assume nonnegativity for the nonlinear terms in the left-hand side of (4.8):

$$\begin{aligned}
0 &\le \left(\frac{(|\nabla\phi_h^{n+1}|^2+|\nabla\phi_h^n|^2)(\nabla\phi_h^{n+1}+\nabla\phi_h^n)}{4}, \nabla(\xi_\phi^{n+1}+\xi_\phi^n)\right) \\
&\quad - \left(\frac{(|\nabla P_h\phi^{n+1}|^2+|\nabla P_h\phi^n|^2)(\nabla P_h\phi^{n+1}+\nabla P_h\phi^n)}{4}, \nabla(\xi_\phi^{n+1}+\xi_\phi^n)\right). \qquad (4.20)
\end{aligned}$$

The same argument as (2.30) leads to

$$
\begin{aligned}
&\frac{\varepsilon}{2}\big(\nabla(\xi_w^{n+1}+\xi_w^n),\nabla(\xi_\phi^{n+1}+\xi_\phi^n)\big)\\
&=\frac{\varepsilon}{2}\|\xi_w^{n+1}+\xi_w^n\|_0^2+\frac{\varepsilon}{2}\big(\xi_w^{n+1}+\xi_w^n,(\eta_w^{n+1}+\eta_w^n)-(\tilde{\eta}_w^{n+1}+\tilde{\eta}_w^n)\big)\\
&\geq\left(\frac{\varepsilon}{2}-2\delta_5\right)\|\xi_w^{n+1}+\xi_w^n\|_0^2-C\|\eta_w^{n+1}+\eta_w^n\|_0^2-C\|\tilde{\eta}_w^{n+1}+\tilde{\eta}_w^n\|_0^2. \qquad (4.21)
\end{aligned}
$$

From (2.29) and (2.31), we have

$$
\begin{aligned}
\frac{1}{2}\|\nabla(\xi_\phi^{n+1}+\xi_\phi^n)\|_0^2 &\leq \frac{1}{2}\|\tilde{\xi}_w^{n+1}+\tilde{\xi}_w^n\|_0\|\xi_\phi^{n+1}+\xi_\phi^n\|_0\\
&\leq \delta_6\|\tilde{\xi}_w^{n+1}+\tilde{\xi}_w^n\|_0^2+\frac{1}{16\delta_6}\|\xi_\phi^{n+1}+\xi_\phi^n\|_0^2\\
&\leq 2\delta_6\|\xi_w^{n+1}+\xi_w^n\|_0^2+C\|\eta_w^{n+1}+\eta_w^n\|_0^2+C\|\tilde{\eta}_w^{n+1}+\tilde{\eta}_w^n\|_0^2\\
&\quad+\frac{1}{16\delta_6}\|\xi_\phi^{n+1}+\xi_\phi^{n+1}\|_0^2. \qquad (4.22)
\end{aligned}
$$

We choose δ_1, δ_2, δ_3, δ_4, δ_5, and δ_6 such that

$$
2\Big(\delta_1+\delta_2+\delta_3+\delta_4+\delta_5+\delta_6\Big)=\frac{\varepsilon}{4}; \qquad (4.23)
$$

e.g., $\delta_1=\delta_2=\delta_3=\delta_4=\delta_5=\delta_6=\varepsilon/48$. Thus combining (4.8), (4.13), and (4.17)–(4.23) leads to

$$
\begin{aligned}
&\left(\frac{\xi_\phi^{n+1}-\xi_\phi^n}{\Delta t},\xi_\phi^{n+1}+\xi_\phi^n\right)+\frac{\varepsilon}{2}\|\xi_w^{n+1}+\xi_w^n\|_0^2\\
&\quad\leq C\Delta t^3\int_{t_n}^{t_{n+1}}\|\phi_{ttt}\|_0^2ds+\frac{C}{\Delta t}\int_{t_n}^{t_{n+1}}\|\partial_t\eta_\phi\|_0^2ds+C\Delta t^3\int_{t_n}^{t_{n+1}}\|\nabla\phi_{tt}\|_0^2ds\\
&\qquad+C\varepsilon\Delta t^3\int_{t_n}^{t_{n+1}}\|\nabla w_{tt}\|_0^2ds+\widetilde{C}\big(\|\xi_\phi^{n+1}\|_0^2+\|\xi_\phi^n\|_0^2\big)+C\|\nabla(\eta_\phi^{n+1}+\eta_\phi^n)\|_0^2\\
&\qquad+C\|\eta_w^{n+1}+\eta_w^n\|_0^2+C\|\tilde{\eta}_w^{n+1}+\tilde{\eta}_w^n\|_0^2+\frac{\varepsilon}{4}\|\xi_w^{n+1}+\xi_w^n\|_0^2, \qquad (4.24)
\end{aligned}
$$

where

$$
\widetilde{C}=1+\frac{1}{2}\left(\frac{1}{\delta_1}+\frac{1}{\delta_2}+\frac{1}{\delta_3}+\frac{1}{\delta_4}+\frac{1}{4\delta_6}\right). \qquad (4.25)
$$

Summing both sides with respect to n gives

$$
\begin{aligned}
&\|\xi_\phi^N\|_0^2-\|\xi_\phi^0\|_0^2+\sum_{n=0}^{N-1}\Delta t\frac{\varepsilon}{4}\|\xi_w^{n+1}+\xi_w^n\|_0^2\\
&\quad\leq C\Delta t^4\int_0^T\|\phi_{ttt}\|_0^2ds+C\Delta t^4\int_0^T\|\nabla\phi_{tt}\|_0^2ds+C\varepsilon\Delta t^4\int_0^T\|\nabla w_{tt}\|_0^2ds\\
&\qquad+C\int_0^T\|\partial_t\eta_\phi\|_0^2ds+2\widetilde{C}\sum_{n=0}^{N}\Delta t\|\xi_\phi^n\|_0^2+C\sum_{n=0}^{N-1}\Delta t\|\eta_w^{n+1}+\eta_w^n\|_0^2\\
&\qquad+C\sum_{n=0}^{N-1}\Delta t\|\nabla(\eta_\phi^{n+1}+\eta_\phi^n)\|_0^2+C\sum_{n=0}^{N-1}\Delta t\|\tilde{\eta}_w^{n+1}+\tilde{\eta}_w^n\|_0^2. \qquad (4.26)
\end{aligned}
$$

Then Gronwall's inequality in Lemma 3.1 yields the desired result (4.7), provided that $2\widetilde{C}\Delta t < 1$. ☐

We close this section by providing one of the main results of this paper, which gives the error bounds for the fully discrete scheme (3.1).

THEOREM 4.2. *Let (ϕ, w) be the solution of (2.4). Assume that $\phi_0 \in H^m_{\text{per}}(\Omega)$ and that the conditions in Lemma 4.1 hold. If the time step size Δt is sufficiently small, then the finite element approximation (ϕ^n_h, w^n_h) of (3.1) has the following error estimate:*

$$\|\phi(\mathbf{x},T) - \phi_h^N\|_0^2 + \frac{\varepsilon}{4}\sum_{k=0}^{N-1} \Delta t \|w(\mathbf{x},t_{k+1}) + w(\mathbf{x},t_k) - (w_h^{k+1} + w_h^k)\|_0^2$$

$$\le C_{\varepsilon,\phi,w}\Big(h^{2m} + \Delta t^4\Big), \tag{4.27}$$

where the constant $C_{\varepsilon,\phi,w}$ is independent of the mesh size h and time step Δt but depends on ε, ϕ, ϕ_0, and w.

Proof. The desired result can be proved by an argument similar to that of Theorem 2.8 and using the triangle inequality. ☐

5. Numerical experiments. In this section, we use the mixed finite element method and the second-order time-stepping scheme (3.1) to solve the MBE model (1.1).

Example 5.1. In this example, we test the convergence results stated in Theorem 4.2. In order to check the convergence order, we consider the following MBE problem:

$$\begin{cases} \frac{\partial \phi}{\partial t} = -\varepsilon\Delta^2\phi - \nabla\cdot[(1-|\nabla\phi|^2)\nabla\phi] + f & \text{in } \Omega\times(0,T), \\ \phi(\mathbf{x},0) = \phi_0(\mathbf{x}) & \text{in } \Omega, \end{cases} \tag{5.1}$$

with $\Omega = [0,1]\times[0,1]$, $T = 1$, 1-periodic boundary condition, and parameter $\varepsilon = 0.1$. We add a source term f to make the exact solution known. Here the initial solution $\phi(\mathbf{x},0)$ and f are chosen such that the exact solution is

$$u(\mathbf{x},t) = 0.1\exp(-t)\sin(\pi x_1)\sin(\pi x_2).$$

In this example, we will check the convergence order for the linear element ($\mathcal{P}_1$) and quadratic element ($\mathcal{P}_2$) on triangulations, and bilinear element ($\mathcal{Q}_1$) and biquadratic element ($\mathcal{Q}_2$) on rectangles.

The linear and quadratic elements on the triangulation $\mathcal{T}_h$ are defined by

$$V_h := \Big\{v_h \in H^1_{\text{per}}(\Omega), v_h|_K \in \mathcal{P}_1 \text{ or } \mathcal{P}_2\ \forall K \in \mathcal{T}_h\Big\},$$

and the bilinear and biquadratic elements on the rectangle $\mathcal{T}_h$ are defined by

$$V_h := \Big\{v_h \in H^1_{\text{per}}(\Omega), v_h|_K \in \mathcal{Q}_1 \text{ or } \mathcal{Q}_2\ \forall K \in \mathcal{T}_h\Big\}.$$

In the convergence order test, the sequence of partitions is produced by the regular refinement from the initial partitions. The error definition

$$\sqrt{\|\phi(\mathbf{x},T) - \phi_h^N\|_0^2 + \frac{\varepsilon}{4}\sum_{k=0}^{N-1}\Delta t\|w(\mathbf{x},t_k) - w_h^k\|_0^2}$$

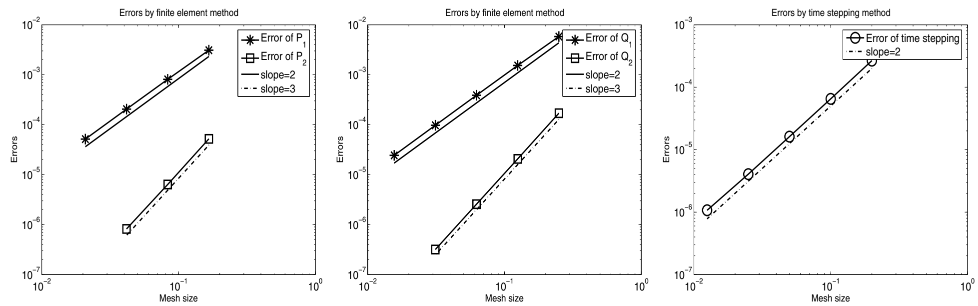

FIG. 1. *Example* 5.1: *The convergence behavior of the spatial discretization with fixed time step size $\Delta t = 10^{-3}$ (left and middle), and the time-stepping method with fixed spatial size $h = \frac{1}{32}$ and $\mathcal{Q}_2$ element (right).*

is adopted in this numerical experiment. The corresponding numerical results are presented in Figure 1, where it is observed that the convergence orders are one order higher than those predicted in Theorem 4.2. This phenomenon needs further consideration in the future.

In this example, we also test the convergence order of the time discretization for the scheme (3.1). The corresponding numerical results are shown in Figure 1. From Figure 1, we can find that the scheme (3.1) has a second-order-accuracy-in-time discretization.

Example 5.2. This example is concerned with a two-dimensional isotropic symmetry current model,

$$\left\{ \begin{array}{rcll} \frac{\partial \phi}{\partial t} & = & -\varepsilon\Delta^2\phi - \nabla\cdot[(1-|\nabla\phi|^2)\nabla\phi] & \text{in } [0,2\pi]^2\times(0,T), \\ \phi(\mathbf{x},0) & = & \phi_0(\mathbf{x}) & \text{in } [0,2\pi]^2, \end{array} \right. \tag{5.2}$$

with 2π-periodic boundary condition and parameter $\varepsilon = 0.1$. The initial condition is chosen as

$$\phi_0(\mathbf{x}) = 0.1(\sin(3x_1)\sin(2x_2) + \sin(5x_1)\sin(5x_2)).$$

This example was studied in [23, 26, 32] to study the solution instability. Here we use the mixed finite element method and CN time-stepping scheme (3.1) to solve this problem. The solution contours given by using the mixed bilinear element and CN time-stepping scheme (3.1) at $t = 0$, $t = 0.05$, $t = 2.5$, $t = 5.5$, $t = 8$, and $t = 30$ (steady state) are plotted in Figure 2, and are in good agreement with those published in [23].

In this example, we also check the energy decay property of the MBE growth model. Figure 3(a) shows the corresponding results, which demonstrate the desired energy decay behavior.

In this example, the roughness of the height function is also checked. The roughness of the height function is defined as

$$R(\phi) = \sqrt{\frac{1}{|\Omega|}\int_\Omega [\phi(\mathbf{x},t) - \bar{\phi}(\mathbf{x},t)]^2 d\Omega}, \quad \text{where } \bar{\phi}(t) = \frac{1}{|\Omega|}\int_\Omega \phi(\mathbf{x},t)d\Omega. \tag{5.3}$$

The corresponding development of roughness is presented in Figure 3(b) and agrees well with the results in [23, 26, 32].

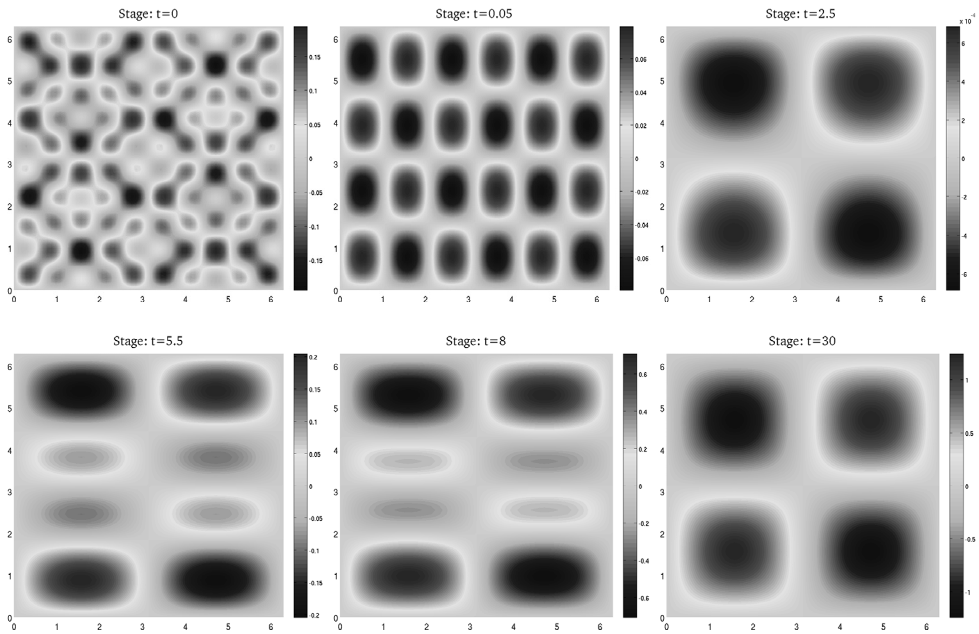

FIG. 2. *Example* 5.2: *Contour plots for height profiles.*

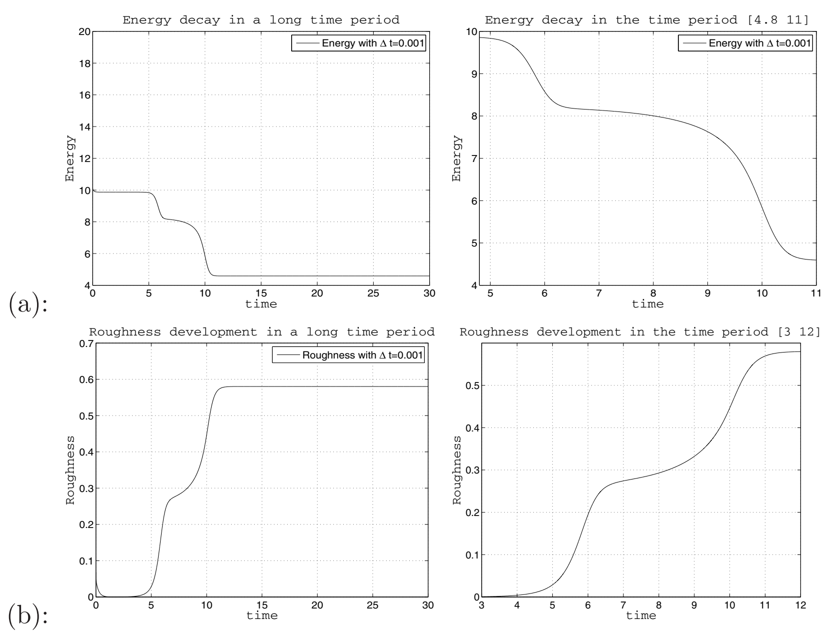

FIG. 3. *Example* 5.2: (a) *The energy decay, and* (b) *the development of the roughness.*

6. Concluding remarks. In this paper, we have developed and analyzed a mixed finite element method for nonlinear diffusion equations modeling epitaxial growth of thin films. The biharmonic operator in the MBE models was decomposed into two Laplacians, which allowed us to use the standard continuous finite element spaces commonly used for elliptic problems. We then concentrated on the gradient flow properties of the corresponding numerical schemes, by establishing the discrete version of the various energy decay properties for the continuous versions. The full stability property, i.e., Theorem 3.5, was then established by using some careful energy estimates. The corresponding error estimates were then obtained based on the stability results. These theoretical predictions for stability and convergence were, finally, confirmed by two numerical experiments.

REFERENCES

[1] R. A. Adams, *Sobolev Spaces*, Academic Press, New York, 1975.

[2] P. Aviles and Y. Giga, *A mathematical problem related to the physical theory of liquid crystal configurations*, Proc. Centre Math. Anal. Austral. Nat. Univ., 12 (1987), pp. 1–16.

[3] G. S. Ball and R. D. James, *Proposed experimental tests of a theory of fine microstructure and the two-well problem*, Philos. Trans. R. Soc. London Ser. A, 338 (1992), pp. 389–450.

[4] H. Brunner, *Collocation Methods for Volterra Integral and Related Functional Differential Equations*, Cambridge University Press, Cambridge, UK, 2004.

[5] R. E. Caflisch, M. F. Gyure, B. Merriman, S. J. Osher, C. Ratsch, D. D. Vvedensky, and J. J. Zinch, *Island dynamics and the level set method for epitaxial growth*, Appl. Math. Lett., 12 (1999), pp. 13–22.

[6] W. Chen, S. Conde, C. Wang, X. Wang, and S. Wise, *A linear energy stable scheme for a thin film model without slope selection*, J. Sci. Comput., 52 (2012), pp 546–562.

[7] W. Chen and Y. Wang, *A mixed finite element method for thin film epitaxy*, Numer. Math., 122 (2012), pp. 771–793.

[8] P. G. Ciarlet and J. L. Lions, eds., *Finite Element Methods*, Handb. Numer. Anal. II., North–Holland, Amsterdam, 1991.

[9] S. Clarke and D. D. Vvedensky, *Origin of reflection high-energy electron-diffraction intensity oscillations during molecular-beam epitaxy: A computational modeling approach*, Phys. Rev. Lett., 58 (1987), pp. 2235–2238.

[10] C. Collins, J. Shen, and S. Wise, *An efficient, energy stable scheme for the Cahn-Hilliard-Brinkman system*, Commun. Comput. Phys., 13 (2013), pp. 929–957.

[11] Q. Du and R. A. Nicolaides, *Numerical analysis of a continuum model of phase transition*, SIAM J. Numer. Anal., 28 (1991), pp. 1310–1322.

[12] C. M. Elliott, D. A. French, and F. A. Milner, *A second order splitting method for the Cahn-Hilliard equation*, Numer. Math., 54 (1989), pp. 575–590.

[13] X. B. Feng and A. Prohl, *Error analysis of a mixed finite element method for the Cahn-Hilliard equation*, Numer. Math., 99 (2004), pp. 47–84.

[14] X. B. Feng and H. J. Wu, *A posteriori error estimates for finite element approximations of the Cahn-Hilliard equation and the Hele-Shaw flow*, J. Comput. Math., 26 (2008), pp. 767–796.

[15] G. Gioia and M. Ortiz, *Delamination of compressed thin films*, Adv. Appl. Mech., 33 (1997), pp. 119–192.

[16] L. Golubovic, A. Levandovsky, and D. Moldovan, *Interface dynamics and far-from-equilibrium phase transitions in multilayer epitaxial growth and erosion on crystal surfaces: Continuum theory insights*, East Asian J. Appl. Math., 1 (2011), pp. 297–371.

[17] Y. He, Y. Liu, and T. Tang, *On large time-stepping methods for the Cahn-Hilliard equation*, Appl. Numer. Math., 57 (2007), pp. 616–628.

[18] W. Jin and R. V. Kohn, *Singular perturbation and the energy of folds*, J. Nonlinear Sci., 10 (2000), pp. 355–390.

[19] S. Kesavan, *Topics in Functional Analysis and Applications*, Wiley Eastern Limited, New Delhi, India, 1989.

[20] R. Kohn, *Energy-driven pattern formulation*, in Proceedings of the International Congress of Mathematicians, Madrid, Spain, 2006, M. Sanz-Sole, J. Soria, J. L. Varona, and J. Verdera, eds., 2007, pp. 359–384.

[21] R. Kohn and S. Müller, *Surface energy and microstructure in coherent phase transitions*, Comm. Pure Appl. Math., 47 (1994), pp. 405–435.

[22] R. Kohn and F. Otto, *Upper bounds on coarsening rates*, Comm. Math. Phys., 229 (2002), pp. 375–395.

[23] B. Li and J.-G. Liu, *Thin film epitaxy with or without slope selection*, European J. Appl. Math., 14 (2003), pp. 713–743.

[24] S. E. Minkoff and N. M. Kridler, *A comparison of adaptive time stepping methods for coupled flow and deformation modeling*, Appl. Math. Modeling, 30 (2006), pp. 993–1009.
[25] D. Moldovan and L. Golubovic, *Interfacial coarsening dynamics in epitaxial growth with slope selection*, Phys. Rev. E, 61 (2000), pp. 6190–6214.
[26] Z. Qiao, Z. Zhang, and T. Tang, *An adaptive time-stepping strategy for the molecular beam epitaxy models*, SIAM J. Sci. Comput., 33 (2011), pp. 1395–1414.
[27] J. Shen, C. Wang, X. Wang, and S. M. Wise, *Second-order convex splitting schemes for gradient flows with Ehrlich–Schwoebel type energy: Application to thin film epitaxy*, SIAM J. Numer. Anal., 50 (2012), pp. 105–125.
[28] G. Söderlind, *Automatic control and adaptive time-stepping*, Numer. Algorithms, 31 (2002), pp. 281–310.
[29] Z. J. Tan, Z. R. Zhang, Y. Q. Huang, and T. Tang, *Moving mesh methods with locally varying time steps*, J. Comput. Phys., 200 (2004), pp. 347–367.
[30] C. Wang, X. Wang, and S. Wise, *Unconditionally stable schemes for equations of thin film epitaxy*, Discrete Contin. Dyn. Syst. Ser. A, 28 (2010), pp. 405–423.
[31] S. M. Wise, C. Wang, and J. S. Lowengrub, *An energy-stable and convergent finite-difference scheme for the phase field crystal equation*, SIAM J. Numer. Anal., 47 (2009), pp. 2269–2288.
[32] C. Xu and T. Tang, *Stability analysis of large time-stepping methods for epitaxial growth models*, SIAM J. Numer. Anal., 44 (2006), pp. 1759–1779.
[33] J. Zhu, L. Q. Chen, and V. Tikare, *Coarsening kinetics from variable-mobility Cahn-Hilliard equations: Application of a semi-implicit Fourier spectral method*, Phys. Rev. E, 60 (1999), pp. 3564–3572.