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GLOBAL SMOOTH SOLUTIONS OF THE THREE-DIMENSIONAL MODIFIED PHASE FIELD CRYSTAL EQUATION*

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Abstract. The Modified Phase Field Crystal (MPFC) equation, a generalized damped wave equation for which the usual Phase Field Crystal (PFC) equation is a special case, is analyzed in detail in three dimensions. A time-discrete numerical scheme, based on a convex splitting for the functional energy, is utilized to construct an approximate solution, which is then shown to converge to a solution of the MPFC equation as the time step approaches zero. In detail, a uniform-in-time bound of the pseudo energy for the numerical solution is obtained owing to the structure of the convex-splitting scheme. As an immediate result, we obtain a bound of the $L_s^\infty(0,T;H_{per}^2)$ norm of the numerical solution. More detailed energy estimates, which are obtained by taking the inner product of the numerical scheme with $(-\Delta)^m(\phi^{k+1}-\phi^k)$, give bounds for the numerical solution and it first and second temporal backward differences in the $L_s^\infty(0,T;H_{per}^{m+3})$, $L_s^\infty(0,T;H_{per}^m)$ and $L_s^\infty(0,T;H_{per}^{m-3})$ norms, respectively. These estimates of the numerical solutions in turn result in a global weak solution (with $m=0$) and a unique global strong solution ($m=3$) upon passage to the limit as the time step size approaches zero. A global smooth solution can also be established by taking arbitrarily large values of m.

Key words. phase field crystal, modified phase field crystal, pseudo energy, nonlinear partial differential equations, global weak solution, global strong solution, global smooth solution

AMS subject classifications. 35G25, 35L75, 65M12

1. Introduction.

The Phase Field Crystal (PFC) model, which is a sixth-order, parabolic-type PDE, was recently proposed in [3] as a new approach to simulating the morphological evolution of crystalline solids at the atomic length scale in space but on a coarse-grained diffusive time-scale. See, for example, the recent review [12] that describes the variety of applications for the PFC approach. Recently, Stefanovic *et al.* [11] introduced a small but important extension of the PFC model known as the Modified Phase Field Crystal (MPFC) equation. This equation is designed to properly account for elastic interactions, which the PFC fails to do, and includes a second-order time derivative:

$$\beta\partial_{tt}\phi+\partial_t\phi=\Delta\left(\phi^3+\alpha\phi+2\Delta\phi+\Delta^2\phi\right)\ , \tag{1.1}$$

where $\beta\geq 0$ and $\alpha>0$. Equation (1.1) is a generalized damped wave equation, though the parabolic PFC equation is recovered in the degenerate case when $\beta=0$. The MPFC approach introduces a separation of time scales that allows for the elastic relaxation of the crystal lattice on a rapid time scale while other processes evolve on a slower diffusion time scale [12, 11].

In the papers [9, 16] we described unconditionally stable, unconditionally solvable and convergent schemes for the PFC equation based on convex-splitting methods. Extending the work from [9, 16], in [15] we devised a convex splitting scheme for the 2-D MPFC equation, proving unconditional energy stability and convergence of the numerical solutions. Here our goal is to prove the unique existence of global smooth solutions to the 3-D MPFC equation. Our approach will be to show that numerical

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