Response to “Comment on ‘Degenerate mobilities in phase field models are insufficient to capture surface diffusion’” [Appl. Phys. Lett. 108, 036101 (2016)]

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Response to “Comment on ‘Degenerate mobilities in phase field models are insufficient to capture surface diffusion’” [Appl. Phys. Lett. 108, 036101 (2016)]

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In our recent paper,1 we argued that degenerate mobilities in phase field models are insufficient to capture surface diffusion. We demonstrated this statement by construction: we showed that the Cahn-Hilliard equation with a quadratic degenerate mobility $M(u) = 1 - u^2$ does not reduce to surface diffusion as its sharp interface limit. Crucially, we did not suggest that phase field models could never capture surface diffusion. As such, the title of our paper is neither misleading nor contradictory to our results, as Voigt argues in his comment.8 In fact, it is important to alert practitioners in the field to the pitfalls of modelling surface diffusion with Cahn-Hilliard equations.

Indeed, there are numerous instances in the literature where the combination of a Cahn-Hilliard equation with this quadratic degenerate mobility and a (polynomial) double well free energy is used to model surface diffusion (e.g., Refs. 2 and 3; note that those are only some examples from the literature). A common misconception in the literature (see, e.g., Refs. 2 and 4) is to apply the classical result by Cahn et al.5 on the sharp interface limit for the double obstacle or deep quench limit of the logarithmic free energy to models with a (polynomial) double well free energy. We note that the matched asymptotic analysis in Ref. 6, cited in Voigt’s comment, contained a significant error. Rather than carrying out the full matched asymptotic analysis, the authors erroneously assume that the outer solution is equal to 0 or 1, i.e., to the pure phases, to all orders. Using this assumption, the authors conclude that all degenerate mobilities (without “stabilizing function”) lead to an inconsistency/contradiction in the derivation. They do not, however, explain what the consistent asymptotic derivation is. Our recent work7 investigates this subtle point in detail and extends the discussion in our brief letter.1 In particular, we carry out a consistent and systematic asymptotic analysis to derive the sharp interface limit of the Cahn-Hilliard equation with a quadratic degenerate mobility and polynomial double well free energy. Our analysis reveals a non-trivial outer solution, as well as additional intermediate layers that necessitate the matching of exponential terms. We concluded that bulk diffusion enters the sharp interface model to leading order for $M(u) = 1 - u^2$ (thus recovering the result in Ref. 1) but not for higher order mobilities. No “stabilizing function” is required to address a contradiction or overspecification of terms in the expansion, as was argued in Ref. 6, hence its role does not appear to be as clear as suggested in Voigt’s comment. Our result for the quadratic mobility is different to Ref. 6, but agrees well with numerical calculations.