Dynamic Density Functional Theory (DDFT) model for nano-crystal growth from fluid phase: The effect of fluid flow
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The Classical Density Functional Theory (CDFT) based models, which include the Phase Field Crystal (PFC) model, have proven to be good approaches to model crystal growth from a fluid phase. These models capture atomic level details including defects and grain boundaries. However these approaches usually involve a phenomenological gradient descent based time evolution and do not take the convection of the fluid phase (fluid flow) into consideration. In this work we start with the Revised Enskog Theory (RET) (an effective kinetic theory) as the definition of time evolution. Then exploiting the connection to CDFT of freezing, we develop evolution equations for the macroscopic density and flow fields. The over damped limit provides us a DDFT model for time evolution of the density field. Some studies of this model and results on crystal growth from fluid phase will be discussed.

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