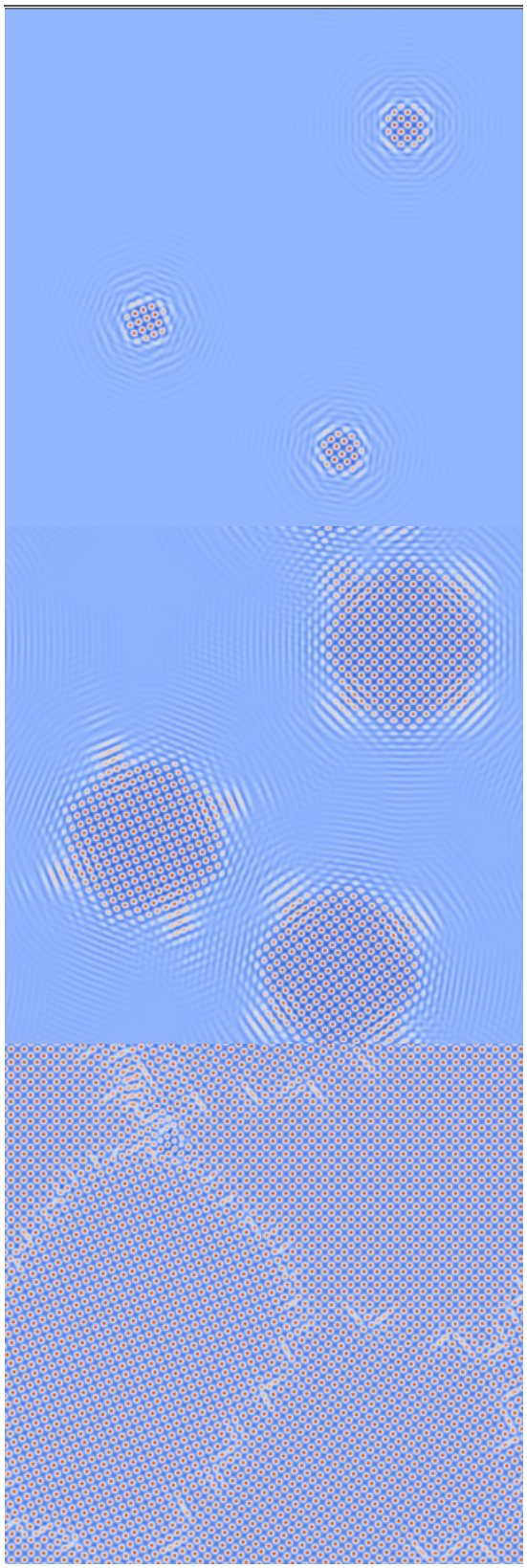

FIG. 3: Simulation of polycrystalline solidification starting from three seeded fcc crystals in a supercooled liquid. The system is fully periodic, and the snapshots are taken at dimensionless times $t = 5 \times 10^2, 3 \times 10^3$, and 10^5. The parameters are $R = 0$, $\epsilon = .00823$, and $\bar{\psi} = -0.06$.

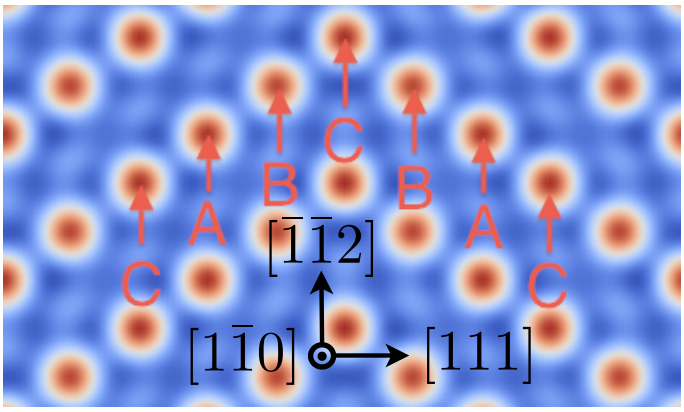

FIG. 4: Simulation of an equilibrium coherent (111) twin boundary for $R = 0$, $\epsilon = 0.00823$, and $\bar{\psi} = -0.06269$.

C. Numerical examples

We now demonstrate the feasibility of the model with some numerical examples of fcc polycrystalline growth and (111) twin growth. The PFC conserved dynamics governed by Eq. (18) with the free-energy defined by Eqs. (19) and (20) was solved using the semi-implicit pseudo-spectral scheme given by Eq. (A2) in Appendix A of Ref. [25]. We used the parameters $R = 0$ and $\epsilon = 0.00823$ obtained from our fit of pure Ni presented later in section IV, together with the grid spacing $\Delta x = \Delta y = \Delta z = 2\pi\sqrt{3}/16$, which determines the number of Fourier modes, and the time step $\Delta t = 0.5$. For this value of R and ϵ, the computations presented in the next section show that the size of the solid-liquid coexistence region is extremely small, i.e. $\bar{\psi}_s - \bar{\psi}_l$ is two orders of magnitude smaller than $(\bar{\psi}_s + \bar{\psi}_l)/2$ as can already be seen from the phase diagram in Fig. 2, and $\bar{\psi}_s \approx \bar{\psi}_l \approx -0.0627$.

The first example in Fig. 3 shows the growth of small fcc crystallites of different orientations for a value of $\bar{\psi} = -0.06 > \bar{\psi}_s$ that is well inside the stable fcc-solid region of the phase diagram. The crystallites grow as expected until they collide to form grain boundaries. The second example in Fig. 4 shows a (111) twin crystal for a value of $\bar{\psi} = -0.06269$ at coexistence and for a system size chosen such that a twin crystal with two stacking faults fits perfectly the periodic boundary conditions in all directions without any liquid present. A computation of the excess free-energy of this twin boundary given in the appendix to this paper yields a value of approximately 30 mJ/m^2 that falls within the range of values typically reported in the literature for fcc metals. Fig. 5 then shows the growth of the same twin crystal in a supercooled liquid for a much larger system with $\bar{\psi} = -0.06$.