Supplementary Material to the article

"Growth of two-dimensional hexagonal lattices in phase-field crystal model"

I. Structure factor of non-Bravais lattices with additional basis. For the non-Bravais lattices, one can write the general condition for the absence of reciprocal lattice points for lattices with an additional basis. For the structure factor $S(\mathbf{K})$ the absence of the described points occurred when $S(\mathbf{K}) = 0$. In the case of two-dimensional honeycomb lattice this correspondent to the following:

$$S(\mathbf{K}) = \sum_j \exp(i\mathbf{K}\cdot\mathbf{b}_j) = 0, \quad j = 1...2, \tag{S1}$$

$$\mathbf{K} = \mathtt{h}\mathbf{q}_1 + \mathtt{k}\mathbf{q}_2 = 2\pi\left\langle \mathtt{h}, -\frac{1}{\sqrt{3}}(\mathtt{h} - 2\mathtt{k})\right\rangle. \tag{S2}$$

Substituting the additional basis vectors $\mathbf{b}_j$ (namely $\mathbf{b}_1 = \langle 0, 0\rangle; \mathbf{b}_2 = a_0\left\langle \frac{1}{2}, -\frac{1}{2\sqrt{3}}\right\rangle$ for honeycomb) one can get this condition as $\mathtt{k} = 2\mathtt{h} - 3/2$. However this condition is never satisfied for Miller indices as the integers in case of honeycomb. This approach should be utilized for the case of any non-Bravais lattices and at least to be checked for such structures as hexagonal close-packed (HCP) lattice when considered in Phase Field Crystal models (PFC-models).

II. Amplitude equations of the one-mode triangle's structure. Using the long-wave approximations given in Eqs. (9), (10) one can write amplitude equations for one-mode amplitudes $j = 1...3$ of triangle's structure as

$$\left(\tau\frac{\partial^2}{\partial t^2} + \frac{\partial}{\partial t}\right)\eta_j = -M\left[\Delta B_0\eta_j + B_0^x\mathcal{G}_j^2\eta_j + 3v(A^2 - |\eta_j|^2)\eta_j - 2a\prod_{i\neq j}\eta_j^*\right], \tag{S3}$$

where $A^2 = 2\sum_j |\eta_j^2|$. The correspondent free energy F for triangle structure is written in the usual way:

$$F = \int d\mathbf{r}\left[\frac{\Delta B_0}{2}A^2 + \sum_j\left\{B_0^x|\mathcal{G}_j\eta_j|^2 - \frac{3v}{2}|\eta_j|^4\right\} + \frac{3v}{4}A^4 - 2a\left(\prod_j\eta_j + \text{C.C.}\right)\right], \tag{S4}$$

here C.C. is stated for complex conjugate.

III. Amplitude equations of the two-mode triangle's structure. Using the similar approximations after the equalization of amplitudes with Eq. (18) $\eta_{j=1..3} = \phi$, $\eta_{j=4..6} = \xi$. The correspondent to the each amplitude component amplitude equations are given for each j-th component:

$$\eta_1: \quad (\tau\partial^2/\partial t^2 + \partial/\partial t)\,\phi = -M\mathbf{G}_1^2\left[(\Delta B_0 + \beta B_0^x\mathcal{G}_1^2)\phi - 2a\,(2\xi + \phi)\,\phi + 3v\left(5\phi^2 + 6\phi\xi + 10\xi^2\right)\phi\right],$$

$$\begin{aligned}\eta_2: \quad (\tau\partial^2/\partial t^2 + \partial/\partial t)\,\phi = -M\mathbf{G}_2^2\Bigg[&(\Delta B_0 + \beta B_0^x\mathcal{G}_2^2)\left\{\left(1 + \frac{8}{9\pi^2}\right)\phi + \frac{8}{9\pi^2}\xi\right\} - \\ &a\left(4\xi\phi + 2\phi^2 + \frac{1}{\pi^2}\left\{\frac{1}{135}(224\xi\phi - 656\phi^2) + \frac{208}{35}\xi^2\right\}\right) + \\ &v\left(15\phi^3 + 18\phi^2\xi + 30\phi\xi^2 + \frac{32}{4725\pi^2}\left\{-15\phi^3 + -1485\xi\phi^2 + 2419\phi\xi^2 - 207\xi^3\right\}\right)\Bigg],\end{aligned}$$

$$\begin{aligned}\eta_3: \quad (\tau\partial^2/\partial t^2 + \partial/\partial t)\,\phi = -M\mathbf{G}_3^2\Bigg[&(\Delta B_0 + \beta B_0^x\mathcal{G}_2^2)\left\{\left(1 - \frac{8}{9\pi^2}\right)\phi - \frac{8}{9\pi^2}\xi\right\} - \\ &a\left(4\xi\phi + 2\phi^2 + \frac{1}{\pi^2}\left\{\frac{1}{135}(-224\xi\phi + 656\phi^2) + \frac{208}{35}\xi^2\right\}\right) + \\ &v\left(15\phi^3 + 18\phi^2\xi + 30\phi\xi^2 + \frac{32}{4725\pi^2}\left\{15\phi^3 + 1485\xi\phi^2 - 2419\phi\xi^2 + 207\xi^3\right\}\right)\Bigg],\end{aligned}$$

$$\eta_4: \quad (\tau\partial^2/\partial t^2+\partial/\partial t)\,\xi = -M\mathbf{G}_4^2\left[(\Delta B_0+\beta B_0^x\mathcal{G}_2^2)\left\{\left(3+\frac{8}{9\pi^2}\right)\xi-\frac{24}{5\pi^2}\phi\right\}-\right.$$
$$a\left(6(\phi^2+\xi^2)+\frac{16}{945\pi^2}\left\{543\phi^2-162\xi\phi+287\xi^2\right\}\right)+$$
$$\left.v\left(18\phi^3+90\phi^2\xi+45\xi^3+\frac{32}{17325\pi^2}\left\{26455\phi^3+20933\xi\phi^2-29349\phi\xi^2+55\xi^3\right\}\right)\right],$$

$$\eta_5: \quad (\tau\partial^2/\partial t^2+\partial/\partial t)\,\xi = -M\mathbf{G}_5^2\left[(\Delta B_0+\beta B_0^x\mathcal{G}_2^2)\left\{\left(3-\frac{8}{9\pi^2}\right)\xi+\frac{24}{5\pi^2}\phi\right\}-\right.$$
$$a\left(6(\phi^2+\xi^2)+\frac{16}{945\pi^2}\left\{543\phi^2-162\xi\phi+287\xi^2\right\}\right)+$$
$$\left.v\left(18\phi^3+90\phi^2\xi+45\xi^3-\frac{32}{17325\pi^2}\left\{26455\phi^3+20933\xi\phi^2-29349\phi\xi^2+55\xi^3\right\}\right)\right],$$

$$\eta_6: \quad (\tau\partial^2/\partial t^2+\partial/\partial t)\,\xi = -M\mathbf{G}_6^2\left[3\left(\Delta B_0+\beta B_0^x\mathcal{G}_6^2\right)\xi-6a\left(\xi^2+\phi^2\right)+3v\left(6\phi^3+30\phi^2\xi+15\xi^3\right)\right].$$

These equations after summation and substitution $\xi=\alpha\phi$ lead to the averaged moving equation for two-mode triangle's structure:

$$\frac{3+3\alpha}{M}\left(\tau\frac{\partial^2}{\partial t}+\frac{\partial}{\partial t}\right)\phi = 12B_0^x\left(1+9\alpha\right)\nabla^2\phi-\Delta B_0(3+9\alpha)\phi+6a(3\alpha^2+2\alpha+4)\phi^2-$$
$$-9v(15\alpha^3+10\alpha^2+36\alpha+11)\phi^3. \tag{S5}$$

Correspondent two-mode triangle's free energy is given by

$$F_{tri-2}=\int d\mathbf{r}\left[2B_0^x\left(\sum_{j=1}^{3}|\mathcal{G}_j\phi|^2+\alpha^2\sum_{j=4}^{6}|\mathcal{G}_j\phi|^2\right)+3\Delta B_0(1+\alpha^2)\phi^2-4a(1+3\alpha+\alpha^3)\phi^3+\right.$$
$$\left.+\frac{45}{2}v\left(\alpha^4+4\alpha^2+\frac{8}{5}\alpha+1\right)\phi^4\right]. \tag{S6}$$

IV. Amplitude equations for two-mode honeycomb's lattice. After the equalization of amplitudes with Eq. (18) $\eta_{j=1..3}=\phi$, $\eta_{j=4..6}=\xi$ one can define the amplitude equations for honeycomb's lattice. The correspondent to the each amplitude component amplitude equations are given for each j-th component:

$$\eta_1: \quad (\tau\partial^2/\partial t^2+\partial/\partial t)\,\phi = -M\mathbf{G}_1^2\left[\left(\Delta B_0+\beta B_0^x\mathcal{G}_1^2\right)\phi-2a\phi^2+3v\left(5\phi^2+8\xi^2\right)\phi\right],$$

$$\eta_2: \quad (\tau\partial^2/\partial t^2+\partial/\partial t)\,\phi = -M\mathbf{G}_2^2\left[(\Delta B_0+\beta B_0^x\mathcal{G}_2^2)\left\{\left(1+\frac{8}{9\pi^2}\right)\phi+\frac{232}{35\pi^2}\xi\right\}-\right.$$
$$a\left(2\phi^2+\frac{16}{51975\pi^2}\left\{15785\phi^2+73062\phi\xi-14315\xi^2\right\}\right)+$$
$$\left.v\left(15\phi^3+24\phi\xi^2+\frac{32}{1576575\pi^2}\left\{-5005\phi^3+2410695\xi\phi^2-2170051\phi\xi^2+3993801\xi^3\right\}\right)\right],$$

$$\eta_3: \quad (\tau\partial^2/\partial t^2+\partial/\partial t)\,\phi = -M\mathbf{G}_3^2\left[(\Delta B_0+\beta B_0^x\mathcal{G}_2^2)\left\{\left(1-\frac{8}{9\pi^2}\right)\phi-\frac{232}{35\pi^2}\xi\right\}-\right.$$
$$a\left(2\phi^2-\frac{16}{51975\pi^2}\left\{15785\phi^2+73062\phi\xi-14315\xi^2\right\}\right)+$$
$$\left.v\left(15\phi^3+24\phi\xi^2-\frac{32}{1576575\pi^2}\left\{-5005\phi^3+2410695\xi\phi^2-2170051\phi\xi^2+3993801\xi^3\right\}\right)\right],$$

$$\eta_4: \quad \left(\tau\partial^2/\partial t^2 + \partial/\partial t\right)\xi = -M\mathbf{G}_4^2\left[\left(\Delta B_0 + \beta B_0^x \mathcal{G}_2^2\right)\left\{\frac{4}{3}\xi - \frac{256}{45\pi^2}\phi\right\} - a\left(\frac{8}{3}\xi^2 - \frac{1024}{225\pi^2}\phi^2 + \frac{68608}{2835\pi^2}\phi\xi\right) + v\left(32\phi^2\xi + 20\xi^3 - \frac{1024}{4729725\pi^2}\phi\left\{292383\phi^2 - 381238\xi\phi + 200907\xi^2\right\}\right)\right],$$

$$\eta_5: \quad \left(\tau\partial^2/\partial t^2 + \partial/\partial t\right)\xi = -M\mathbf{G}_5^2\left[\left(\Delta B_0 + \beta B_0^x \mathcal{G}_2^2\right)\left\{\frac{4}{3}\xi + \frac{256}{45\pi^2}\phi\right\} - a\left(\frac{8}{3}\xi^2 + \frac{1024}{225\pi^2}\phi^2 - \frac{68608}{2835\pi^2}\phi\xi\right) + v\left(32\phi^2\xi + 20\xi^3 + \frac{1024}{4729725\pi^2}\phi\left\{292383\phi^2 - 381238\xi\phi + 200907\xi^2\right\}\right)\right],$$

$$\eta_6: \quad \left(\tau\partial^2/\partial t^2 + \partial/\partial t\right)\xi = -M\mathbf{G}_6^2\left[\frac{4}{3}\left(\Delta B_0 + \beta B_0^x \mathcal{G}_6^2\right)\xi - \frac{8}{3}a\left(\xi^2 + \phi^2\right) + 4v\left(8\phi^2\xi + 5\xi^3\right)\right].$$

These six equations describe the first and second sublattices by their amplitudes $\eta_1 ... \eta_3$ and $\eta_4 ... \eta_6$, respectively, for the honeycomb as the two-dimensional hexagonal lattice.