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Supplementary Information: Regulation of Microtubule Disassembly by Spatially Heterogeneous Patterns of Acetylation

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S1. Determining the parameters used in the simulations

1) For a lattice consisting entirely of GTP-bound tubulin subunits, the lateral interaction energies are estimated to be in the range $-6k_BT \leq g_l \leq -3k_BT$ in Stukalin *et al* [1, 2]. In our simulations we fix the lateral interaction energy of the completely deacetylated GTP-lattice to be $-4.5k_BT$.

2) The mean disassembly rate of a GTP lattice measured from experiments is $\approx 0.5 \mu \text{m min}^{-1}$ [3]. Accordingly, R_d is fixed from the simulations at $432 \mu \text{m}$ min⁻¹ (α is assumed to be 0 in all our simulations).

3) The mean growth rate of a GTP lattice measured from a set of experiments is $\approx 0.17 \mu M^{-1} \mu m \min^{-1}$ [3]. Accordingly, R_a is fixed from the simulations at $0.17 C \mu m \min^{-1}$ (since $\alpha = 0$), where C is the concentration of the free tubulin.

4) With R_d fixed, the lateral interaction energy of the completely deacetylated lattice consisting of only GDP-subunits, is fixed at $g_l^0 = -2.85k_BT$ such that the disassembly rate is $\approx 8\mu \text{m min}^{-1}$ as measured from experiments [4].

5)

i) In vitro experiments have observed that the presence of acetylation reduces the lateral interaction between neighbouring protofilaments [4]. In order to accommodate this in the model, we consider that if the i^{th} subunit is acetylated or if any of the neighbours (lateral and longitudinal) of this subunit in the lattice is acetylated, then the lateral interaction energy associated with u_i and w_i are modified accordingly.

ii) In the experiments of Portran *et al* [4], it was observed that in the presence of 96% acetylation, the disassembly rate of the MT lattice is $\approx 20 \mu \text{m min}^{-1}$, three fold increased compared to the case at zero percent acetylation. Assuming that this disassembly rate is composed of the depolymerisation rate of GDP-subunits

alone, the modified lateral interaction energy of the GDP-subunits under the effect of acetylation is fixed at $g_l^{ac} = -2.25k_BT$ such that at 100% acetylation, disassembly rate of the filament is $\approx 20\mu \text{m min}^{-1}$.

References

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