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"Twist-state" transitions in parallel actin bundles induced by crosslinking proteins HOMIN SHIN, GREGORY GRASON, University of Massachusetts Amherst — Parallel actin bundles are common structural motifs in many crucial cellular specializations, from filopodia to mechanosensory bundles of the inner ear. Here, we study a model of actin bundles, crosslinked by compact globular bundling proteins, known to modify the torsional state of filaments due to frustration between helical structure of the filaments and in-plane ordering of the bundle. Our coarse-grained model of parallel bundles maps the linker-induced "twist-state" transition of actin filament onto a *commensurate-incommensurate* phase transition, described by an effective Frenkel-Kontorowa model. We predict that the transition from the uncrosslinked, incommensurate helical symmetry to fully crosslinked, commensurate symmetry is highly sensitive to linker flexibility: flexible crosslinking smoothly distorts the twist state of bundled filaments, while rigidly crosslinked bundles undergo a phase transition, rapidly overtwisting filaments over a narrow range of free crosslinker concentrations. Additionally, we predict a rich spectrum of intermediate structures, composed of alternating domains of sparsely bound (untwisted) and strongly bound (overtwisted) filaments. This model reveals that subtle differences in crosslinking agents themselves modify not only the detailed structure of parallel actin bundles, but also the thermodynamic pathway by which they form.

Homin Shin
University of Massachusetts Amherst

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