## Abstract Submitted for the NEF10 Meeting of The American Physical Society

Actin – myosin interaction CYNTHIA PRUDENCE, YANA RESHET-NYAK, OLEG ANDREEV, URI — Muscle contraction is resulted from the interaction of myosin with actin and ATP. The study of kinetics of binding of myosin subfragment 1 (S1) to F-actin revealed the two step binding, which were modeled by initial binding of S1 to one actin monomer (state 1) and then to the second neighboring monomer (state 2). The results of time-resolved cross-linking of S1 and F-actin upon their rapid mixing in stopped flow apparatus directly demonstrated that myosin head initially binds through the loop 635-647 to the N-terminus of one actin and then through the loop 567-574 to the N-terminus of the second actin (Andreev & Reshetnyak, 2007, J. Mol. Biol. 365(3), 551-554). The computational docking of S1 with F-actin demonstrated that both actin monomers are located in the same strand of F-actin with the first and second actins being close to the pointed and barbed ends of F-actin, respectively. The closing of the main cleft in 50 kDa of S1 might prevent binding of S1 with two actins since the distance between loops 635-647 and 567-574 became too short to interact with N-termini of two actins simultaneously. Depending on degree of saturation of F-actin with S1s there are two structurally different complexes are formed: at complete saturation each S1 binds only one actin and its cleft is closed while at partial saturation S1 interacts with two actins and its cleft is opened. The transition between one- and two-actin binding states of myosin accompanying with opening the cleft in central domain of S1 might be associated with force generation. The formation of actin-myosin interface would be associated with the energy release that might be used in part for the generation of force in muscle.

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