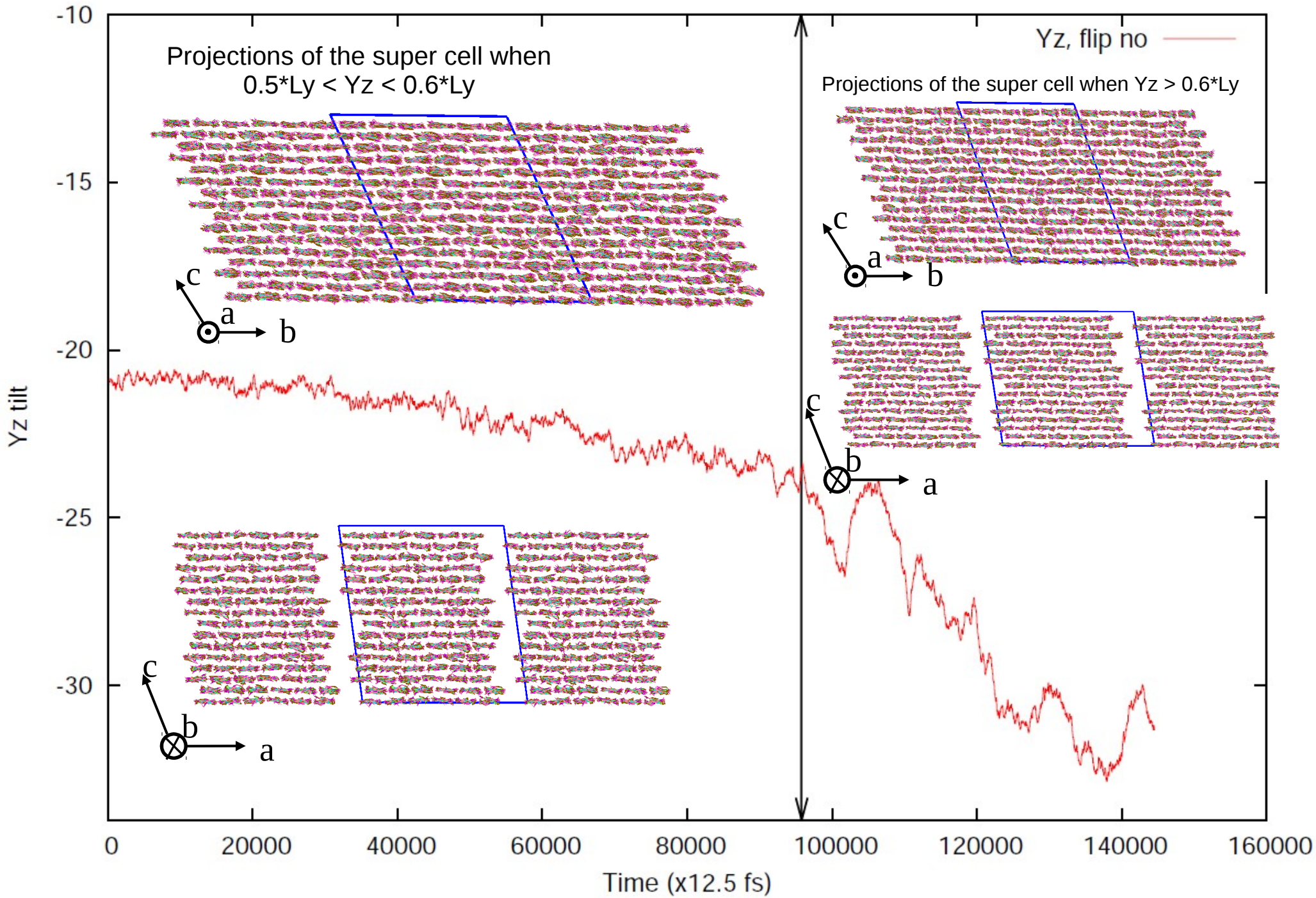
Projections of the super cell when
0.5*Ly < Yz < 0.6*Ly
Yz, flip no
Projections of the super cell when Yz > 0.6*Ly
c
a
b
Yz tilt
Time (x12.5 fs)
-10
-15
-20
-25
-30
0
20000
40000
60000
80000
100000
120000
140000
160000