Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

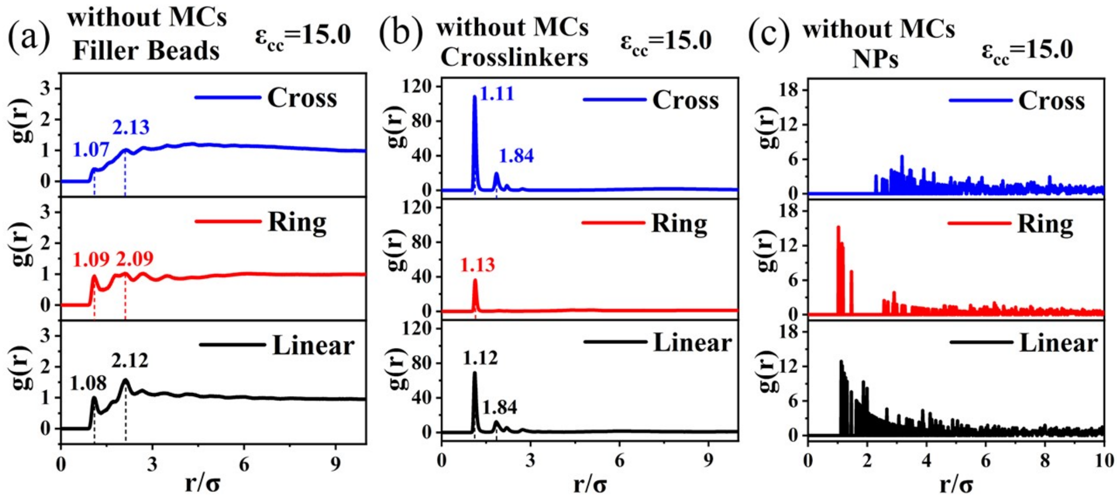


Figure S1. In configurations without MCs. (a) The RDF of filler beads at ε_{cc} = 15.0, (b) the RDF of Crosslinkers at ε_{cc} = 15.0 and (c) the RDF of whole NPs at ε_{cc} = 15.0.

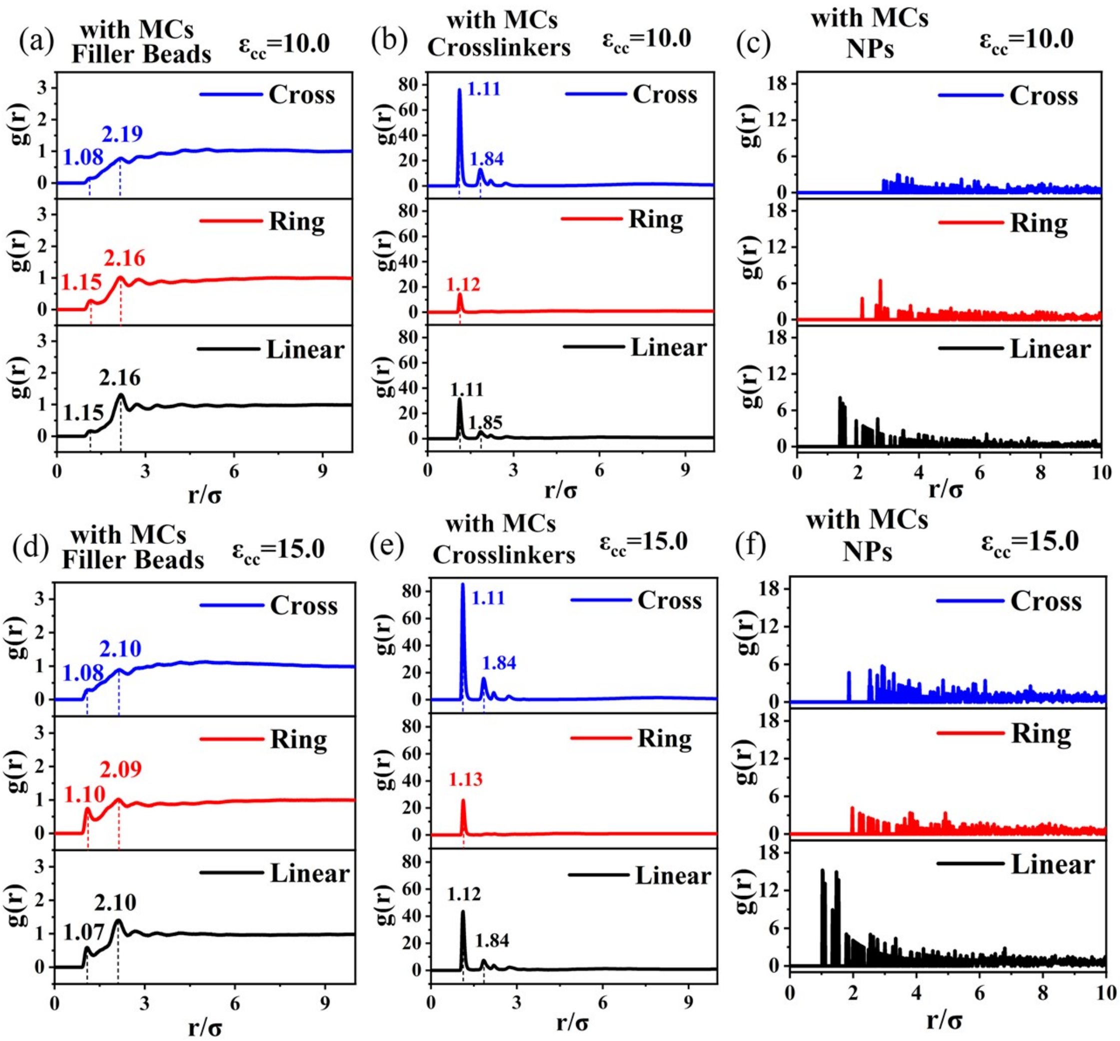


Figure S2. In configurations with MCs. The RDF of (a) filler beads, (b) Crosslinkers and (c) whole NPs at ε_{cc} = 10.0.

The RDF of (d) filler beads, (e) Crosslinkers and (f) whole NPs at ε_{cc} = 15.0.

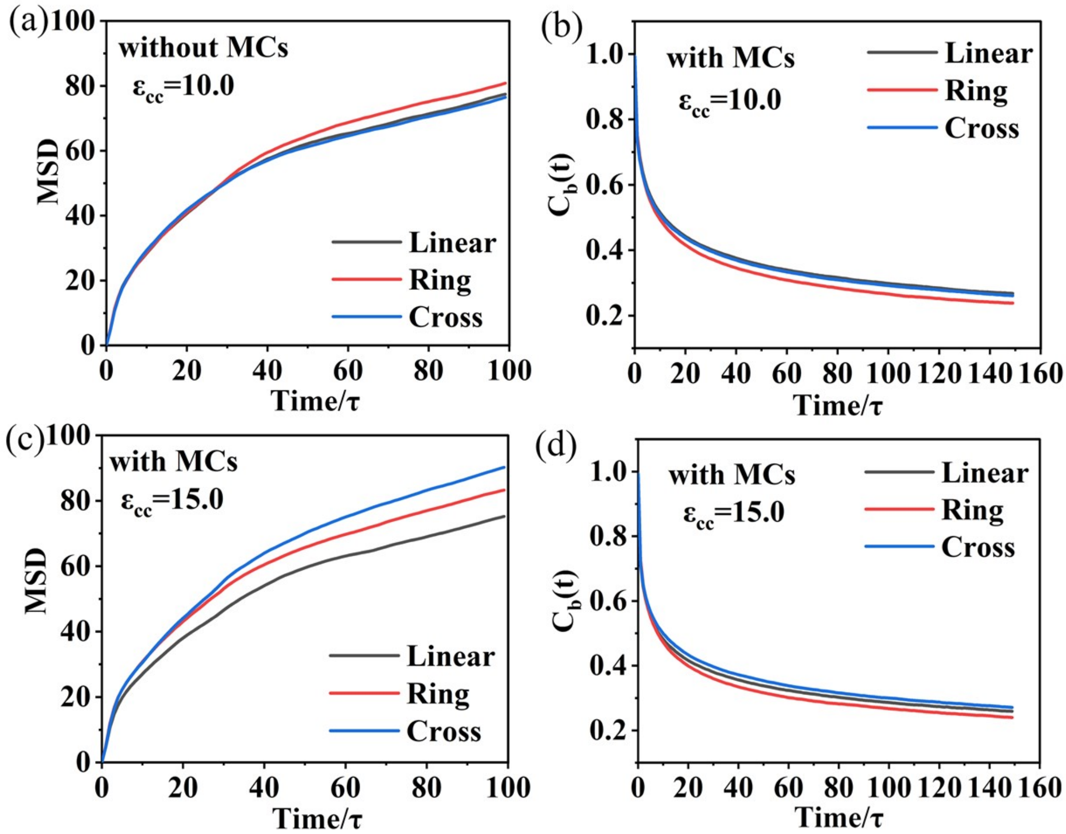


Figure S3. In configuration with MCs, the (a) MSD and (b) the bond autocorrelation function at ε_{cc} = 10.0. The (c) MSD and (d) the bond autocorrelation function at ε_{cc} = 15.0.

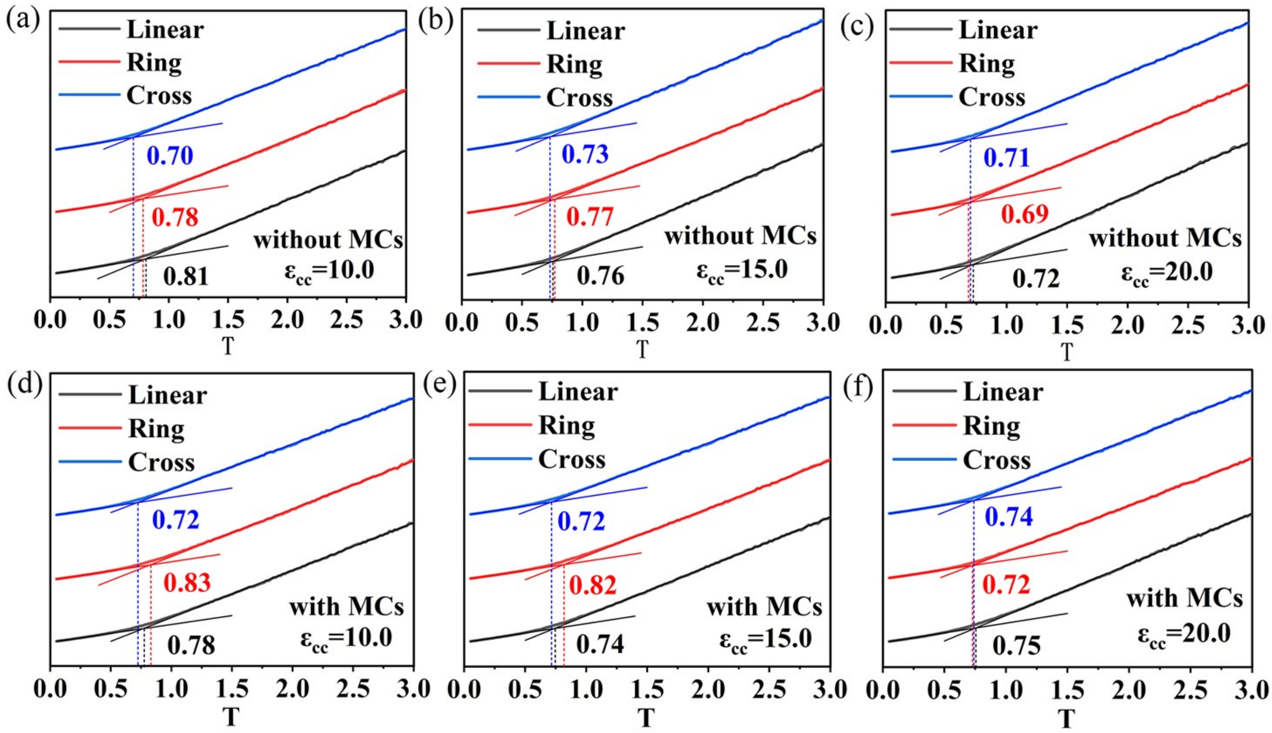


Figure S4. The fitting curves of the function about the volume and temperature: (a) without MCs at ε_{cc} = 10.0, (b) without MCs at ε_{cc} = 15.0, (c) without MCs at ε_{cc} = 20.0 and (d) with MCs at ε_{cc} = 10.0, (e) with MCs at ε_{cc} = 15.0, (f) with MCs at ε_{cc} = 20.0.

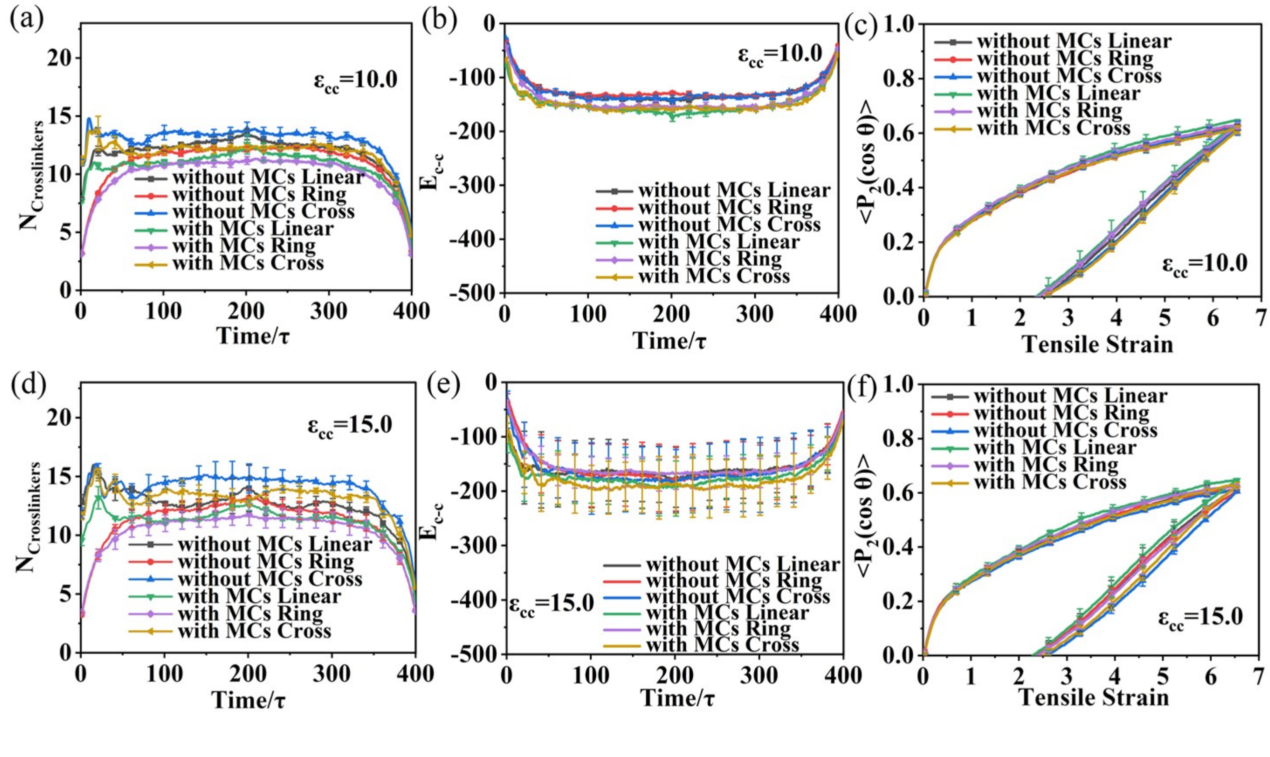


Figure S5. During the uniaxial tension and recovery process. (a) The average number of neighbor Crosslinkers, (b) the total interaction energy between Crosslinkers and (c) the matrix chains orientation at ε_{cc} = 10.0. (d) The average number of neighbor Crosslinkers, (e) the total interaction energy between Crosslinkers and (f) the matrix chains orientation at ε_{cc} = 15.0.

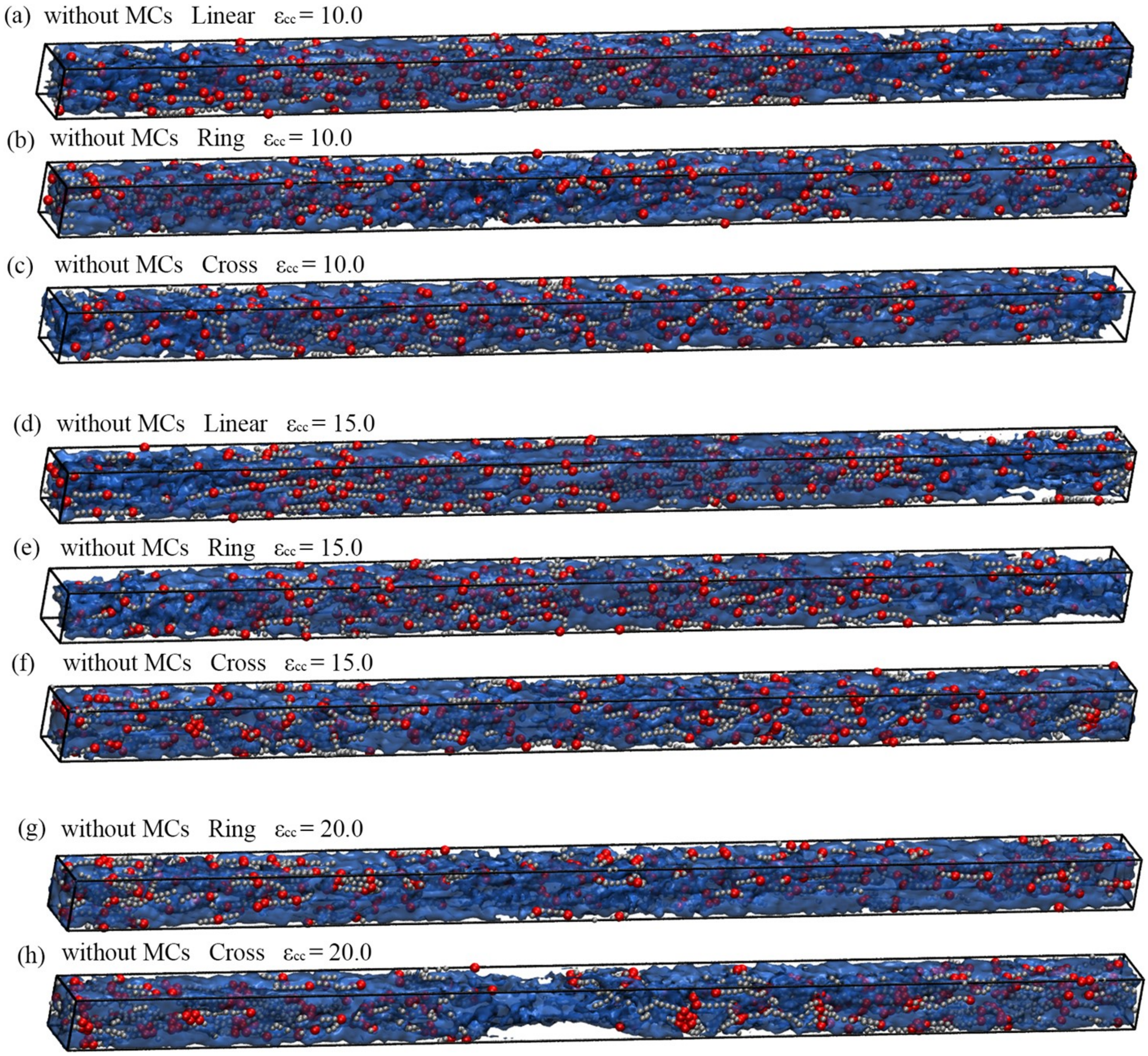


Figure S6. The snapshots at maximum uniaxial strain of (a) Linear, (b) Ring and (c) Cross structure PNCs without MCs at ε_{cc} = 10.0. (d) Linear, (e) Ring and (f) Cross structure PNCs without MCs at ε_{cc} = 15.0. (g) Ring and (h) Cross structure PNCs without MCs at ε_{cc} = 20.0.

Figure S7. The snapshots at maximum uniaxial strain of (a) Linear, (b) Ring and (c) Cross structure PNCs with MCs at ε_{cc} = 10.0. (d) Linear, (e) Ring and (f) Cross structure PNCs with MCs at ε_{cc} = 15.0. (g) Ring and (h) Cross structure PNCs with MCs at ε_{cc} = 20.0.

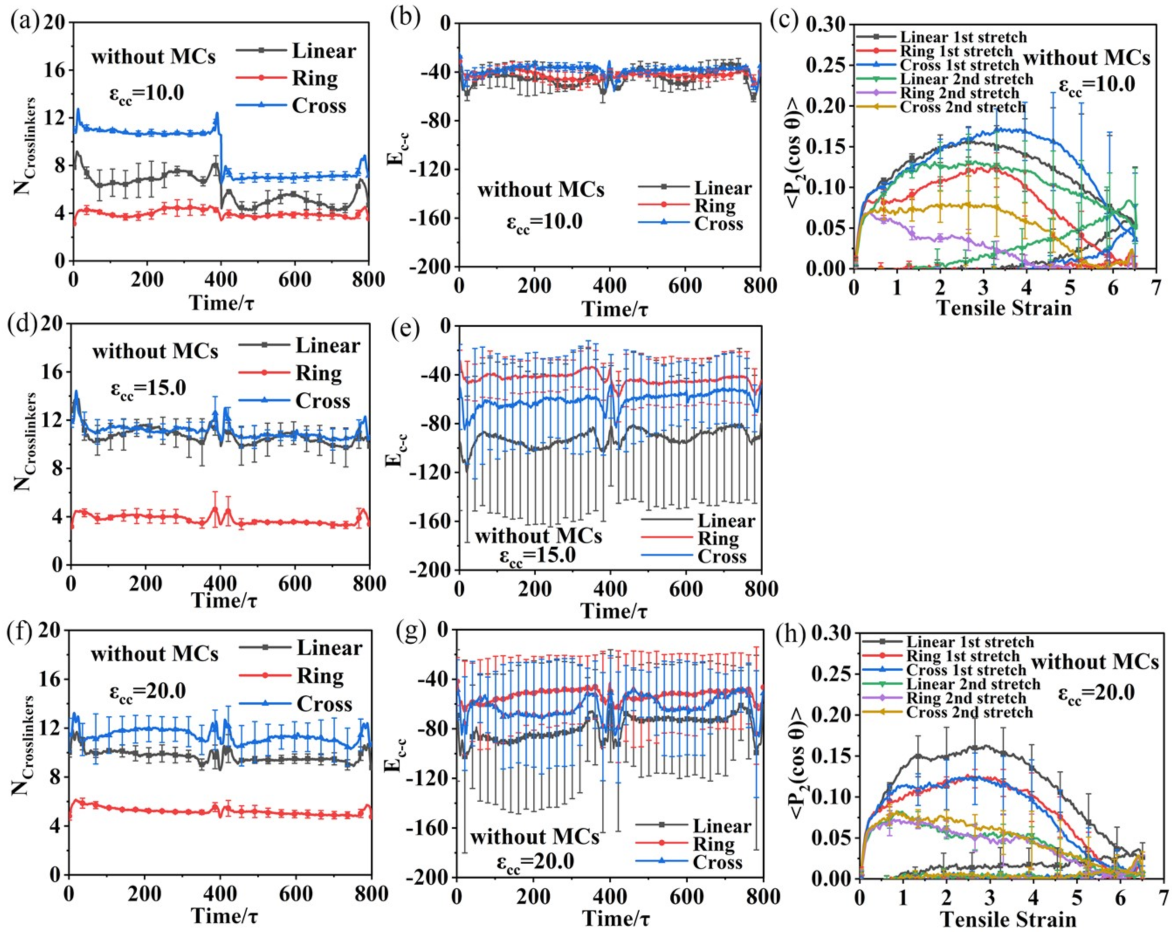


Figure S8. In the configurations without MCs, during the twice approximate triaxial tension and recovery process. (a) The average number of neighbor Crosslinkers, (b) total interaction energy between Crosslinkers and (c) the matrix chains orientation at ε_{cc} = 10.0. (d) The average number of neighbor Crosslinkers and (e) total interaction energy between Crosslinkers ε_{cc} = 15.0. (f) The average number of neighbor Crosslinkers, (g) total interaction energy between Crosslinkers and (h) the matrix chains orientation at ε_{cc} = 20.0.

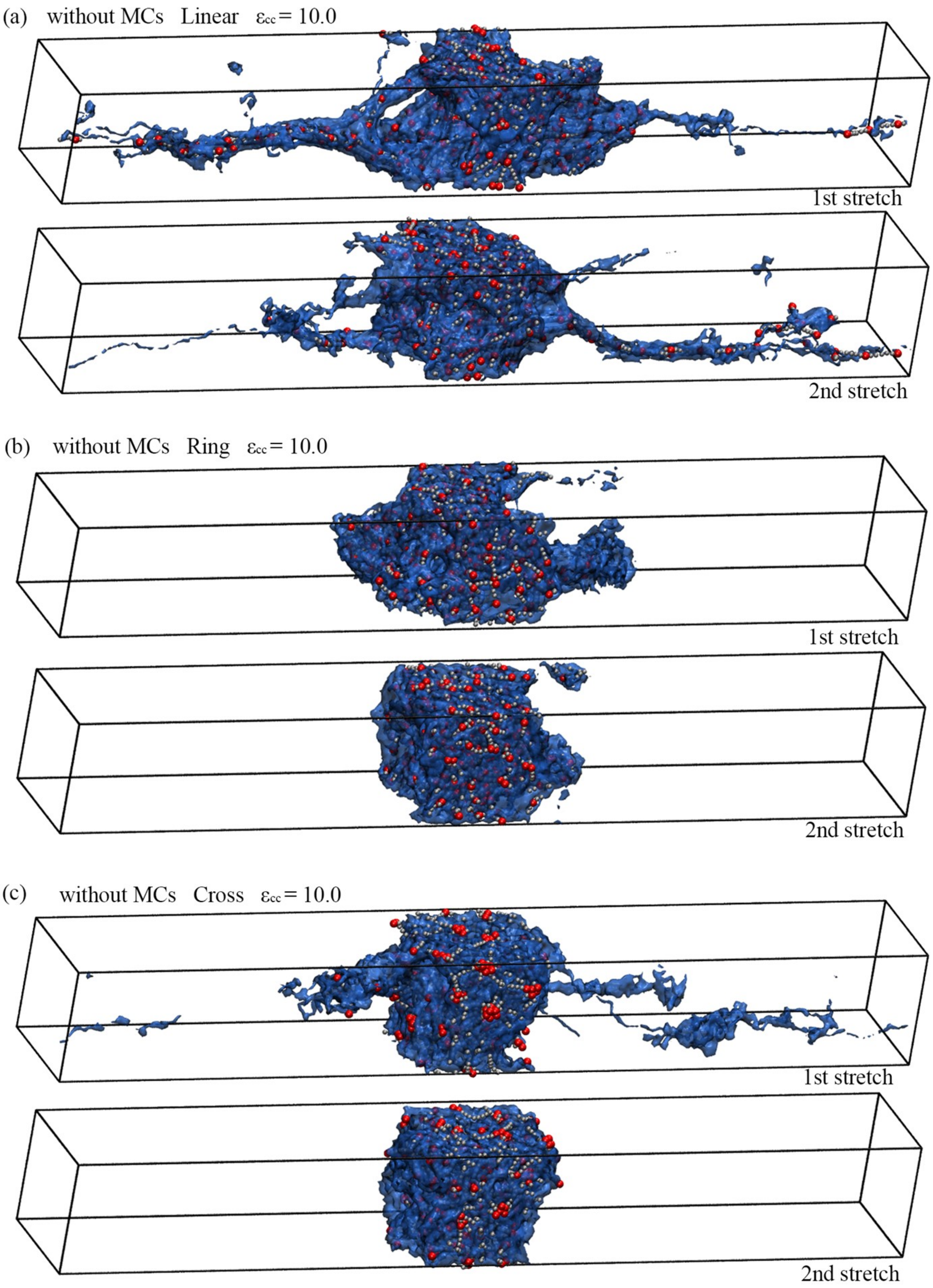
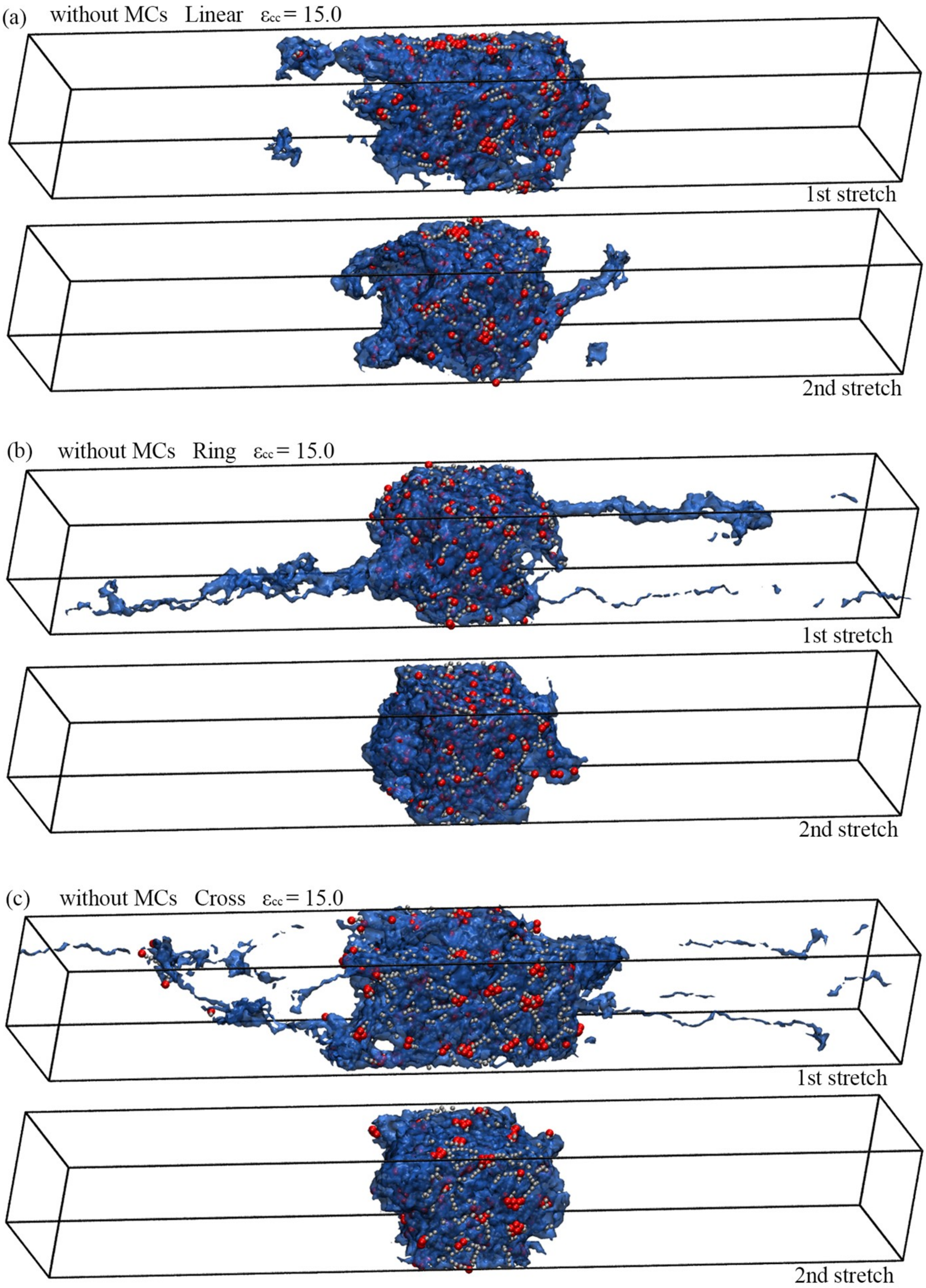


Figure S9. In the configurations without MCs. The snapshots at maximum strain of (a) Linear, (b) Ring and (c) Cross structure PNCs at ε_{cc} = 10.0 in approximate triaxial tension and recovery process.



(a) without MCs Linear εcc = 15.0
1st stretch
2nd stretch
(b) without MCs Ring εcc = 15.0
1st stretch
2nd stretch
(c) without MCs Cross εcc = 15.0
1st stretch
2nd stretch

Figure S10. In the configurations without MCs. The snapshots at maximum strain of (a) Linear, (b) Ring and (c) Cross structure PNCs at ε_{cc} = 15.0 in approximate triaxial tension and recovery process.

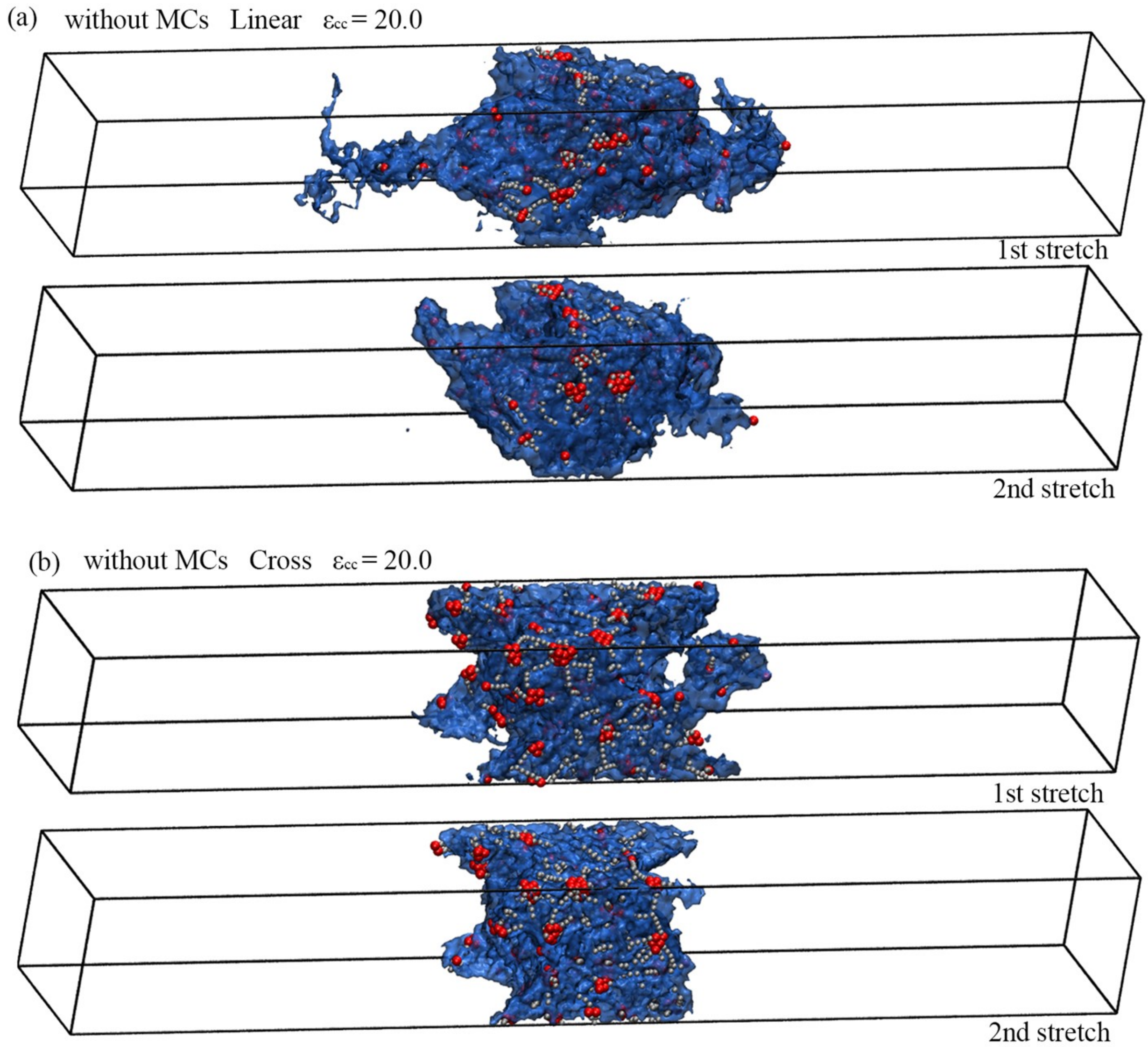


Figure S11. In the configurations without MCs. The snapshots at maximum strain of (a) Linear and (b) Cross structure PNCs at ε_{cc} = 20.0 during approximate triaxial tension and recovery process.

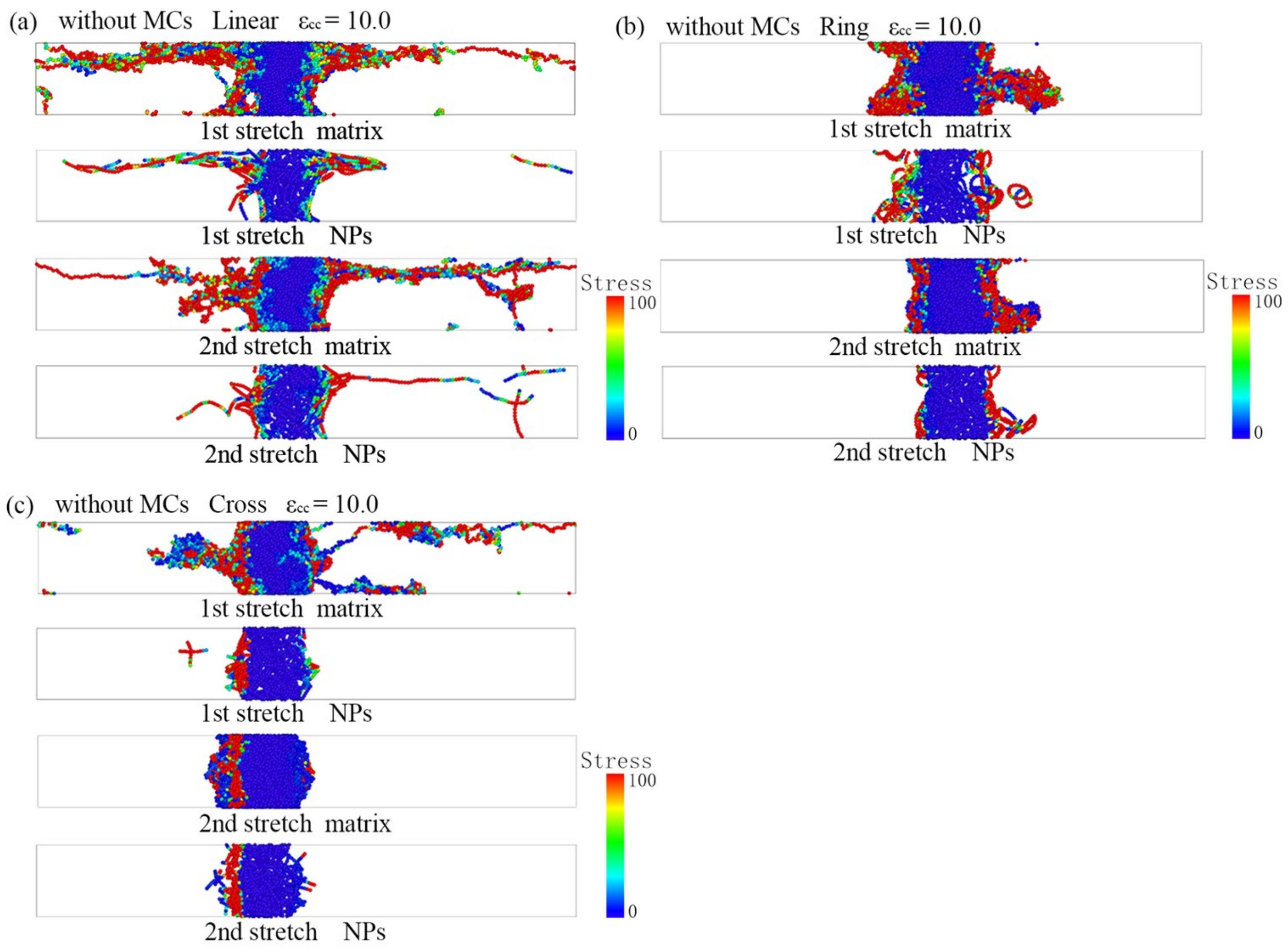


Figure S12. In the configurations without MCs. The heatmaps of matrix and NPs of (a) Linear, (b) Ring and (c) Cross structure PNCs at ε_{cc} = 10.0 during approximate triaxial tension and recovery process when stretched to maximum strain.

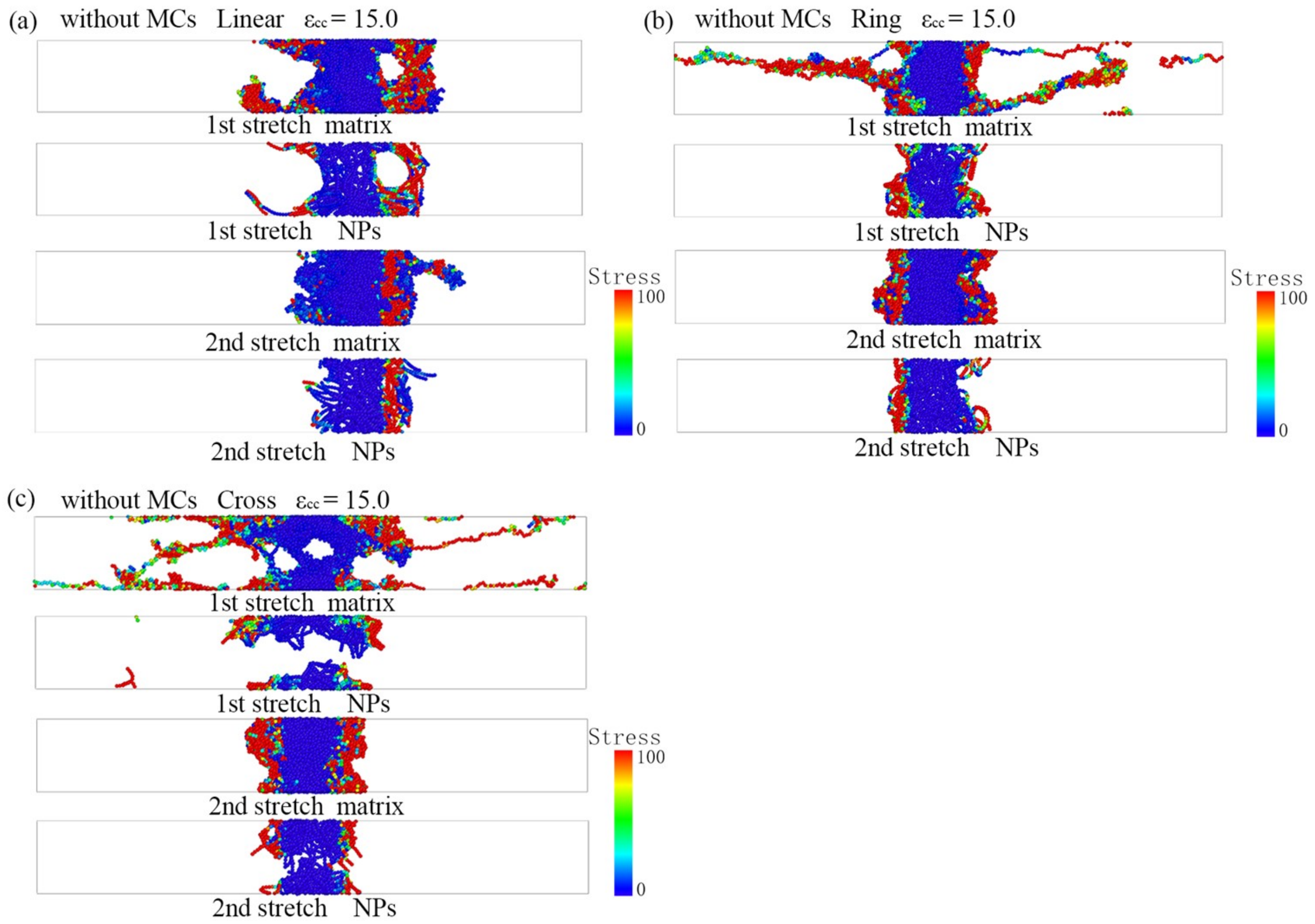


Figure S13. In the configurations without MCs. The heatmaps of matrix and NPs of (a) Linear, (b) Ring and (c) Cross structure PNCs at ε_{cc} = 15.0 during approximate triaxial tension and recovery process when stretched to maximum strain.

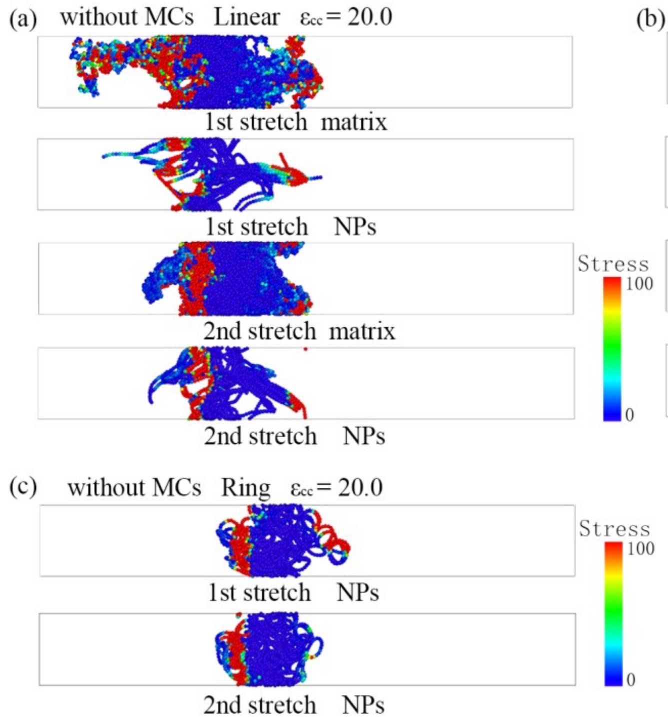


Figure S14. In the configurations without MCs. The heatmaps of matrix and NPs of (a) Linear and (b) Cross structure PNCs at ε_{cc} = 20.0, and (c) the heatmaps of NPs of Ring structure PNCs at ε_{cc} = 20.0 during approximate triaxial tension and recovery process when stretched to maximum strain.

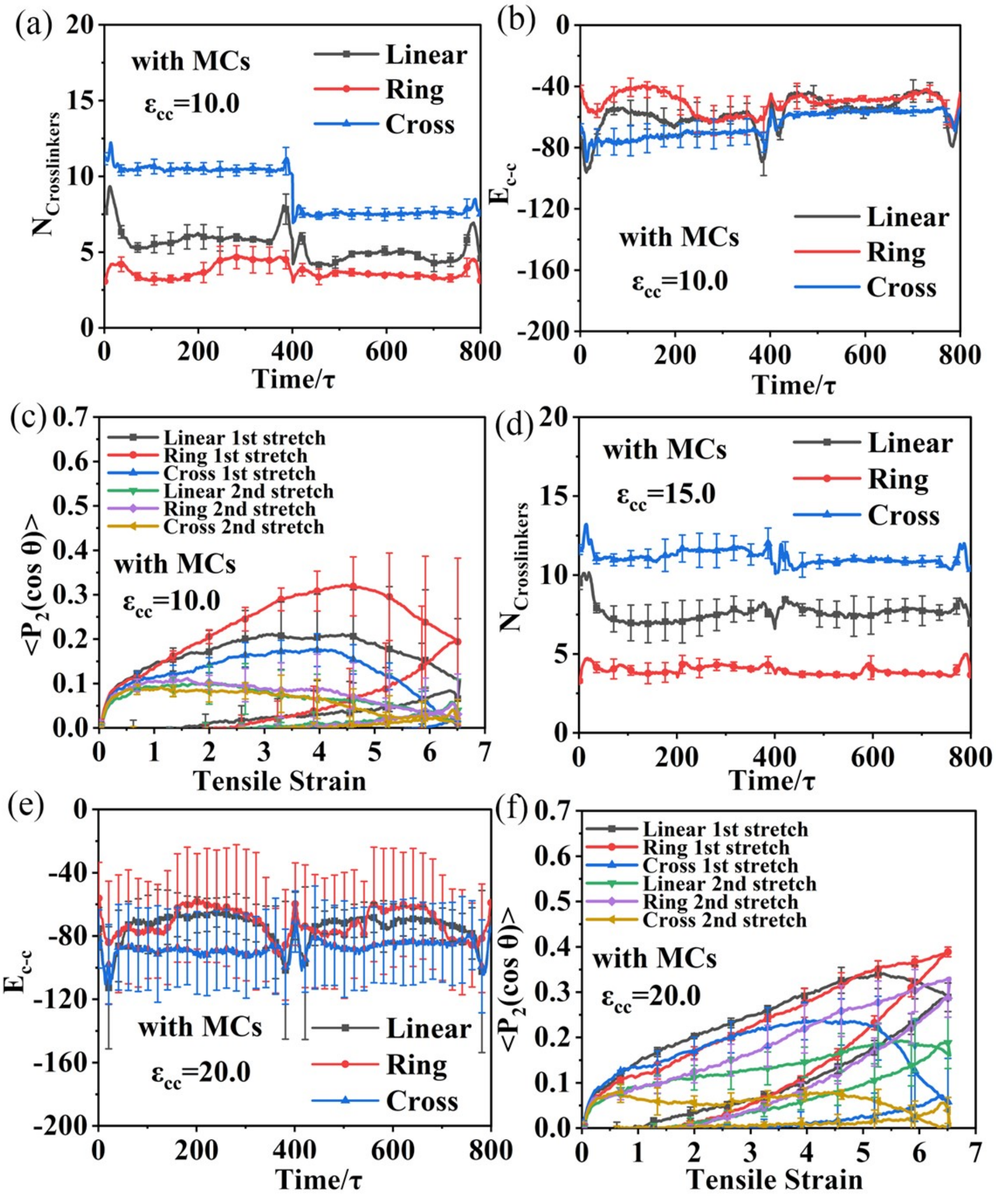


Figure S15. In the configurations with MCs, during the twice approximate triaxial tension and recovery process. (a) The average number of neighbor Crosslinkers, (b) total interaction energy between Crosslinkers and (c) the matrix chains orientation at ε_{cc} = 10.0. (d) The average number of neighbor Crosslinkers at ε_{cc} = 15.0. (e) The total interaction energy between Crosslinkers and (f) the matrix chains orientation at ε_{cc} = 20.0.

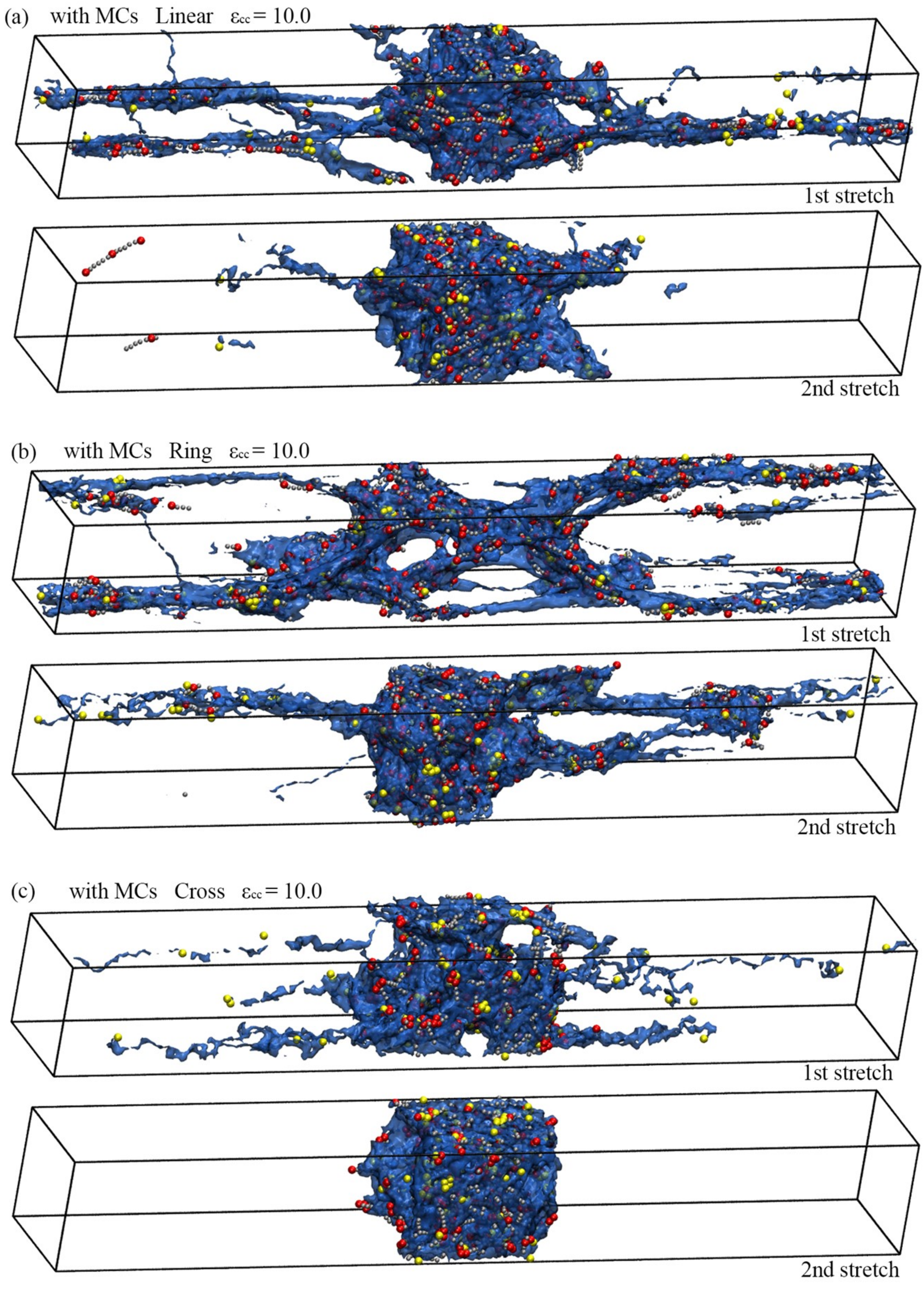


Figure S16. In the configurations with MCs. The snapshots at maximum strain of (a) Linear, (b) Ring and (c) Cross structure PNCs at ε_{cc} = 10.0 during approximate triaxial tension and recovery process.

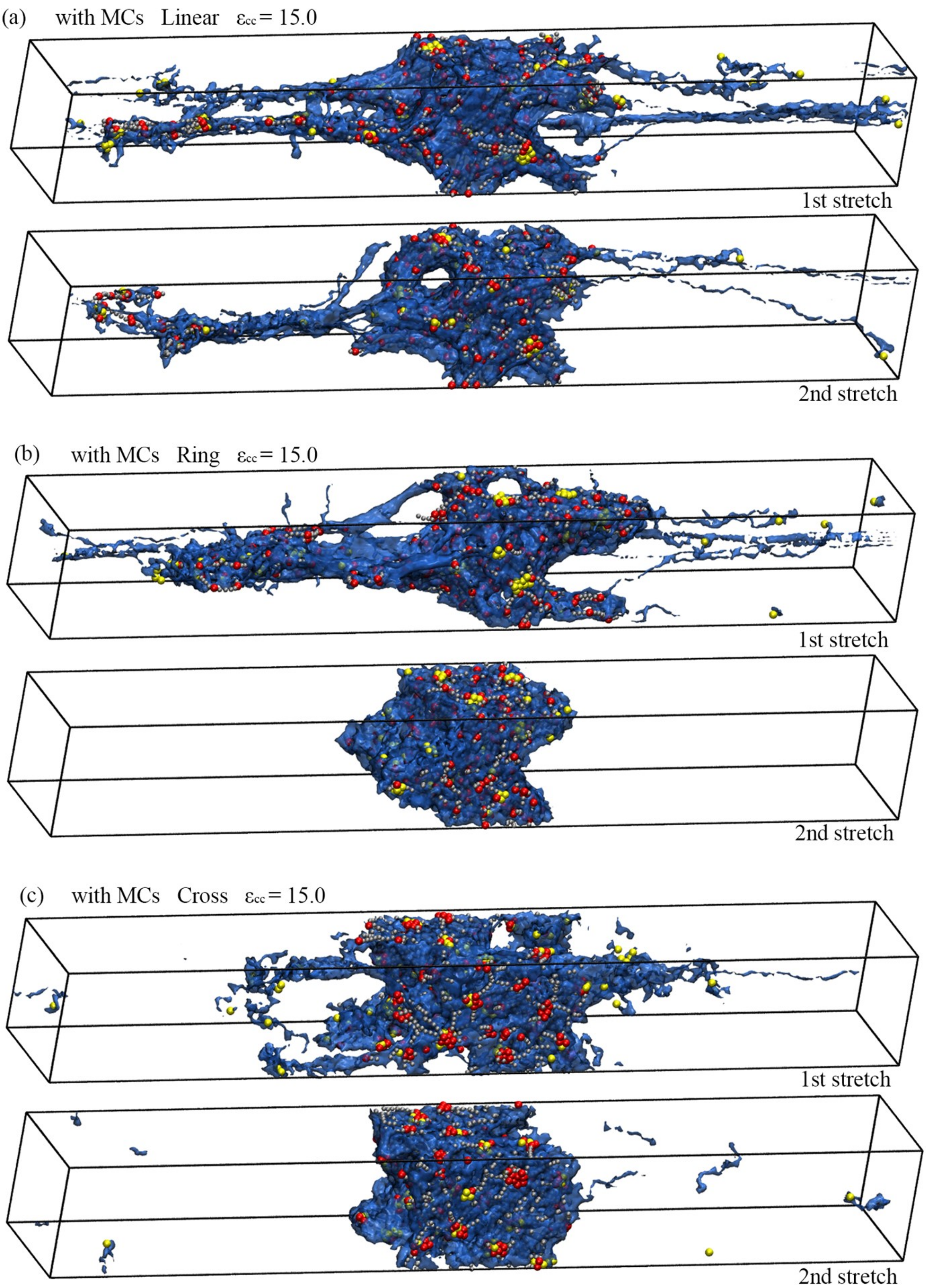

(a) with MCs Linear εcc = 15.0
1st stretch
2nd stretch
(b) with MCs Ring εcc = 15.0
1st stretch
2nd stretch
(c) with MCs Cross εcc = 15.0
1st stretch
2nd stretch

Figure S17. In the configurations with MCs. The snapshots at maximum strain of (a) Linear, (b) Ring and (c) Cross structure PNCs at ε_{cc} = 15.0 during approximate triaxial tension and recovery process.

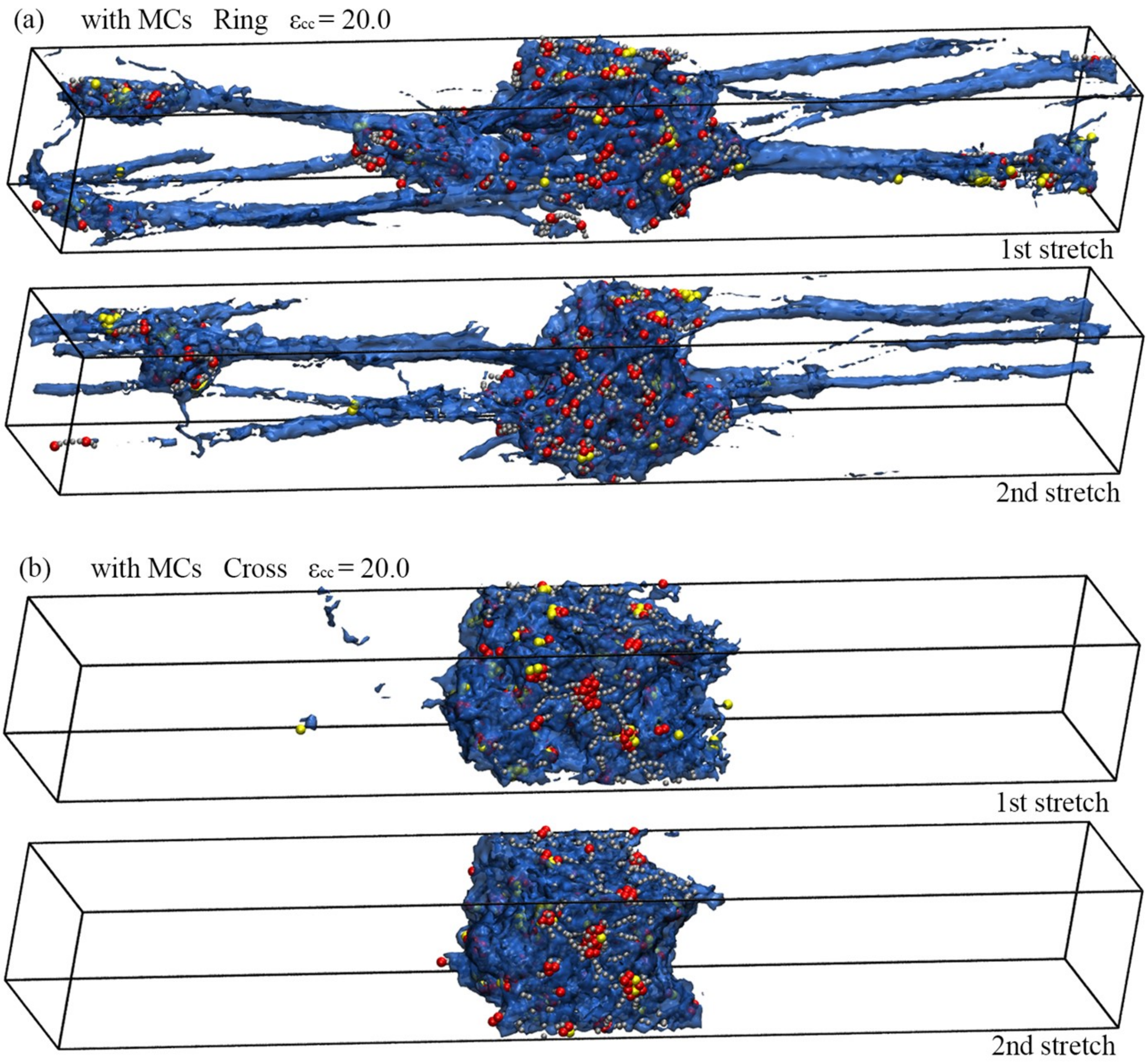


Figure S18. In the configurations with MCs. The snapshots at maximum strain of (a) Ring and (b) Cross structure PNCs at ε_{cc} = 20.0 during approximate triaxial tension and recovery process.

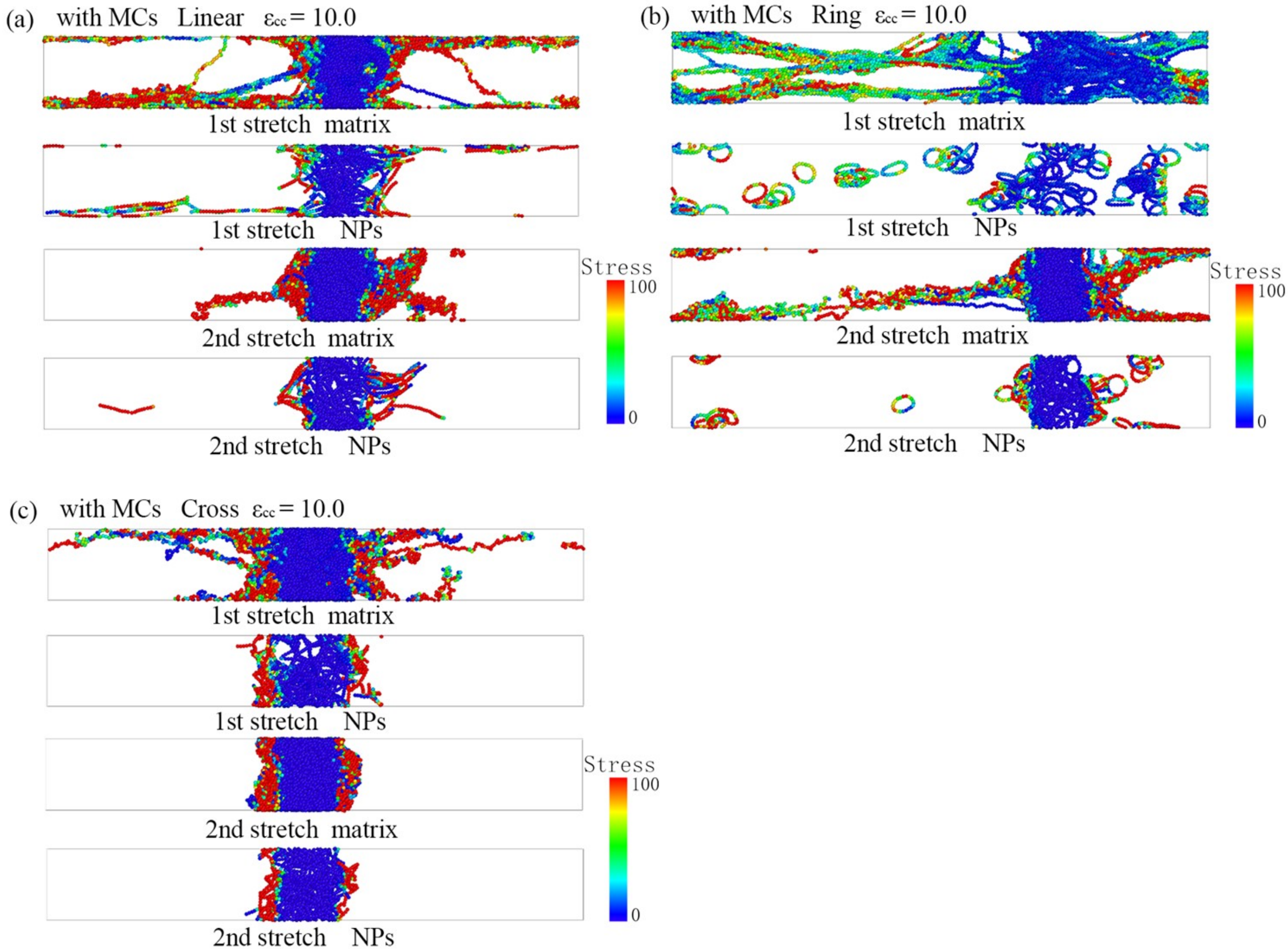


Figure S19. In the configurations with MCs. The heatmaps of matrix and NPs of (a) Linear, (b) Ring and (c) Cross structure PNCs at ε_{cc} = 10.0 during approximate triaxial tension and recovery process when stretched to maximum strain.

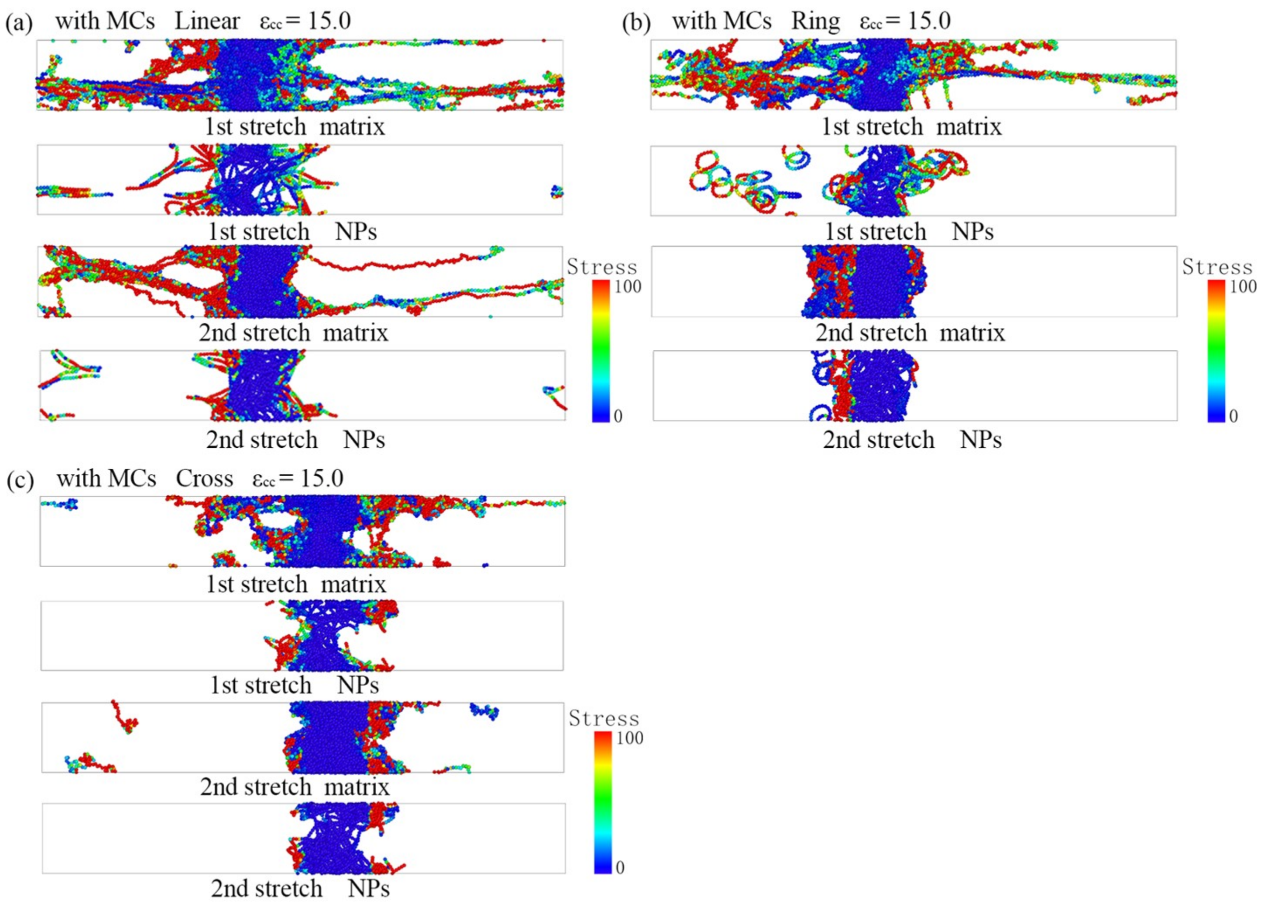


Figure S20. In the configurations with MCs. The heatmaps of matrix and NPs of (a) Linear, (b) Ring and (c) Cross structure PNCs at ε_{cc} = 15.0 during approximate triaxial tension and recovery process when stretched to maximum strain.

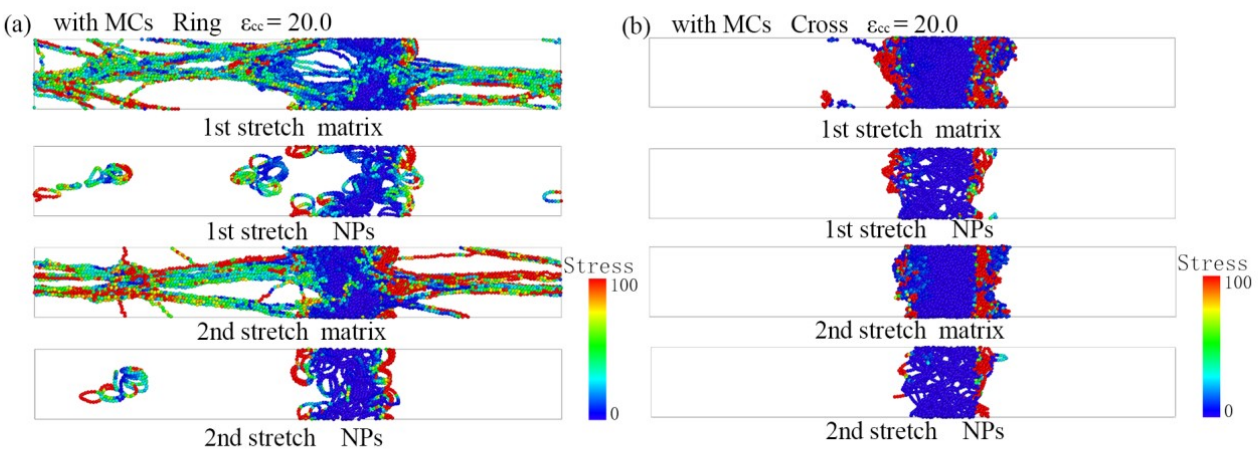


Figure S21. In the configurations with MCs. The heatmaps of matrix and NPs of (a) Ring and (b) Cross structure PNCs at ε_{cc} = 20.0 during approximate triaxial tension and recovery process when stretched to maximum strain.

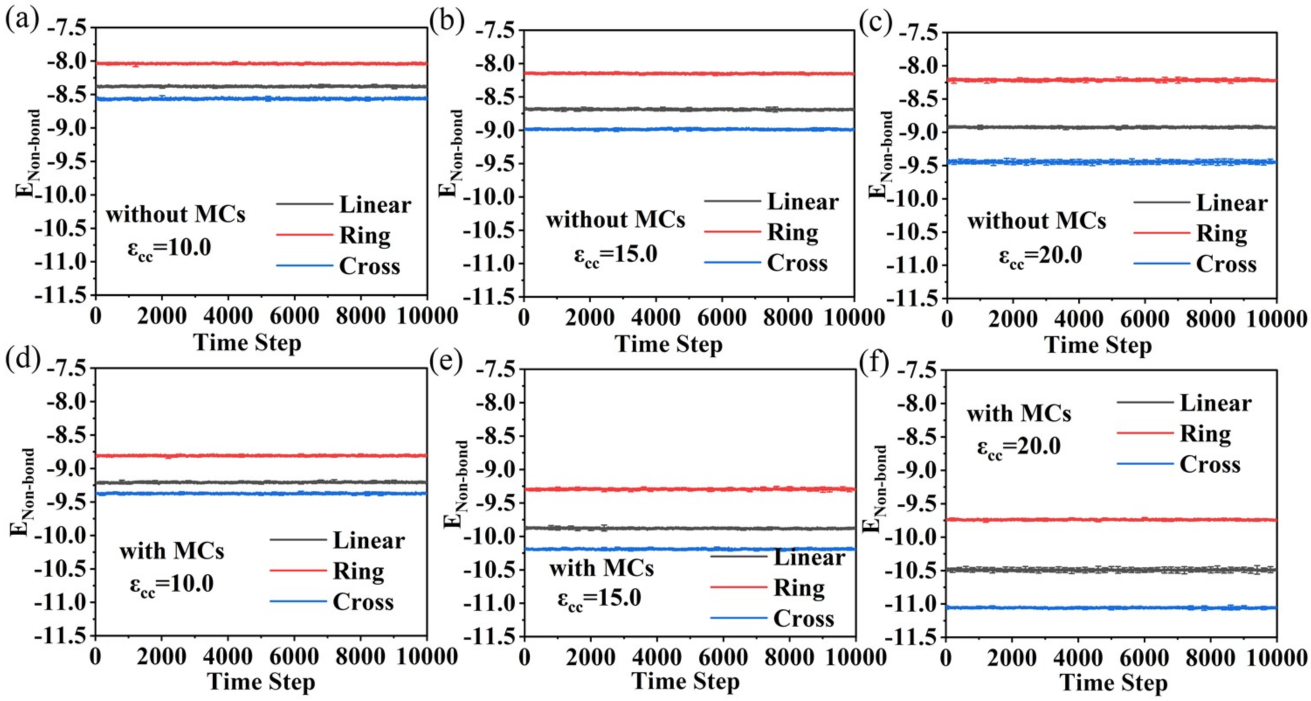


Figure S22. The last 10,000 steps of the equilibrium process of non-bond interaction energy curve: configures without MCs at (a) ε_{cc} = 10.0, (b) ε_{cc} = 15.0, (c) ε_{cc} = 20.0, and configurations with MCs at: (d) ε_{cc} = 10.0, (e) ε_{cc} = 15.0, (f) ε_{cc} = 20.0.