

Appendix A. Supplementary data

1. ReaxFF forcefield parameters can be found at [ffield.reax.CaSiOHC](https://fffield.reax.CaSiOHC)
2. Total energy of each system over time during the relaxation process

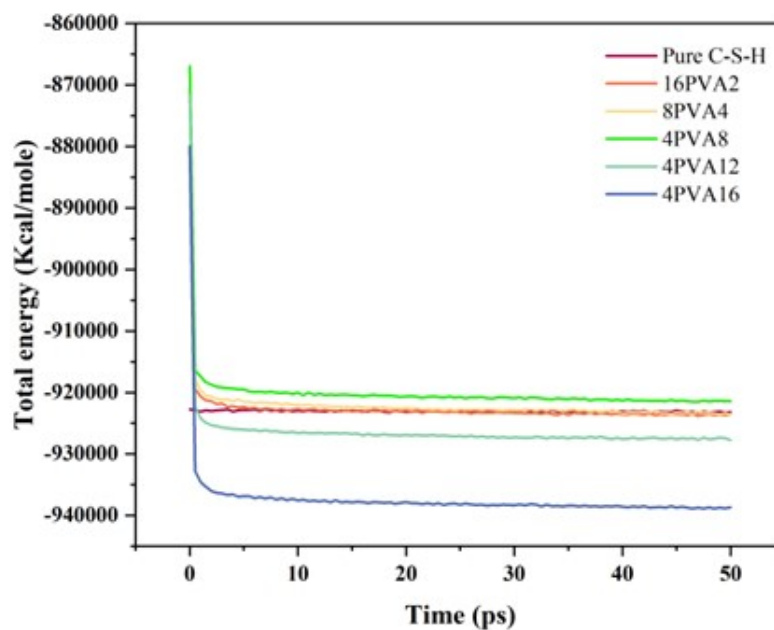


Figure (a). The variation of total energy of each system over time during the relaxation process. In the relaxation process, the total energy of each system tends to be stable with time, which indicates that the system reaches the equilibrium state.

3. The stress distribution diagrams during the tensile deformation along the X-axis, with significant crack occurrence (strain \approx 0.35).

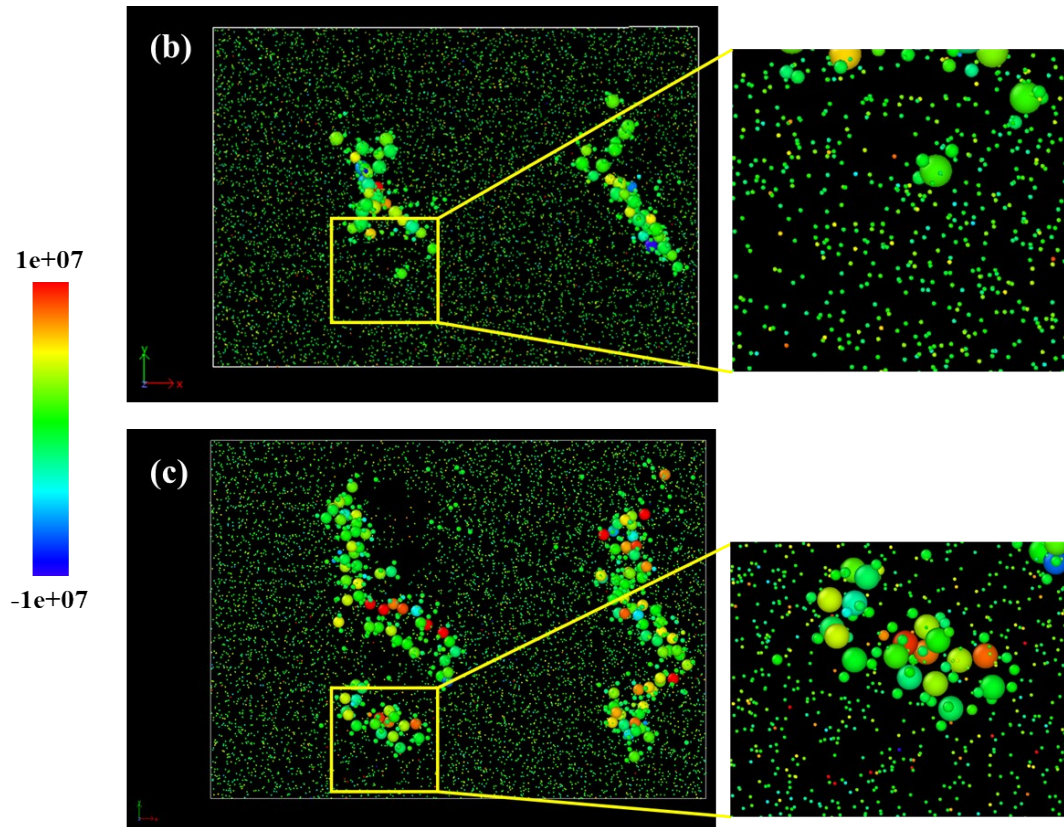
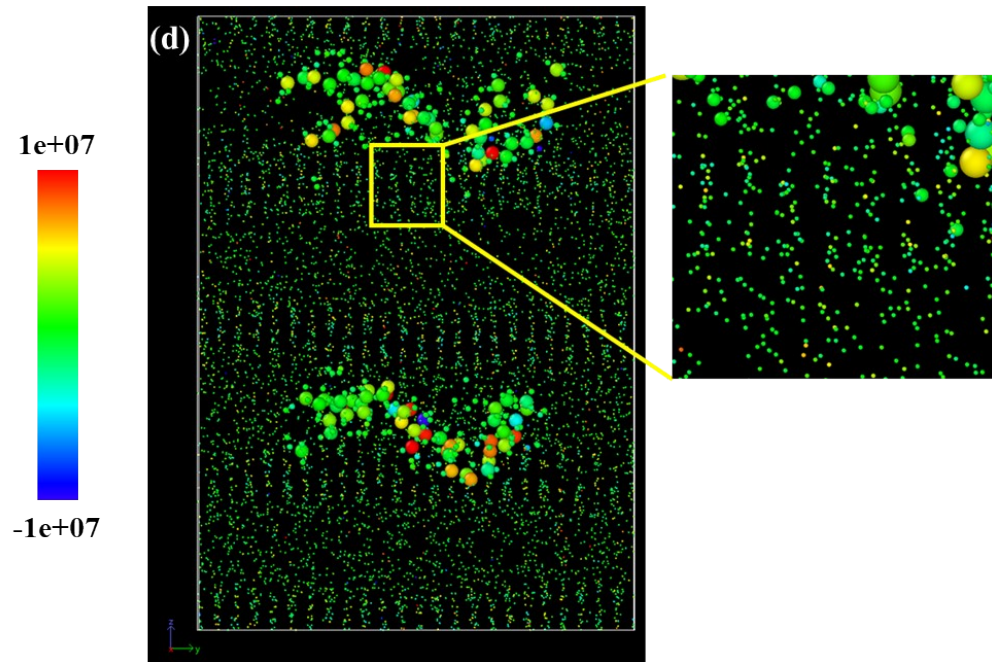
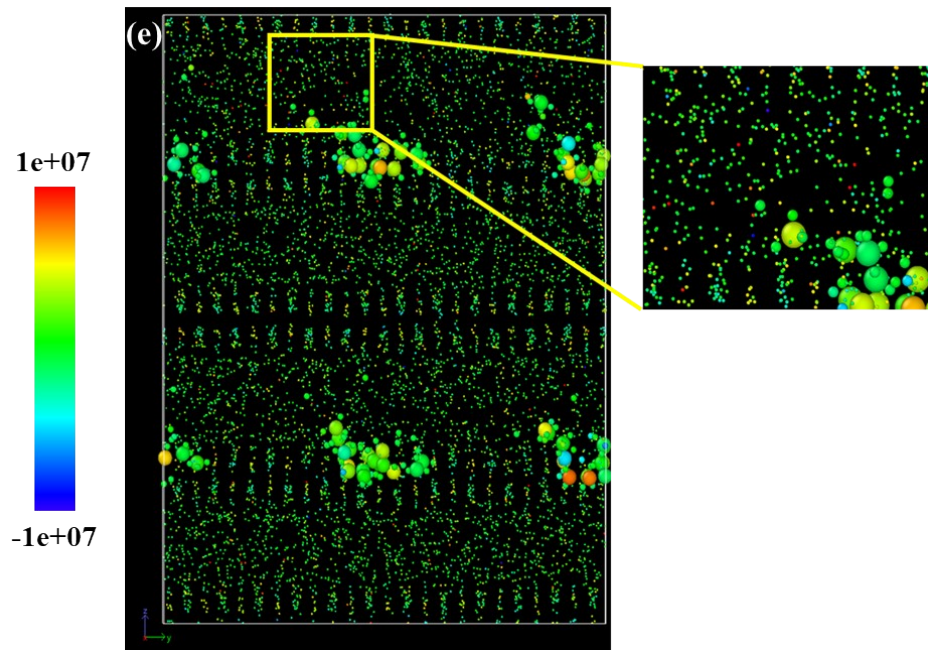


Figure (b) and (c). (b) The 4PVA8 system exhibits good mechanical performance, without significant stress concentration; (c) The 4PVA16 system demonstrates poor mechanical performance and considerable stress concentration.

4. The stress distribution diagrams during the tensile deformation along the Z-axis, with significant crack occurrence (strain \approx 0.35).



(d) The 4PVA12 system exhibits good mechanical performance, without significant stress concentration.



(e) The 8PVA4 system demonstrates poor mechanical performance and significant stress concentration.