materials

MDPI

Supplementary

Phase Transition of Single-Layer Molybdenum Disulfide Nanosheets under Mechanical Loading Based on Molecular Dynamics Simulations

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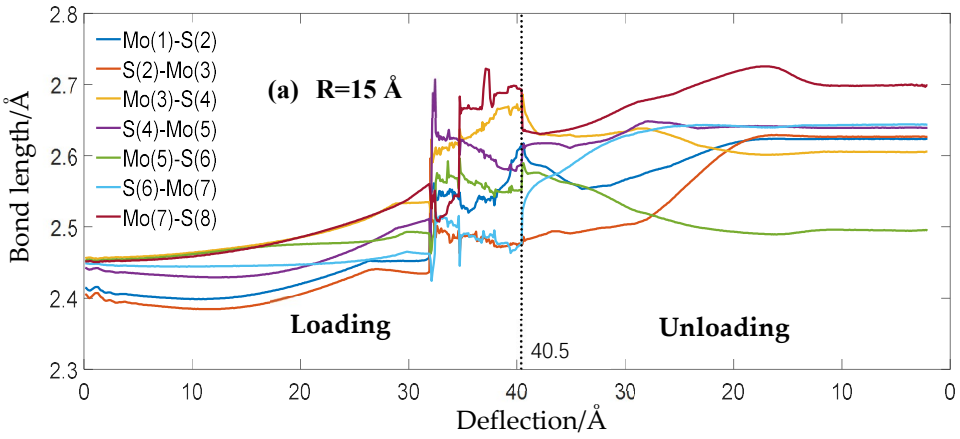
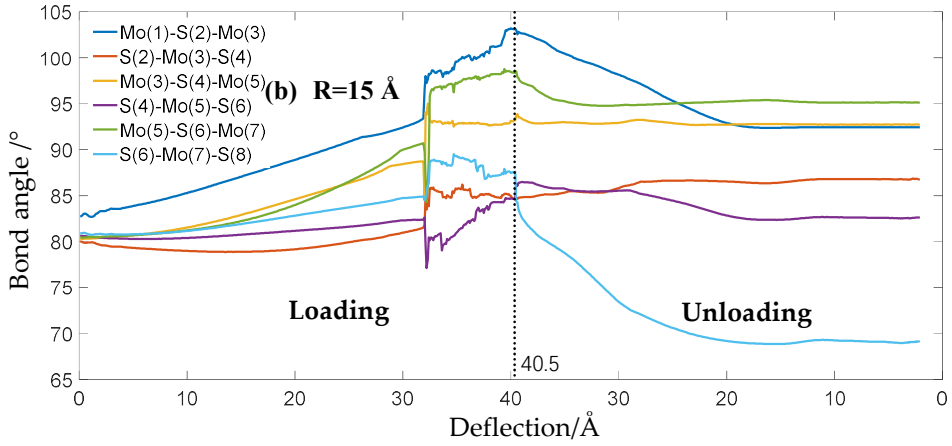
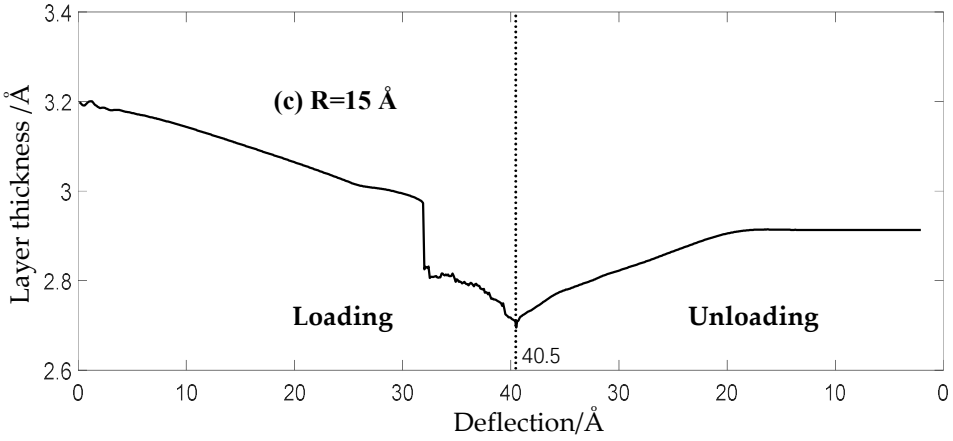
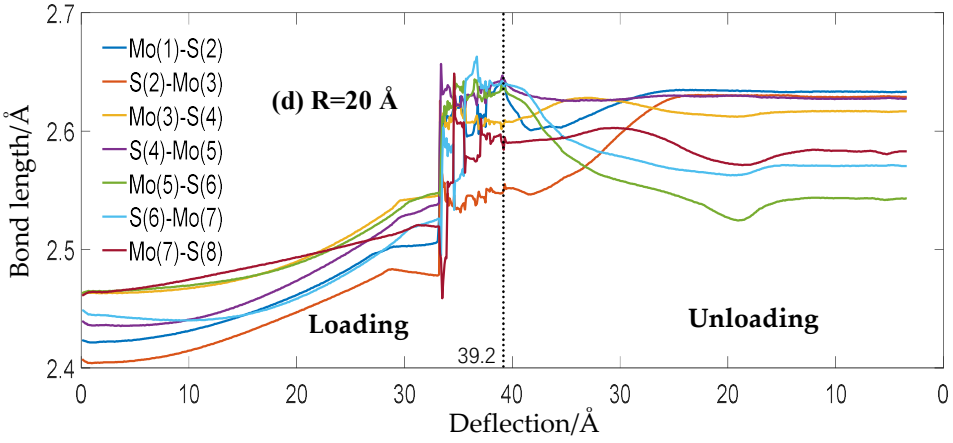
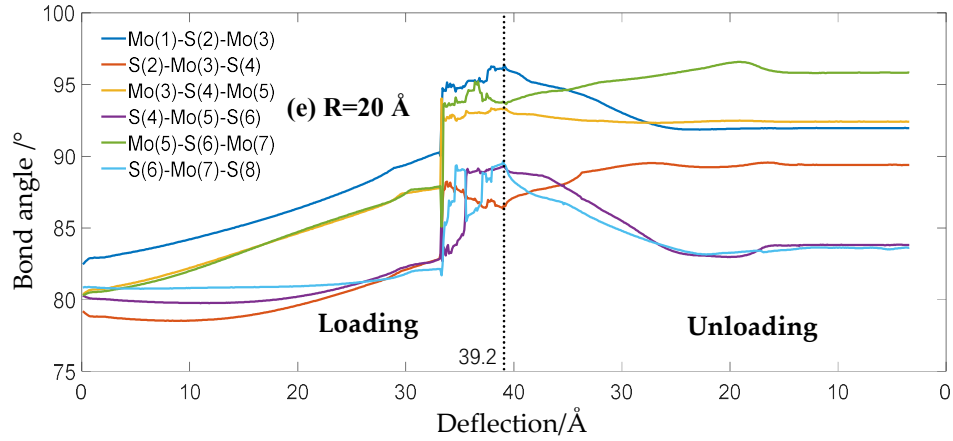
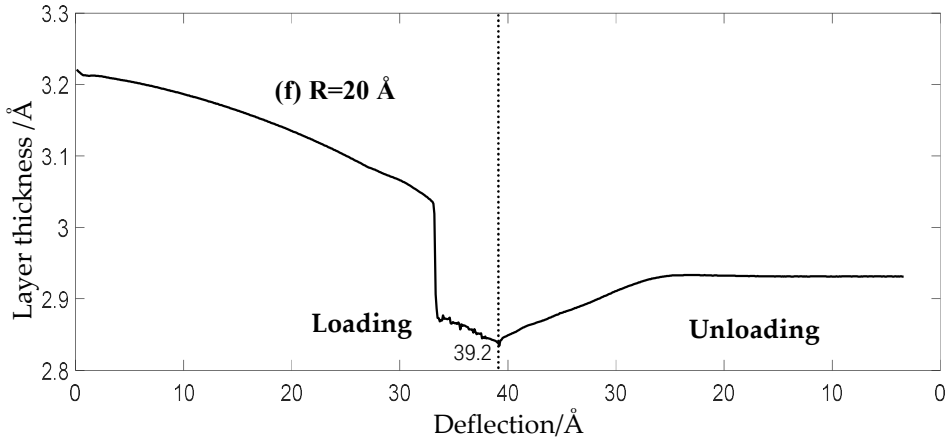


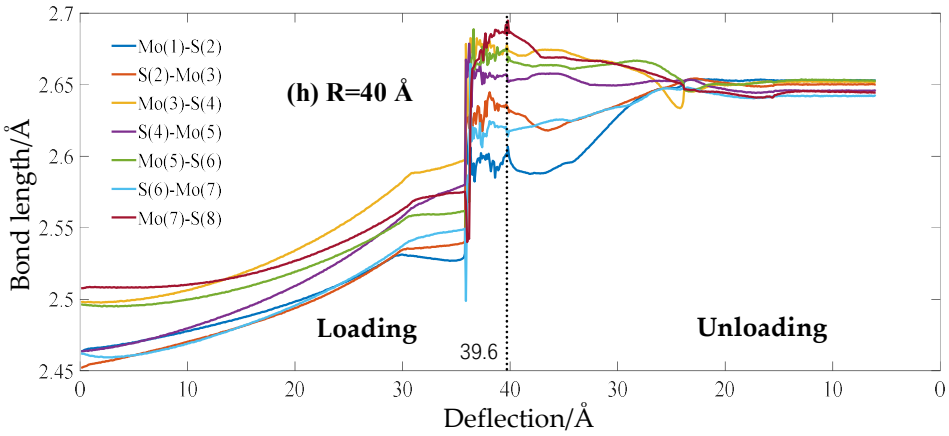

Mo(1)-S(2)-Mo(3)
S(2)-Mo(3)-S(4)
Mo(3)-S(4)-Mo(5)
S(4)-Mo(5)-S(6)
Mo(5)-S(6)-Mo(7)
S(6)-Mo(7)-S(8)
(b) R=15 Å
Loading
Unloading
40.5
Bond angle /°
Deflection/Å

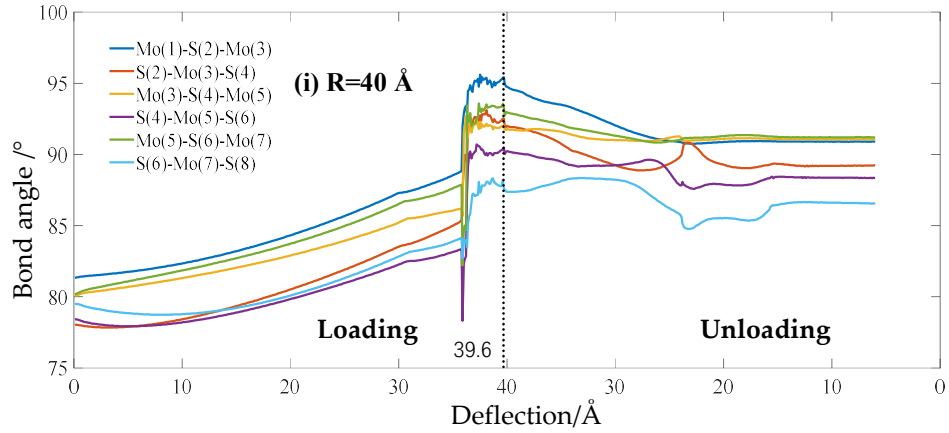

(c) R=15 Å
Loading
Unloading
40.5
Layer thickness /Å
Deflection/Å


Mo(1)-S(2)
S(2)-Mo(3)
Mo(3)-S(4)
S(4)-Mo(5)
Mo(5)-S(6)
S(6)-Mo(7)
Mo(7)-S(8)
(d) R=20 Å
Loading
Unloading
39.2
Bond length/Å
Deflection/Å


Mo(1)-S(2)-Mo(3)
S(2)-Mo(3)-S(4)
Mo(3)-S(4)-Mo(5)
S(4)-Mo(5)-S(6)
Mo(5)-S(6)-Mo(7)
S(6)-Mo(7)-S(8)
(e) R=20 Å
Loading
Unloading
39.2
Bond angle /°
Deflection/Å


(f) R=20 Å
Layer thickness /Å
Deflection/Å
Loading
Unloading
39.2


(h) R=40 Å
Bond length/Å
Deflection/Å
Mo(1)-S(2)
S(2)-Mo(3)
Mo(3)-S(4)
S(4)-Mo(5)
Mo(5)-S(6)
S(6)-Mo(7)
Mo(7)-S(8)
Loading
Unloading
39.6


(i) R=40 Å
Bond angle /°
Deflection/Å
Mo(1)-S(2)-Mo(3)
S(2)-Mo(3)-S(4)
Mo(3)-S(4)-Mo(5)
S(4)-Mo(5)-S(6)
Mo(5)-S(6)-Mo(7)
S(6)-Mo(7)-S(8)
Loading
Unloading
39.6

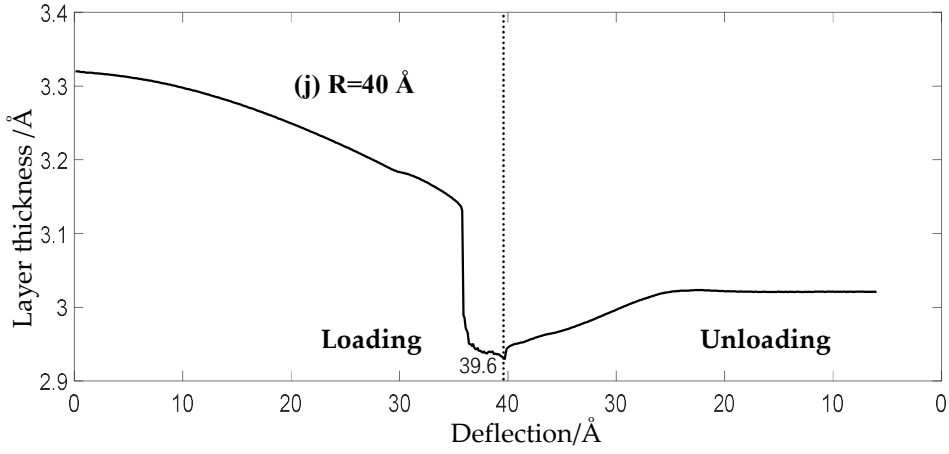

(j) R=40 Å
Layer thickness /Å
Deflection/Å
Loading
Unloading
39.6

Figure 1. The Mo-S and S-Mo bond lengths (a, d and h), S-Mo-S bond angles and Mo-S-Mo angles (b , e and i), and layer thickness of S-S (c, f and j) versus deflection during the loading process and unloading process with indenter radii of 15 Å, 20 Å and 40 Å (The labeled atoms are shown in Figure 3.).