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

Supporting information for

Structural evolution and mechanical stabilities of head-to-side nanowelding of Cu-Ag bimetallic nanowires via atomistic simulations

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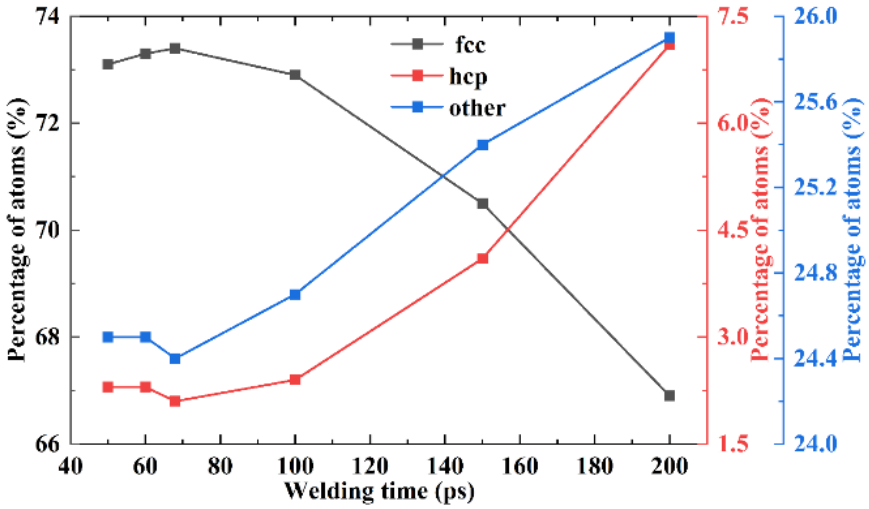

Figure S1. Effect of welding time on percentage of fcc and hcp atoms of joined nanowire after holding process

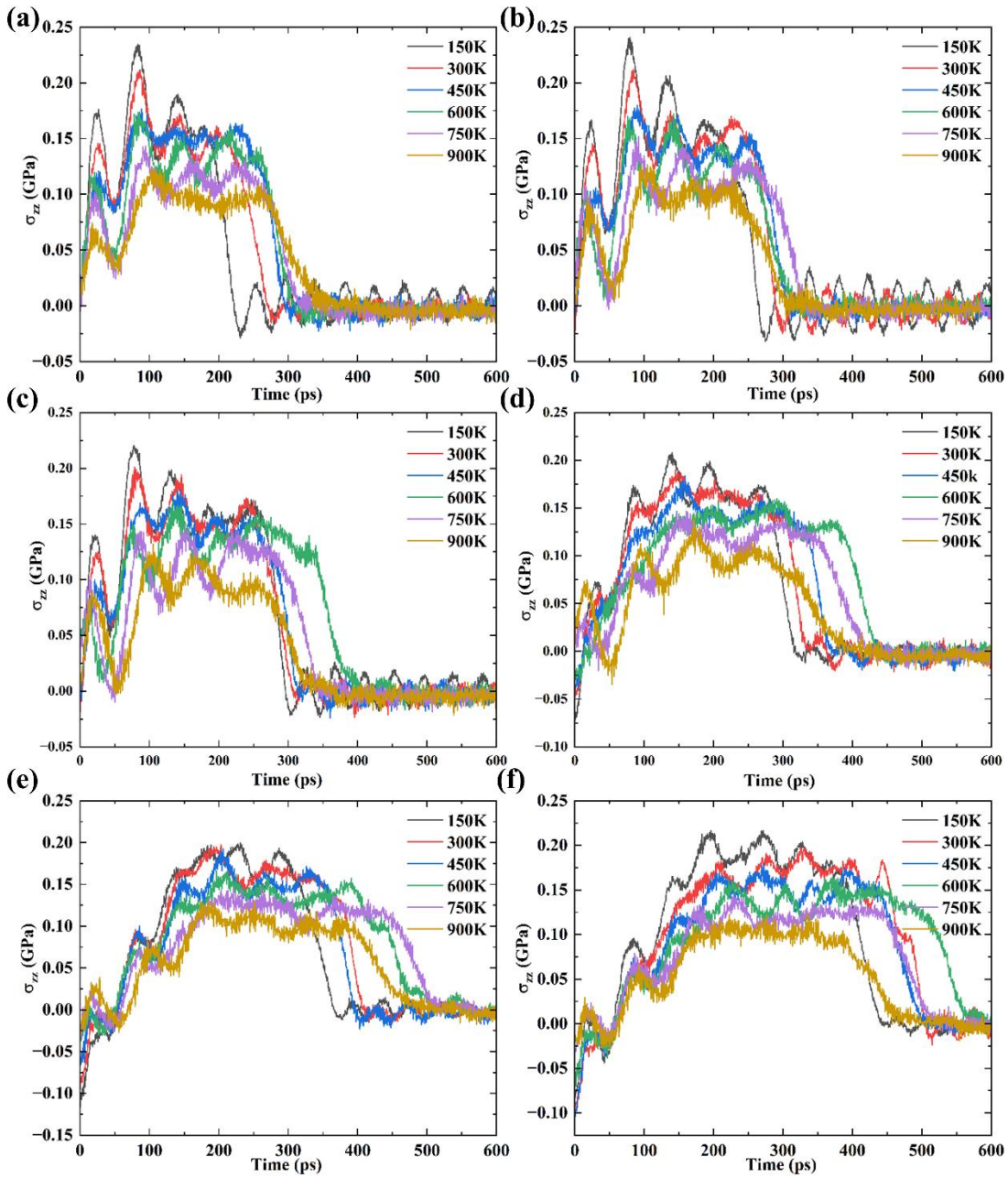

Figure S2. Variation of stress tensor of simulation system with time during stretching process along Z-direction. The welding time is (a) 50 ps, (b) 60 ps, (c) 68 ps, (d) 100 ps, (e) 150 ps and (f) 200 ps, respectively.

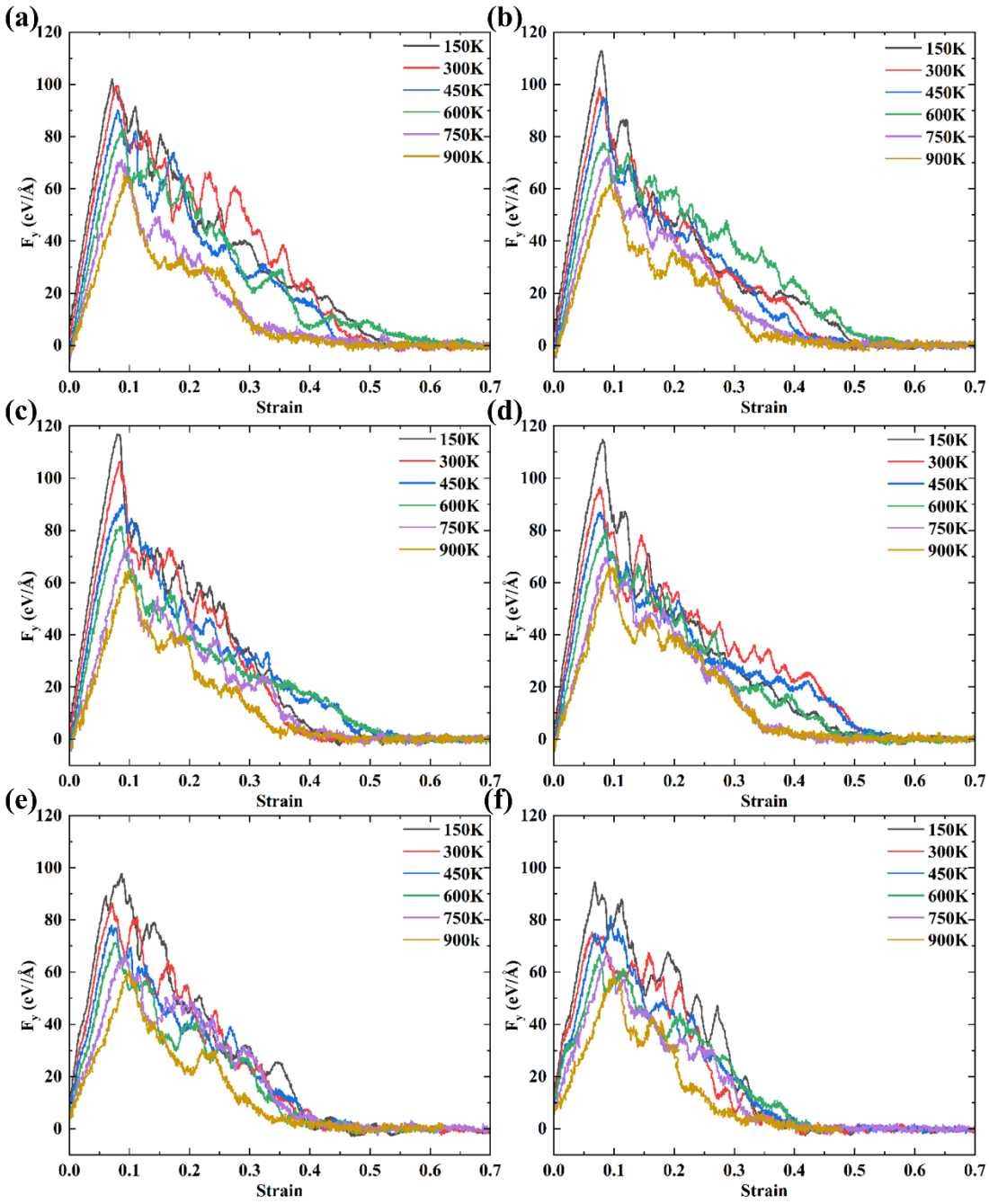

Figure S3. Variation of $F_y - \varepsilon$ curves under uniaxial tensile strain along Y-direction. The welding time is (a) 50 ps, (b) 60 ps, (c) 68 ps, (d) 100 ps, (e) 150 ps and (f) 200 ps, respectively.

Table S1 Simulation parameters of effect of welding time

Group No.	Welding time (ps)	Holding time (ps)	Stretching time (ps)	Stretching direction	Welding velocity (m/s)	Stretching velocity (m/s)	Welding temperature (K)
i	50 60 68 100 150 200	100	600	*Z*-direction	30	30	300
ii	50 60 68 100 150 200		800	*Y*-direction			

Table S2 Simulation parameters of effect of welding temperature

Group No.	Welding time (ps)	Holding time (ps)	Stretching time (ps)	Stretching direction	Welding velocity (m/s)	Stretching velocity (m/s)	Welding temperature (K)
iii	50-200	100	600	*Z*-direction	30	30	150
			800	*Y*-direction			
iv			600	*Z*-direction			450
			800	*Y*-direction			
v			600	*Z*-direction			600
			800	*Y*-direction			
vi			600	*Z*-direction			750
			800	*Y*-direction			
vii			600	*Z*-direction			900
			800	*Y*-direction			