

## Supporting Information

### Reaction mechanism of aluminum nanoparticles in explosives under high temperature and high pressure by shock loading

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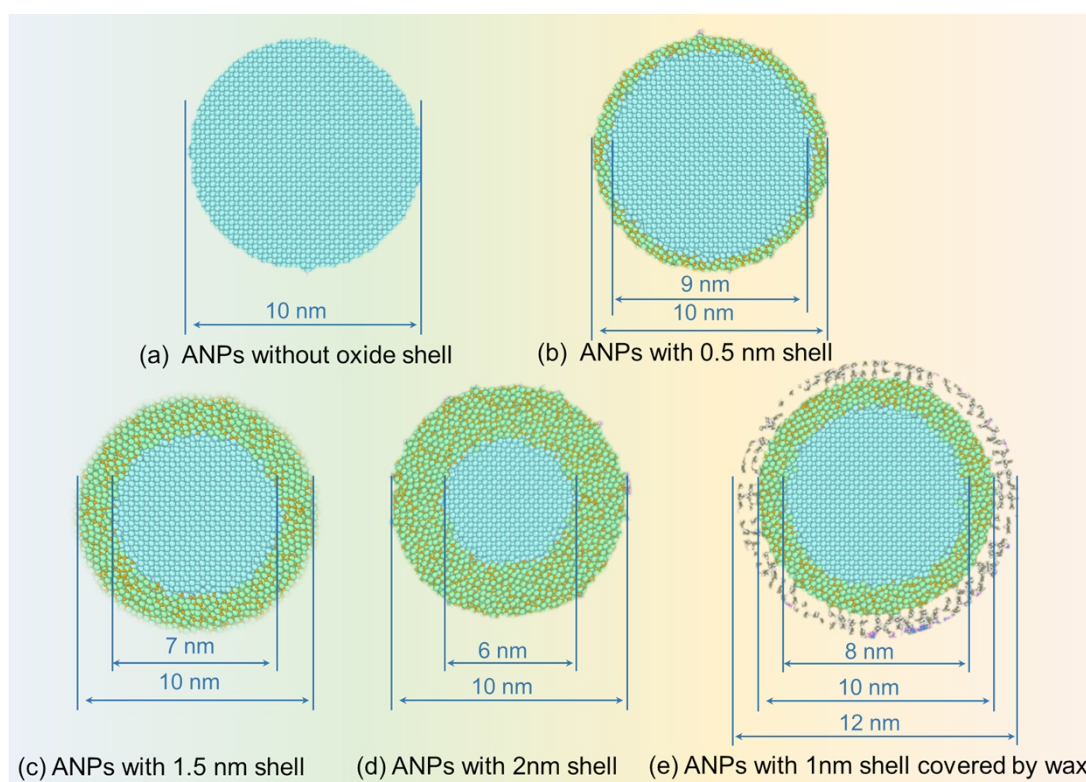


Figure S1 ANPs without an oxide shell, with 0.5-nm, 1.5-nm, and 2-nm oxide shells, and with a 1-nm oxide shell covered by wax.

Table S1 Pressures at which the supercell was compressed to the maximum state under shock loading at various velocities.

Velocity /(m·s <sup>-1</sup> )	Pressure/GPa				Average Pressure
	0.5-nm	1-nm	1.5-nm	2.5-nm	
1000	12.88335	12.08772	12.40477	12.44085	12.45417
1500	20.22598	19.72184	20.22808	20.12653	20.07561
2000	29.21973	29.38643	31.6445	31.32196	30.39315
2500	42.36073	42.25341	44.90553	44.15776	43.41936
3000	55.64892	56.22771	59.25028	60.40227	57.88229