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


# Investigation of the shock-induced chemical reaction (SICR) in Ni + Al nanoparticle mixtures

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Supplementary information contains 4 figures and a movie.

1. Supplementary figures

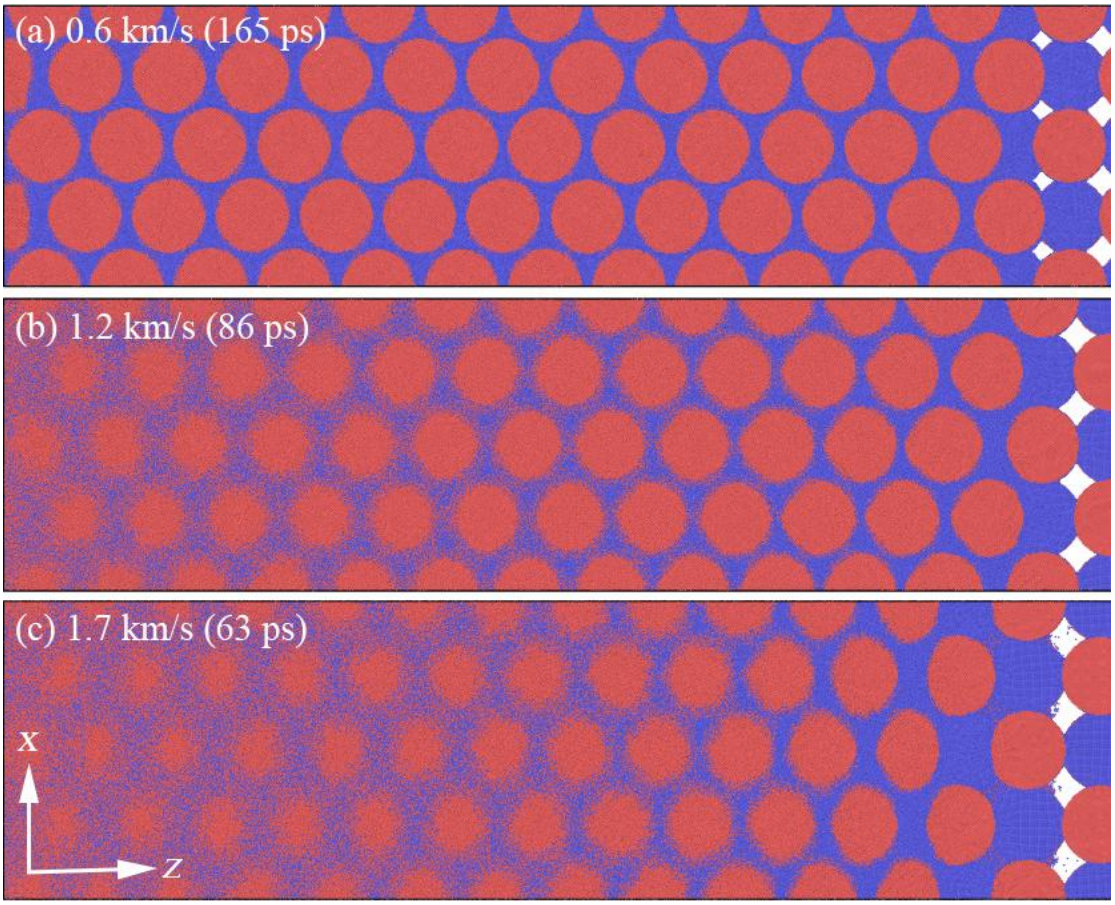


Figure S1. Particle-level responses of 10 nm case under shock loading for $U_p$ = 0.6, 1.2 and 1.7 km/s (from top to bottom). The piston on the left induced shock waves propagating from left to right.

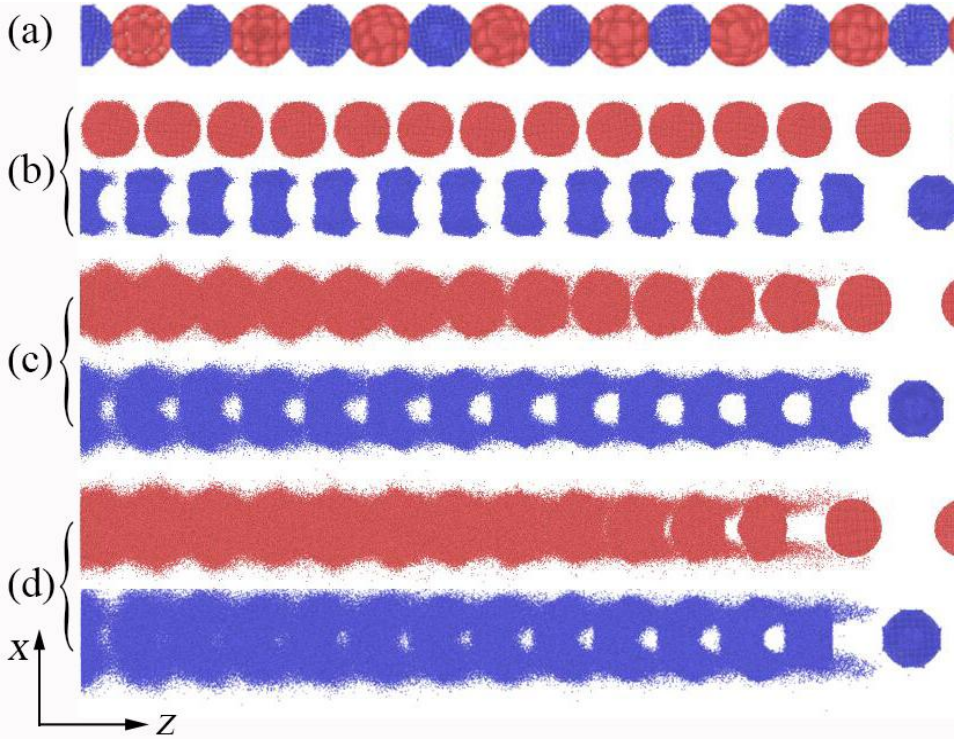


Figure S2. Particles extracted from the samples (10 nm case) that subjected to different piston velocities (corresponding to those in Figure S1). The extracted initial configuration before loading (0 ps) is shown in (a), and the separated Ni (red) and Al (blue) atoms under different piston velocities: (b) $U_p$ = 0.6 km/s (165 ps), (c) $U_p$ = 1.2 km/s (86 ps), and (d) $U_p$ = 1.7 km/s (63 ps).

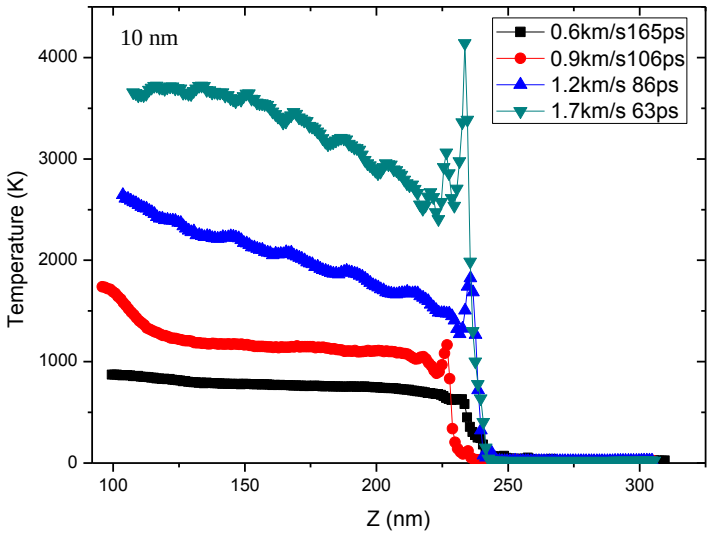


Figure S3. Temperature profiles for 10 nm case at various piston velocities during shock compression.

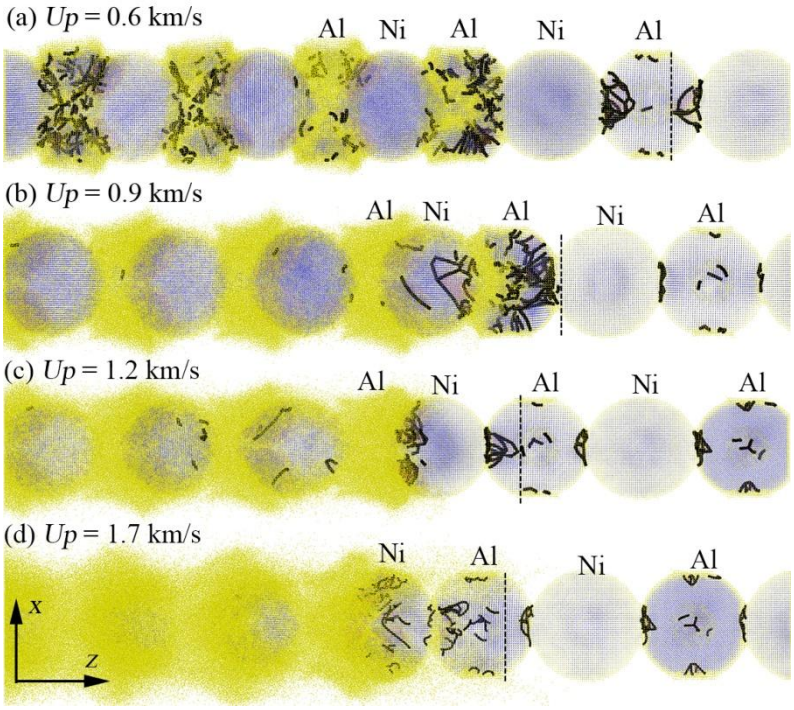


Figure S4. The evolution of dislocations in Ni and Al particles (10 nm case, the location of Ni and Al particles are indicated by "Ni" and "Al", respectively) at different loading velocities. The particles are extracted as describe in section 3.3, and only the particles in the vicinity of shock front are displayed. All the dislocations are colored in dark, while atoms are coded according to the structure type, as in Figure. 2(b). All atoms are zoomed out so that the dislocations can be clearly seen. The dashed line roughly indicates the position of shock wave front.

## 2. Supplementary movie

Movie 1 shows the evolution of dislocations in Ni and Al particles at $U_p$ = 1.2 km/s. The particles are extracted as describe in section 3.3, and only the particles in the vicinity of shock front are displayed (particles from left to right are Ni, Al, Ni, Al ...). All the dislocations are colored in dark, while atoms are coded according to the structure type, as in Figure. 2(b). All atoms are zoomed out so that the dislocations can be clearly seen.

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