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Supplementary Information

Shock-induced ejecta transport and breakup in reactive gas

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1. Interaction potential formulations and verifications

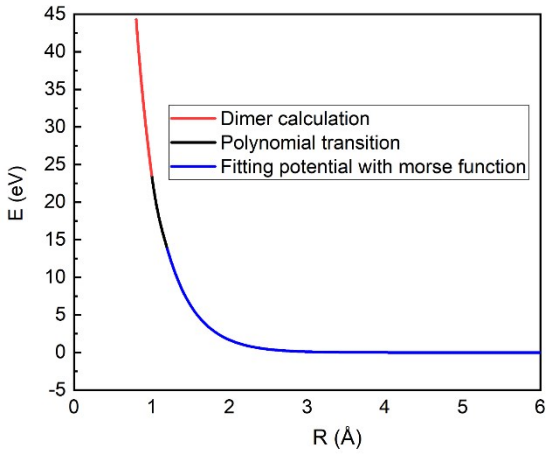

Fig. S1. Pair potential of Al-Ne obtained by fitting ab initial calculations.

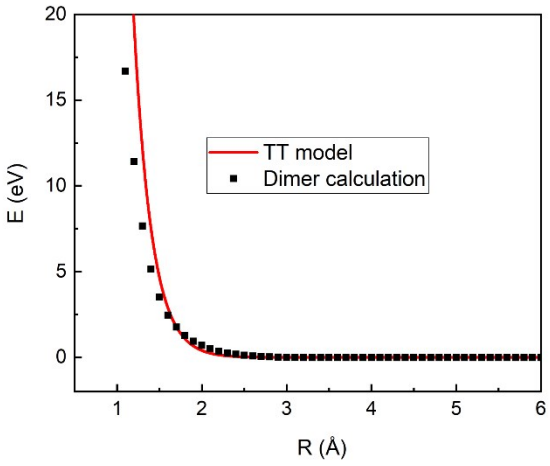

Fig. S2. Comparison of Ne-Ne potential between TT model and dimer calculation.

2. Comparisons for cases with different time step.

In order to test whether the time step has an influence on the calculation results, we recalculate the reactive case for gas density of 0.0029 g/cm^3 with smaller time step of 0.2 and 0.5 fs, respectively, and make comparison with the case of time step 1 fs. In particular, we chose 0.1 fs in the compression process of the bulk Al collision with wall. The total energy drifts upward slowly in our simulations as shown in Fig S3. It should be noted that the total energy drift does not exceed 0.2%. The rapid rise in the total energy at the beginning is caused by the compression process of the bulk Al collision with wall, which can be eliminated by using a time step of 0.1 fs. Noted that our main concern is the subsequent transport of ejecta in the gas, and more importantly, as shown in the later, this energy rise in the beginning does not influence the conclusion we made. As the time step decreases, the energy drift gradually decreases, and the energy remains almost conserved with time step of 0.2 fs. Now we are more concerned about whether the conclusion drawn in the case of 1 fs time step is consistent with that of 0.2 fs time step. Here, we compared ejecta velocity, shock position in the gas and temperature profile as shown in Fig S4, S5 and S6(a). It can be seen that for cases with different time step of 1 fs and 0.2 fs, the spike velocities and the positions of the shock wave generated in the gas almost overlap in the plots. Moreover, we can see that the temperature distributions (see Fig. R6(a)) are almost the same. All these comparisons show that the choice of time step of 1 fs in our simulations does not affect the conclusion we made, though the total energy drift upward slowly. Considering that the calculation is very time-consuming when using small time step, and even beyond our computation power, we think a time step of 1 fs is acceptable.

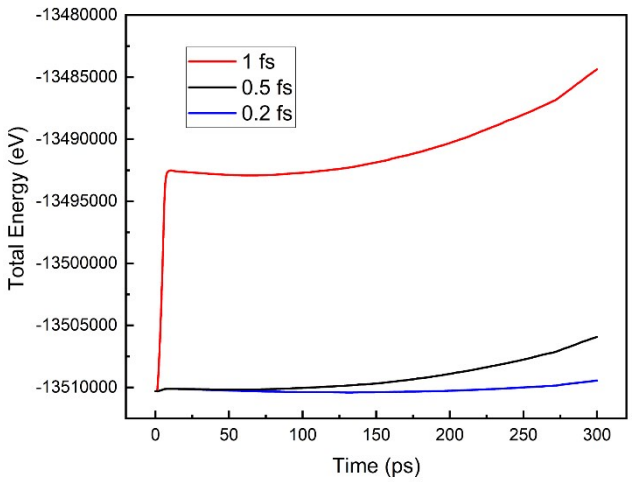

Fig. S3. The total energy vs time for test case of O gas density of 0.0029 g/cm^3 with different time step.

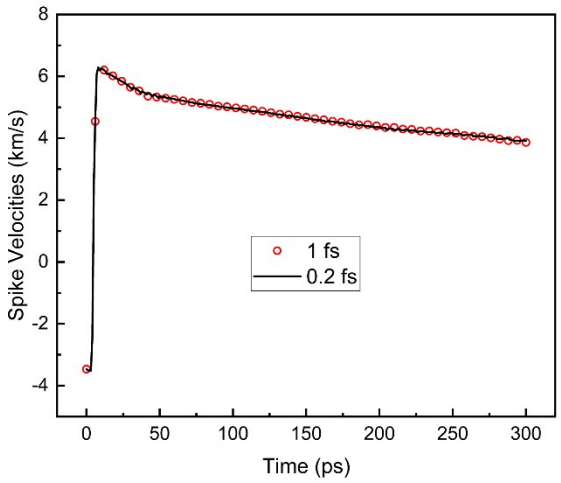

Fig. S4. Comparison of spike velocities for test case of O gas density of 0.0029 g/cm^3 with different time step.

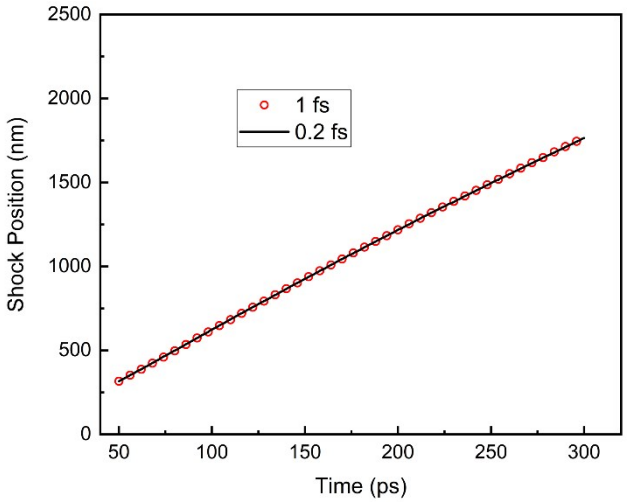

Fig. S5. Comparison of shock positions for test case of O gas density of 0.0029 g/cm^3 with different time step.

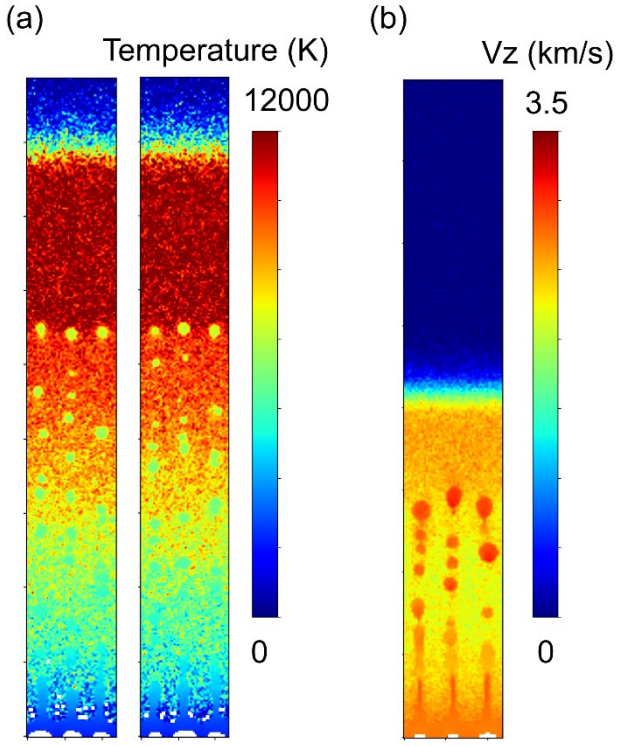

Fig. S6. (a) Comparison of Temperature distributions for test case of O gas density of 0.0029 g/cm^3 with different time step (left: 0.2 fs and right: 1 fs). (b) Velocity along z direction for case of Ne gas density of 0.0143 g/cm^3 at 200 ps.

3. Simulation results.

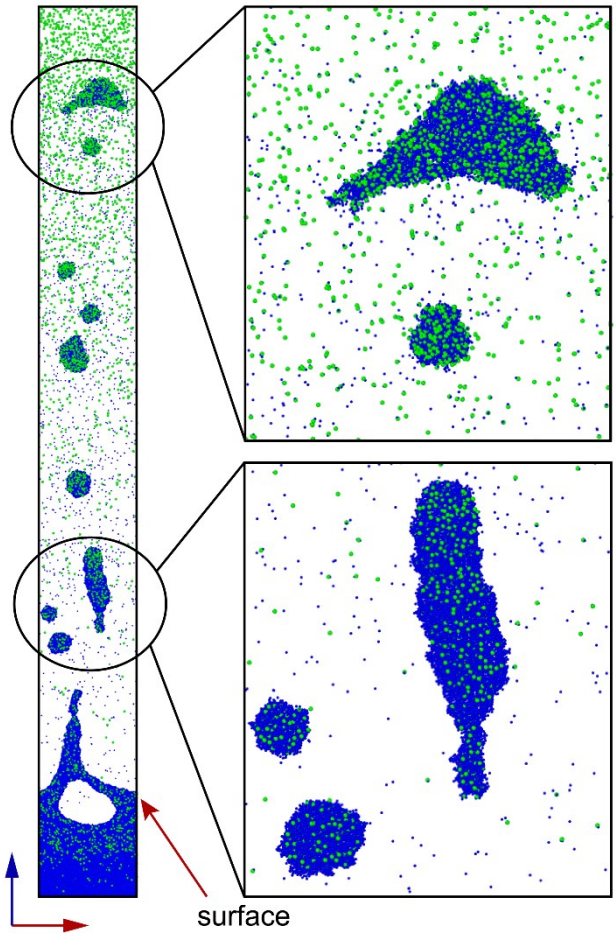

Fig. S7. The Atomic image of ejecta oxidation in O gas at 150 ps for the case of gas density of 0.0029 g/cm^3. Al and O atoms are colored in blue and green respectively.

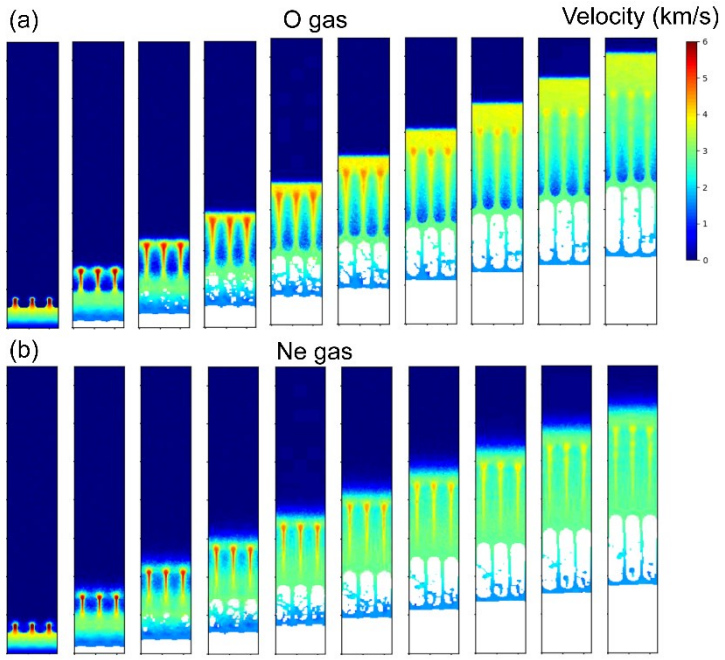

Fig. S8. Velocity contour plots of the time evolution of ejections from 10 ps to 100 ps at 10 ps intervals for case with initial gas density of 0.0143 g/cm^3.

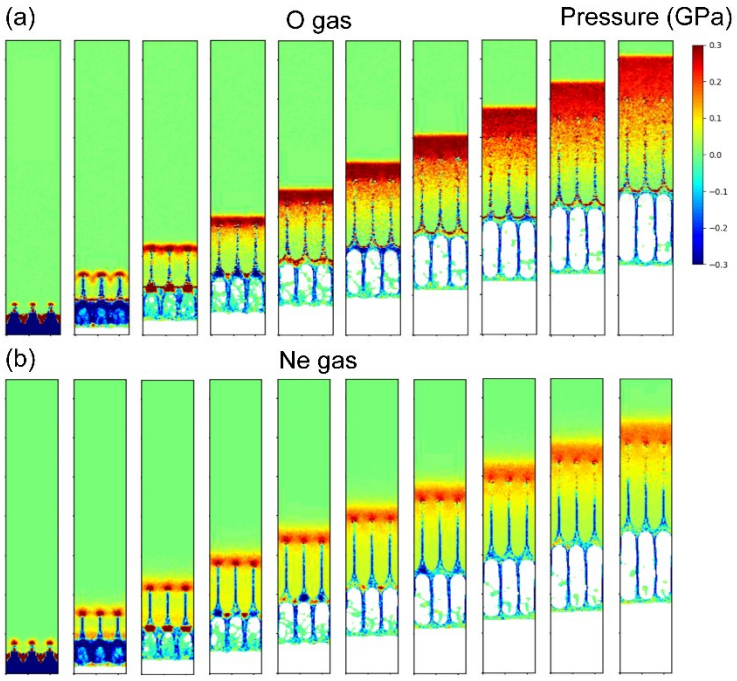

Fig. S9. Pressure contour plots of the time evolution of ejections from 10 ps to 100 ps at 10 ps intervals for case with initial gas density of 0.0143 g/cm^3.

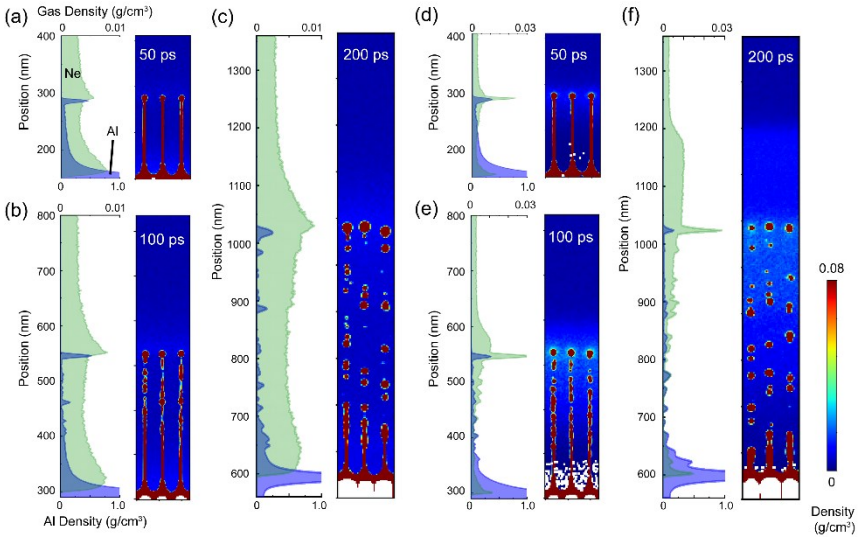

Fig. S10. Density contour plots of ejections transporting in (a)-(c) inert gas and (d)-(f) reactive gas at initial gas density of 0.0029 g/cm^3. The ejecta-gas mixing is illustrated by density plots shown as functions of distance for both Al and gas (Ne or O) on the left sides of the contour plots.

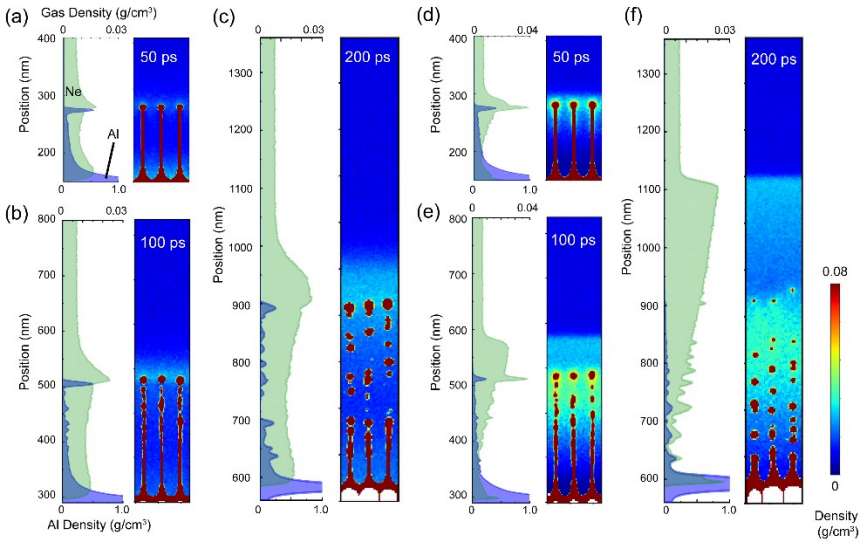

Fig. S11. Density contour plots of ejections transporting in (a)-(c) inert gas and (d)-(f) reactive gas at initial gas density of 0.0072 g/cm^3. The ejecta-gas mixing is illustrated by density plots shown as functions of distance for both Al and gas (Ne or O) on the left sides of the contour plots.