Electronic Supplementary Information for

Shaped-Controlled Growth of Metal Nanoparticles: An Atomistic View

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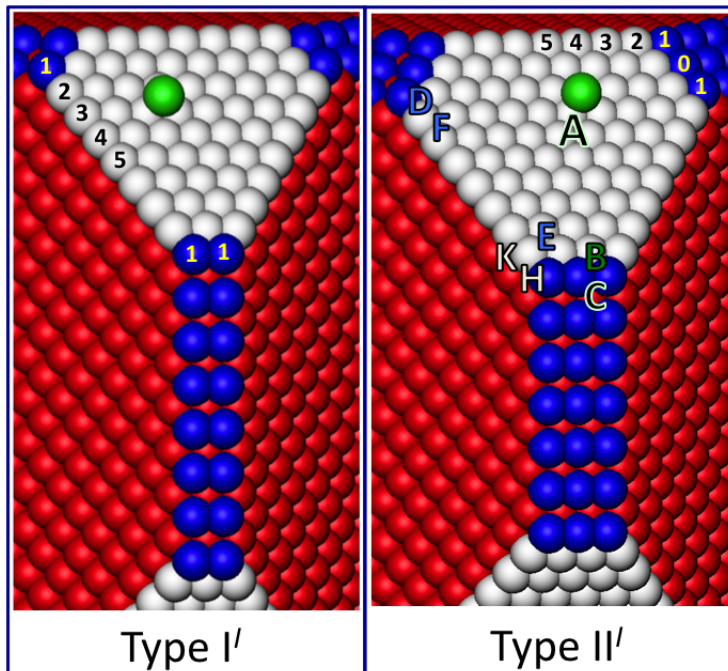*Sabancı University, Tuzla 34950 Istanbul, Turkey*

Fig. S1. The geometries of larger cubic Ag nano-clusters. The length of a side for each computational cells is 6.1 nm. The capital letters represent the selected adsorption sites and regarding adsorption energies are listed in Table S1.

Table S1. Adsorption energies, relative to the energy for the center site A, of various sites on the facets of cubic Ag clusters. For the selected adsorption sites (indicated in paranteses) see Fig. S1.

Adsorption site	Type I	Type II	Type I$'$	Type II$'$
Center on $\{111\}$ facet, *fcc* (A)	0.000	0.000	0.000	0.000
$\{110\}$ / $\{100\}$ submit on $\{111\}$ facet, *hcp* (D)	-0.012	-0.016	-0.015	-0.017
Edge on $\{111\}$ facet, *fcc* (E)	-0.017	-0.021	-0.018	-0.018
Edge on $\{111\}$ facet, *hcp* (F)	-0.004	——	-0.006	-0.007
Corner on $\{111\}$ facet, *fcc* (B)	-0.024	-0.018	-0.023	-0.014
Corner on $\{110\}$ facet, (C)	-0.541	-0.526	-0.540	-0.524
Edge on $\{100\}$ facet close to $\{110\}$ / $\{100\}$, (H)	-0.269	-0.270	-0.268	-0.268
Edge on $\{100\}$ facet, (K)	-0.260	——	-0.258	-0.258

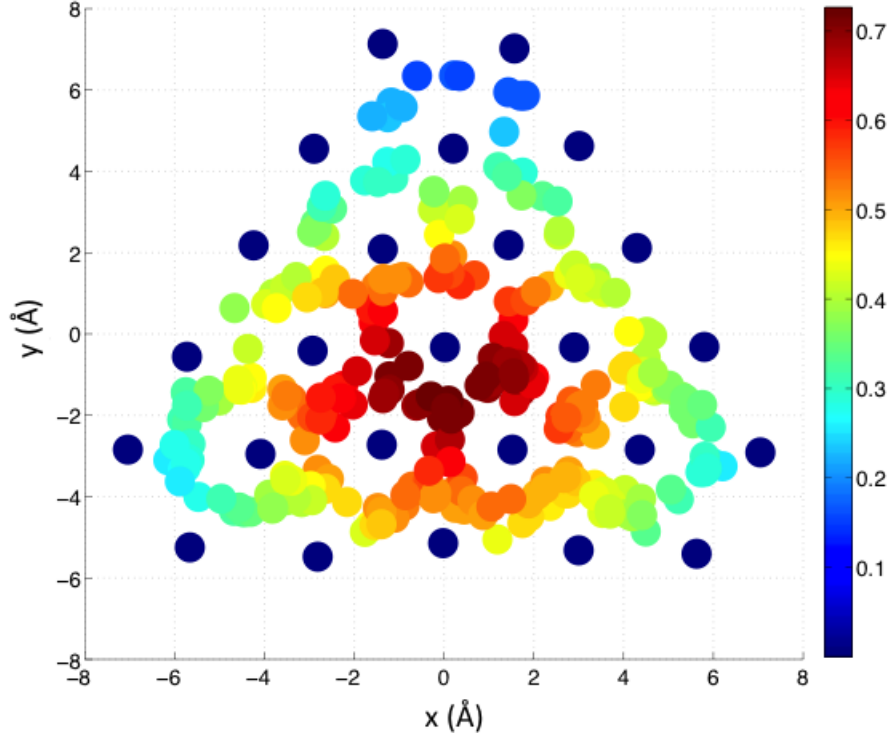Fig. S2. The landing position distribution of adatoms on the {111} facet of Type I system. Dark blue circles denote atomic positions of the {111} facet whereas the coded colors, ranging from light blue to red, represent the probability of the adatom landing on specific sites on the corner facet. The relation between the color code and the probability is given by the scale on the right. Statistical distribution is over 300 repeated single atom events at 500 K.

Table S2. Average diffusion times for number of atoms resulting from 300 repeated simulations on various clusters type at 500 K.

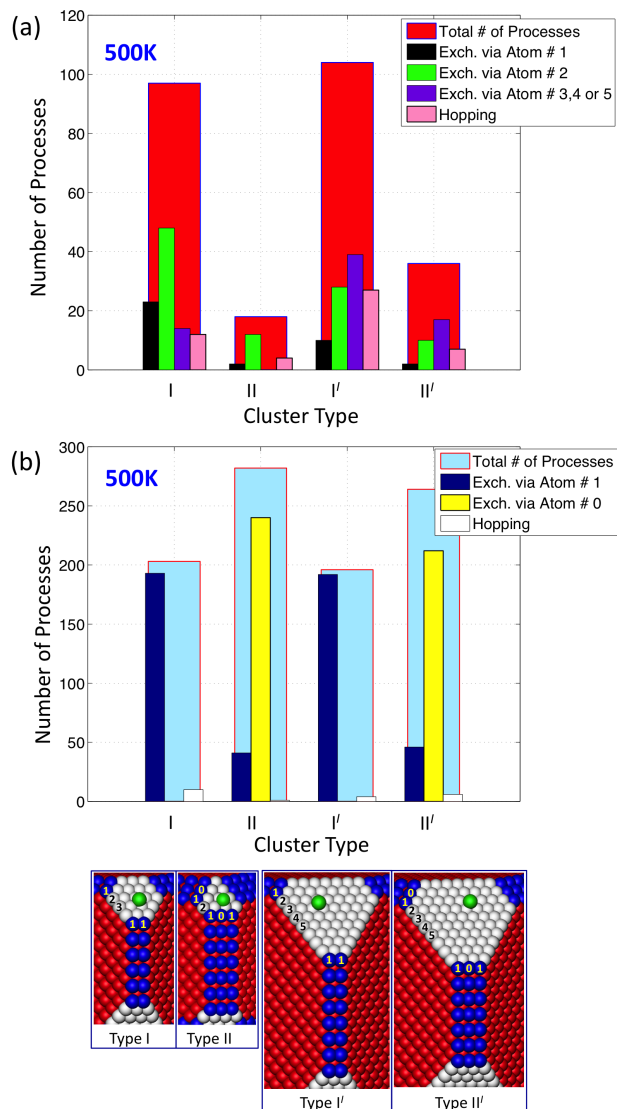| 500K	Type I	Type II	Type I′	Type II′
From (111) to (110)	(203) 254.1 ps	(282) 76.4 ps	(196) 646.6 ps	(264) 406.25 ps
From (111) to (100)	(97) 252.7 ps	(18) 106.9 ps	(104) 636.8 ps	(36) 512.90 ps

Fig. S3. Statistical characteristics of 300 repeated events on various cluster types at 500 K: (a) number of diffusion events from {111} to {100} facets, (b) number of diffusion events from {111} to {110} facets, (c) corner views of the cluster types.
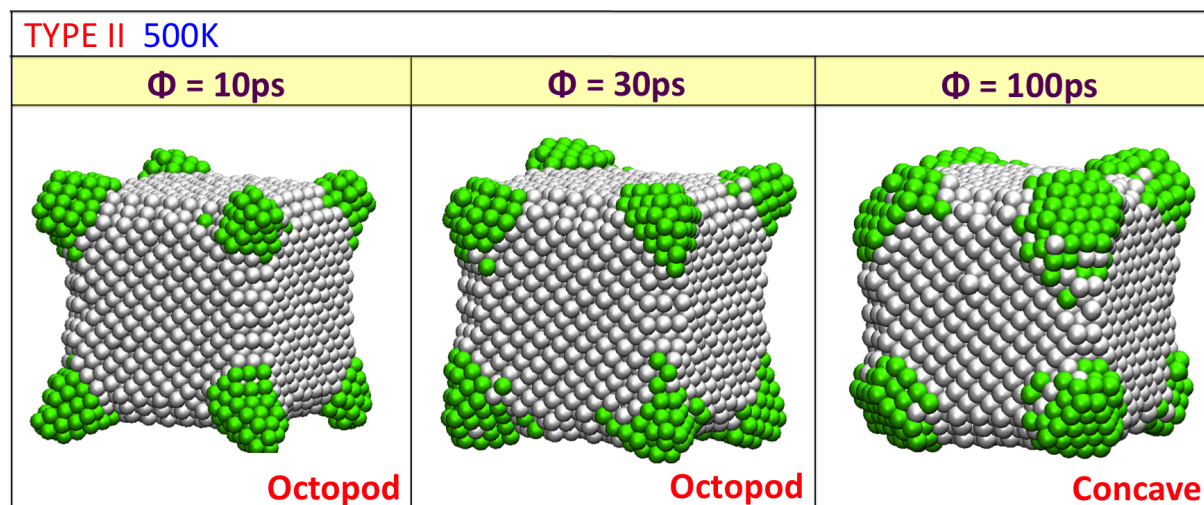
Fig. S4. Two specific growth modes of cubic-Ag Type II system obtained at 500 K: Octopod with deposition rates 10 ps or 30 ps and concave with a deposition rate of each atom 100 ps.