Supplementary Material

S1. Sutton-Chen Potential

In the Sutton-Chen form of EAM potential, the total internal energy of pure metals was expressed in terms of Finnis-Sinclair form, as follows:

$$E = \varepsilon \left[\frac{1}{2} \sum_{i \neq j} \sum V(r_{ij}) - c \sum_i \sqrt{\rho_i} \right]$$

(1)

where $V(r) = (a/r)^n$ is the pair potential and $\rho_i = \sum_{j \neq i} (a/r_{ij})^m$ is the electron density function. Here, r_{ij} is the spacing between atoms i and j, c is a positive dimensionless parameter, ε is a parameter with unit of energy, a is the lattice parameter and m and n are positive integers. The parameters ε, c, m and n as well as lattice parameter a and cohesive energy E_c for Ni, Ag and Pt are listed in Table 1.

	ε (eV)	c	m	n	a	E_c (eV)
Ni	1.5713×10^{-2}	39.755	6	9	3.52	4.44
Ag	2.5415×10^{-3}	145.658	6	12	4.09	2.96
Pt	1.9835×10^{-2}	34.428	8	10	3.92	5.86

Table 1 Potential parameters for pure fcc metals Ni, Ag and Pt [58, 59]

For an A-B alloy system, parameters ε^{AA}, c^{AA}, m^{AA}, n^{AA}, a^{AA} and ε^{BB}, c^{BB}, m^{BB}, n^{BB}, a^{BB} are simply taken with the parameters of pure A metal and pure B metal from Table 1, respectively. A simple arithmetic and geometric means are employed to estimated the parameters for A-B interactions, i.e.,

$$m^{AB} = \frac{1}{2}\left(m^{AA} + m^{BB}\right)$$

$$n^{AB} = \frac{1}{2}\left(n^{AA} + n^{BB}\right)$$

$$a^{AB} = \left(a^{AA}a^{BB}\right)^{1/2} \tag{2}$$

$$\varepsilon^{AB} = \left(\varepsilon^{AA}\varepsilon^{BB}\right)^{1/2}$$

S2. Van Hove Correlation Function

The self-part of the van Hove correlation function $G_s(r, \Delta t)$ describes the probability distribution of the position r of an atom after a time Δt. Mathematically, the van Hove correlation function can be written as:

$$G_s(\mathbf{r}, \Delta t) = \frac{1}{N}\left\langle \sum_{i=1}^{N} \delta\left(\mathbf{r}_i(\Delta t) - \mathbf{r}_i(0) - \mathbf{r}\right)\right\rangle.$$

When Δt is small, $G_s(r, \Delta t)$ is Gaussian, meaning the atom undergoes harmonically localized motion. As the time interval Δt increases, generally we expect to observe non-Gaussian behavior. By looking at $G_s(r, \Delta t)$ at different time intervals, we can trace the path that the atom takes as it moves through the system and quantify these changes in terms of atomic displacement.

Figure S1 shows the self-part of the van Hove correlation function of N=2899 NP at $T = 1400$ K with $\Delta t = 20$ ps. The displacement for each atom has been resolved into two components, the displacement along radial direction $r_{//}$ and the displacement perpendicular to the radial direction $r_\perp$. As discussed in above, the multiple peaks centering at successive nearest-neighbor distances in $G_s(r)$ implies a 'hopping' motion to preferentially quantized distances. However, this feature disappears when the temperature arises above the melting point, as shown in the inset. Since mobile atoms predominantly

occur on the NP surface, it is perhaps not surprising to see that the displacement

perpendicular to the radial direction is the major contribution to the overall atomic
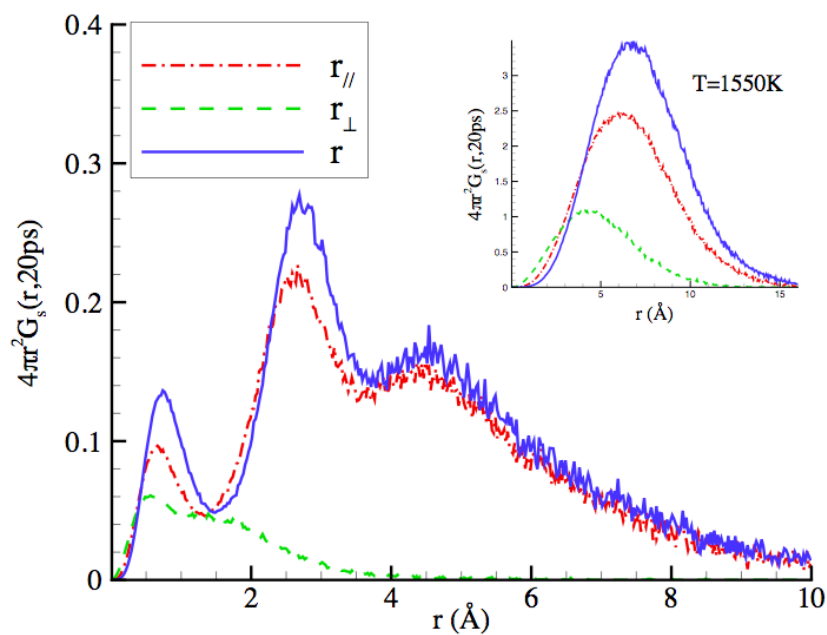
displacement.

Figure S1. The self-part of the van Hove correlation function of N=2899 NP at T=1400K with Δt = 20ps. The inset shows $G_s(r, \Delta t)$ of the same NP at T = 1550K.