In-Situ Observation of Plasmon Tuning in a Single Gold Nanoparticle During Controlled Melting
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Supporting Information

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Details on the simulation results

The simulation results shown in Fig. 5 were obtained using the Discontinuous Galerkin Time-Domain method [1, 2]. A mesh consisting of third order tetrahedral elements was used. For the spherical particle, we used a diameter of 80 nm, which is a typical value observed in the experiment. For the transformed particles, typical heights measured are around 110 nm. Assuming volume conservation and a prolate spheroidal shape, we arrive at short half-axes of 34 nm. To accurately model the particle geometry, elements sizes down to 5 nm were used, the entire setup consists of roughly 40.000 elements.

The permittivity of the gold particle was approximated by an analytical fit to measured values [3]. We used one Drude term plus three Lorentz terms

$$\varepsilon(\omega) = \varepsilon_\infty - \frac{\omega_D^2}{\omega(\omega + i\gamma_D)} + \sum_{i=1}^{3} \frac{\Delta_i \Omega_i^2}{\Omega_i^2 - i\Gamma\omega - \omega^2} \qquad (1)$$

which gives a reasonably accurate approximation. For the substrate, we assumed a permittivity of 2.32.

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	ε_∞	ω_D (s^{-1})	γ_D (s^{-1})
Drude	6.40	$1.37 \cdot 10^{16}$	$1.16 \cdot 10^{14}$
	Δ_i	Ω_i (s^{-1})	Γ_i (s^{-1})
Lorentz 1	$1.51 \cdot 10^{15}$	$4.42 \cdot 10^{15}$	$1.54 \cdot 10^{15}$
Lorentz 2	$1.02 \cdot 10^{15}$	$5.56 \cdot 10^{15}$	$1.83 \cdot 10^{15}$
Lorentz 3	$0.80 \cdot 10^{15}$	$6.72 \cdot 10^{15}$	$1.79 \cdot 10^{15}$

Table 1: Parameters for the Drude-Lorentz model used in the simulations

The particle was excited with a plane wave with a Gaussian profile in time, which is incident under an angle of 7° relative to the substrate, just as in the experiment.

References

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