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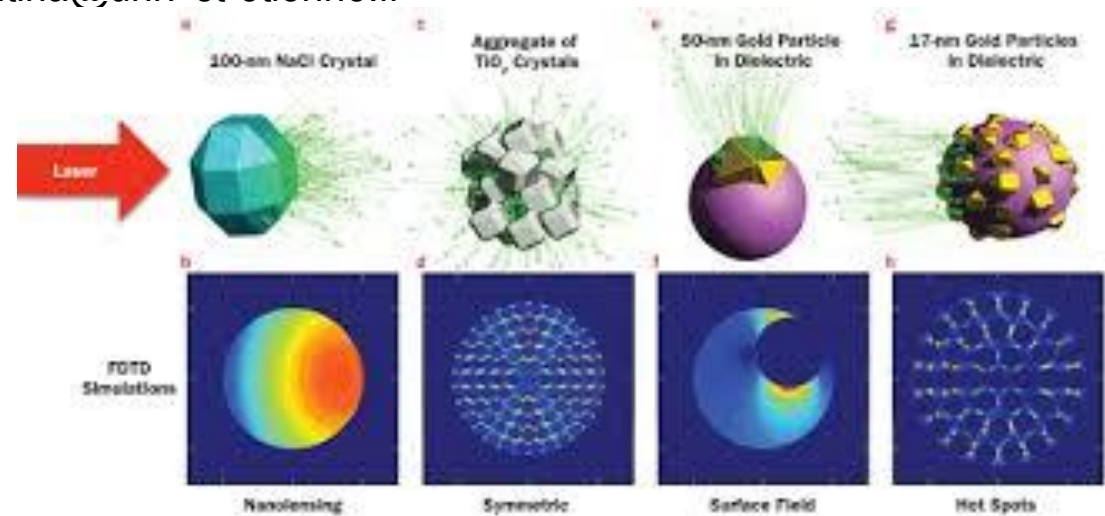
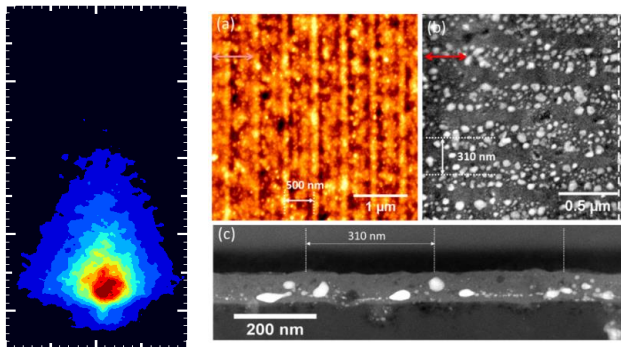
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Numerical simulation of laser interactions with surfaces and nanoparticles

Tatiana E. ITINA

Laboratoire Hubert Curien, UMR CNRS 5516, Saint-Etienne, France

tatiana.itina@univ-st-etienne.fr



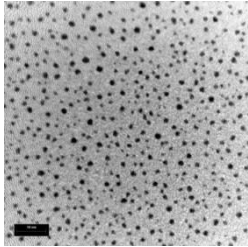
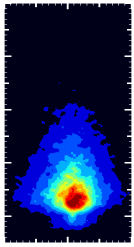
experiments : LP3, LabHC, ITMO

https://www.photonics.com/Articles/Nanoparticles_Probing_the_Plasma_Threshold/a57306

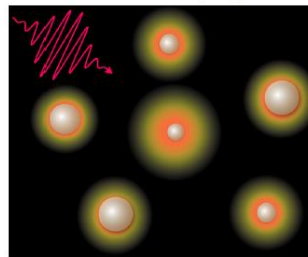
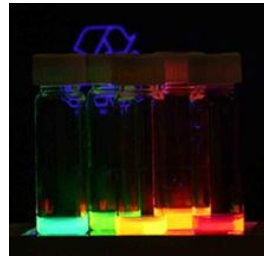
From laser plume to nanoparticles and nanostructures

Main research directions

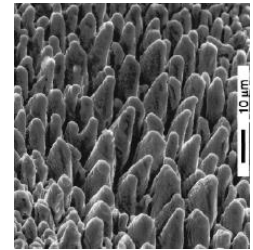
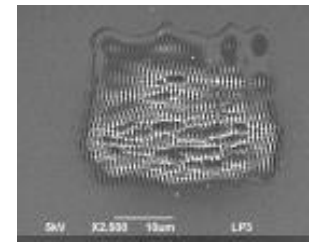
- **Laser-induced formation and modification of nanoparticles, monohybrids and nanostructures: modeling vs experiments**



Pulsed laser interactions

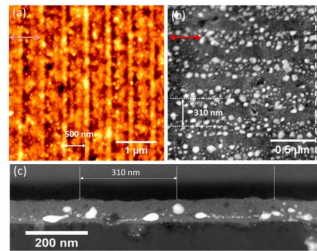


Laser ablation/fragmentation

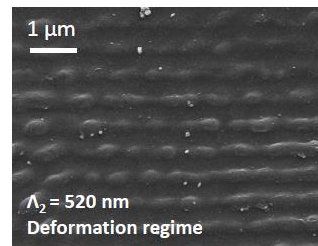


Laser-induced surface/volume structures

- **Laser-assisted formation of nanocomposite materials and metasurfaces**



Nanoparticles inside

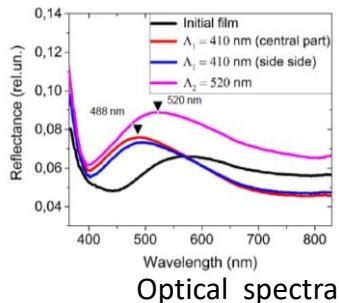


Nanoparticles on the surface

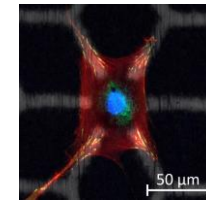
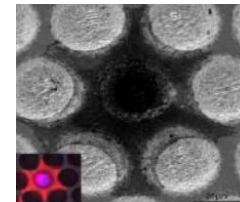
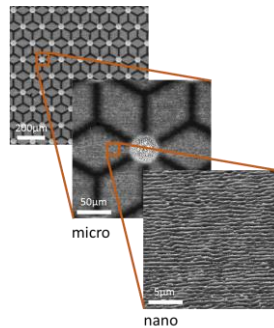


Hierarchical surface structures

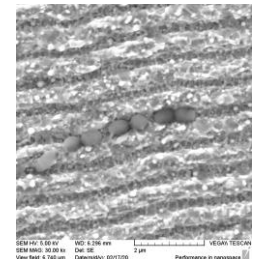
- **Properties and applications of the obtained materials: optical properties, wettability, cells and bacterial adhesion/repulsion**



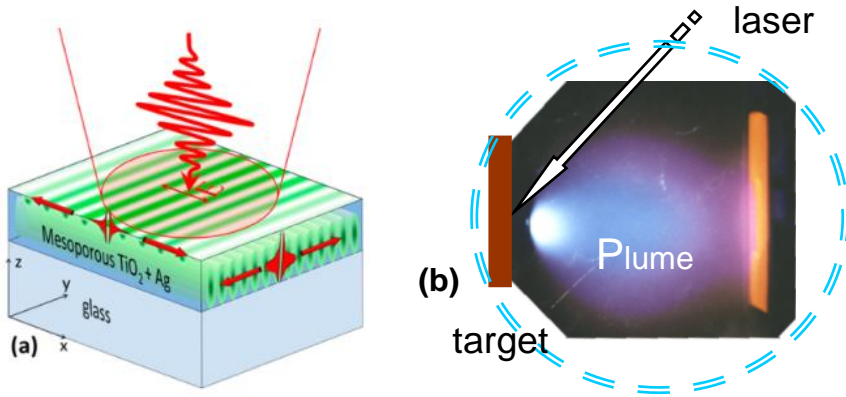
Wettability



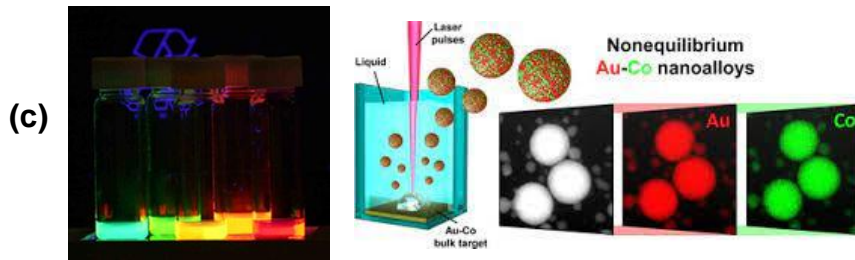
cell and bacteria adhesion on



Laser Interactions



In gas or in vacuum with different geometry



In liquids or in the presence of a colloids

Laser interaction commonly involve:

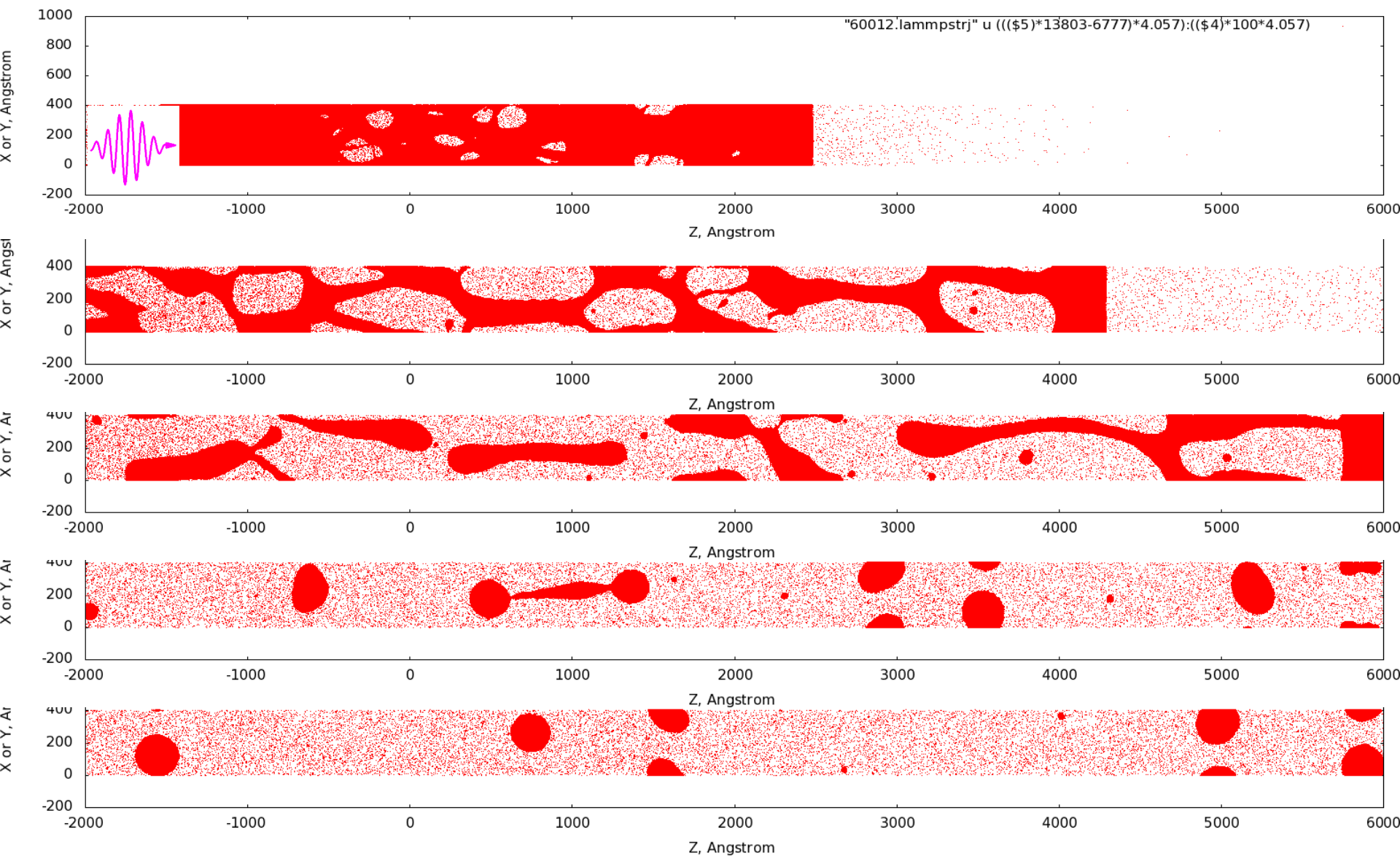
- Energy propagation, electronic excitation, light scattering, reflection and absorption
- Electron-phonon relaxation, heat diffusion, pressure wave propagation, rarefaction and tensile stress, phase transitions, mechanical fragmentation
- Material removal (ablation), plasma plume expansion, reactions, clustering, etc...
- Often multi-pulse irradiation is used with various scanning and focusing conditions

Laser-induced nanoparticle formation

- Green synthesis methods, bio-compatibility
- Control over NP properties
- Scaling-up possibilities
- Possibility to create stable ultra-structures, nanoalloys, hybrids, etc.
- **Additional laser-particle interactions involve many physical and chemical processes**



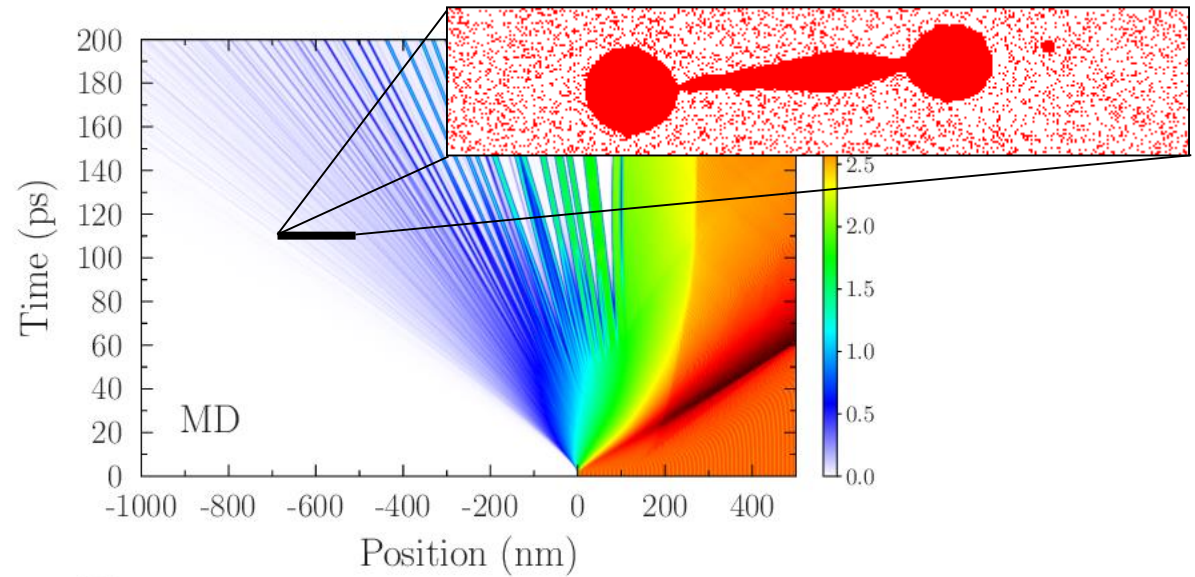
Ablation & Nanoparticles (10M atoms, $F=1 \text{ J/cm}^2$, Al)



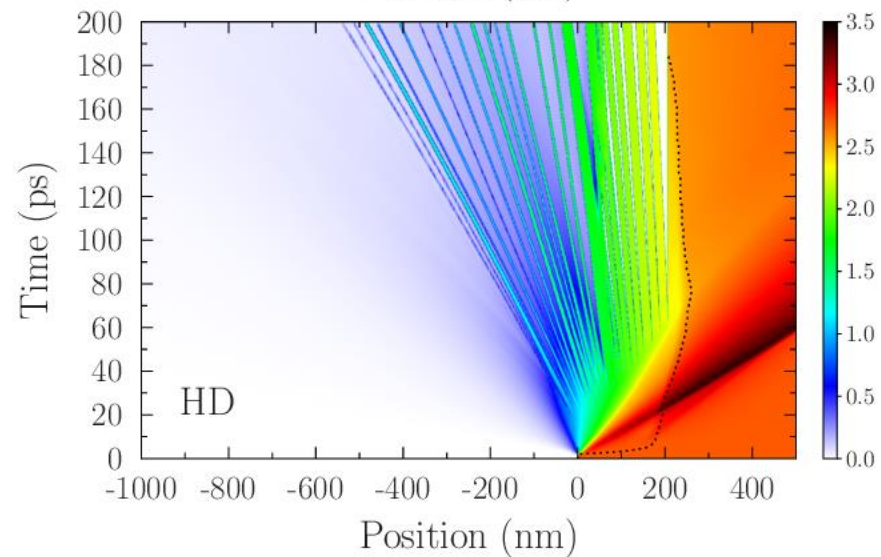
Density

$$\text{Al}, F = 2 \text{ J/cm}^2$$

TTM-MD

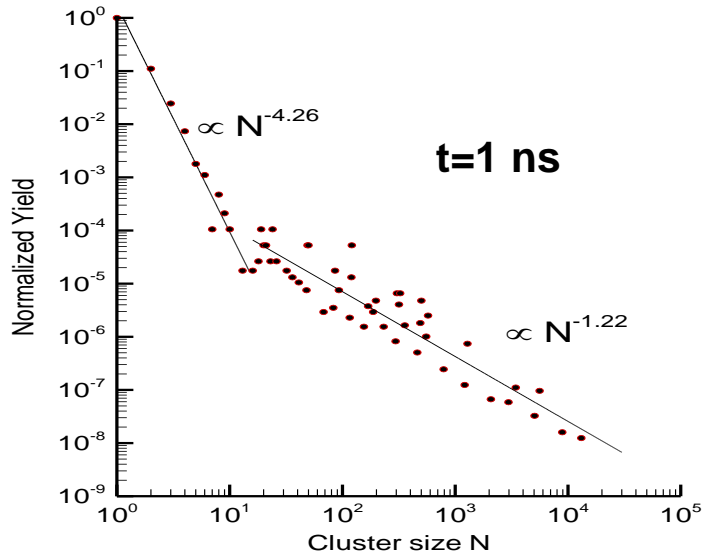


Hydrodynamics

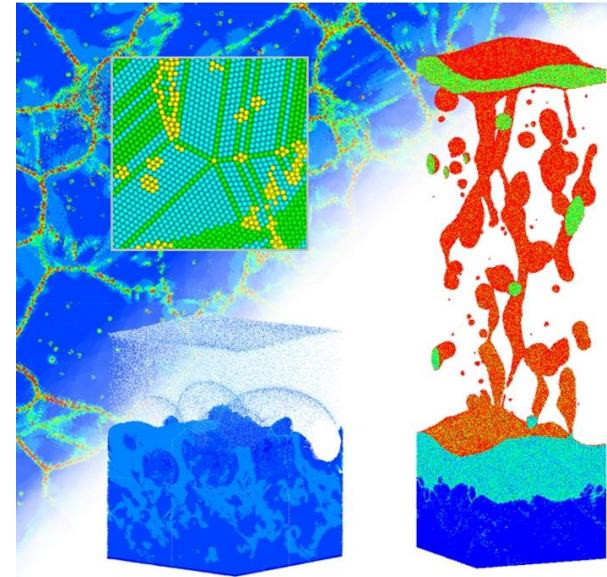
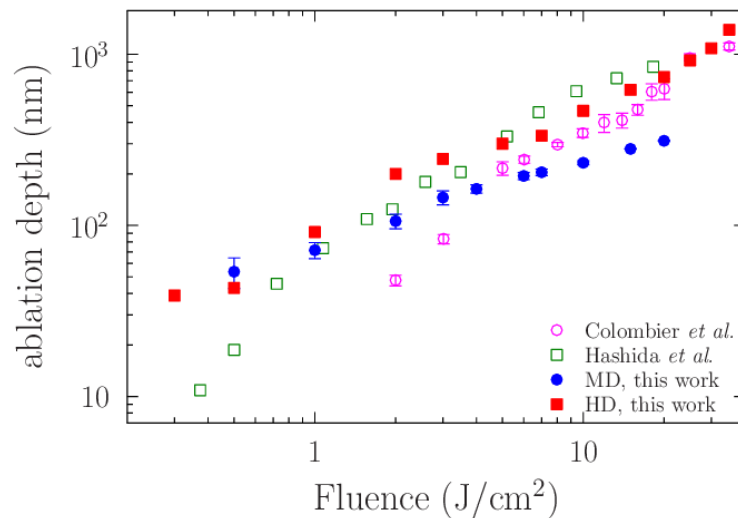


Molecular Dynamics Simulations

Allow to get nanoparticle size distributions and describe non-equilibrium processes



$\tau = 15 \text{ ps}$, $F \sim 2 \text{ Fth}$, $40 \times 10 \text{ nm}$, $t = 1 \text{ ns}$

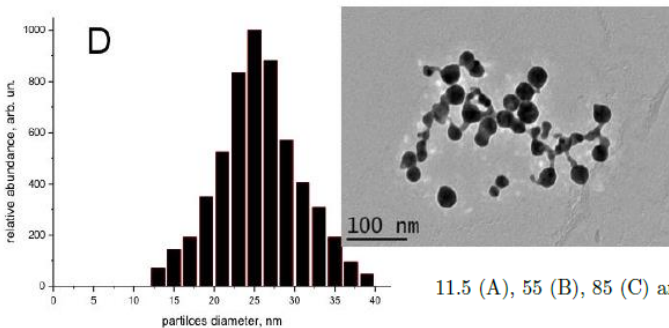
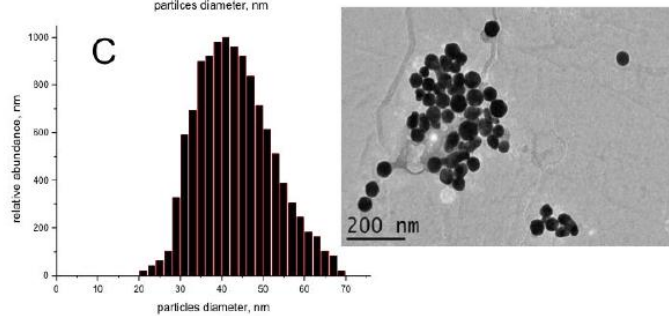
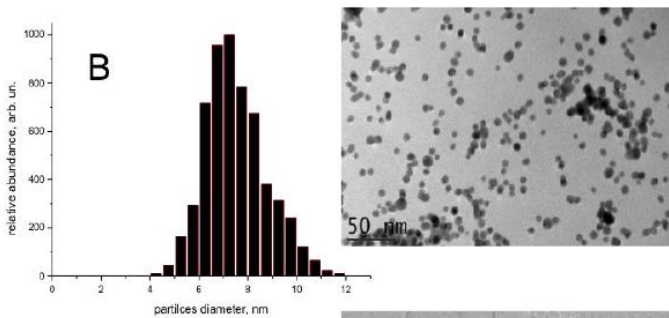
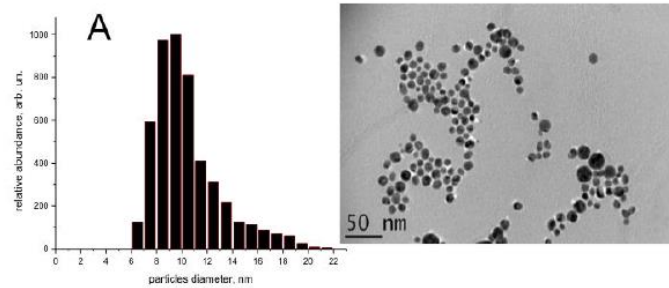


Collaboration with L.V. Zhigilei et al. (Virginia State University, USA)

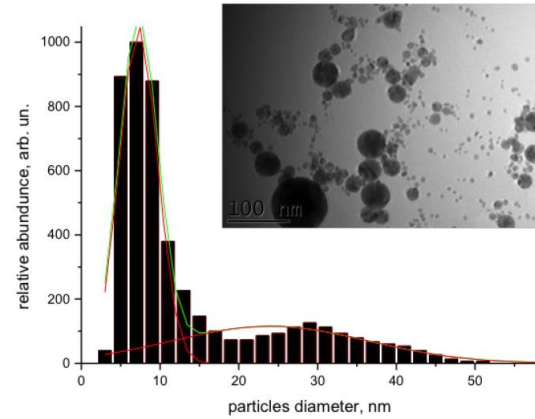
Practically all the molten material is ablated

$$Labl \sim L_0 \ln(F_{abs}/F_0), \quad E > E_b$$

Non-linear Effects in fs Laser Interactions with Au NPs



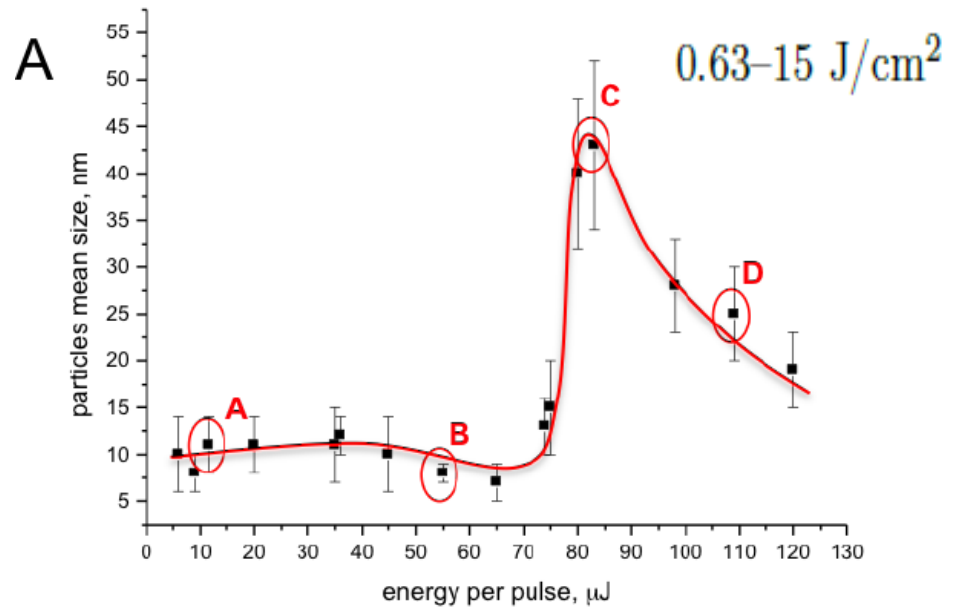
11.5 (A), 55 (B), 85 (C) and 109 (D) μJ



*Upon ablation
1064 nm*

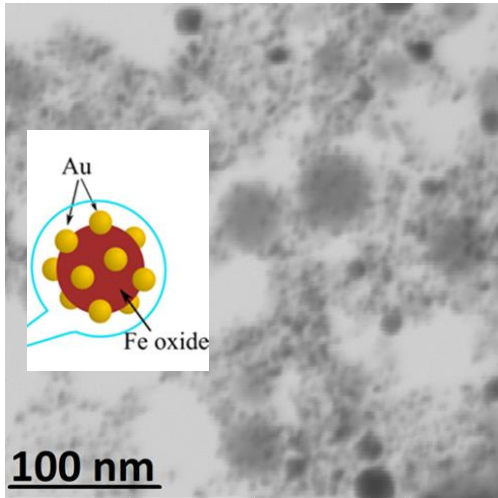
*Additional
fragmentation*

Role of laser energy: non-linear dependency

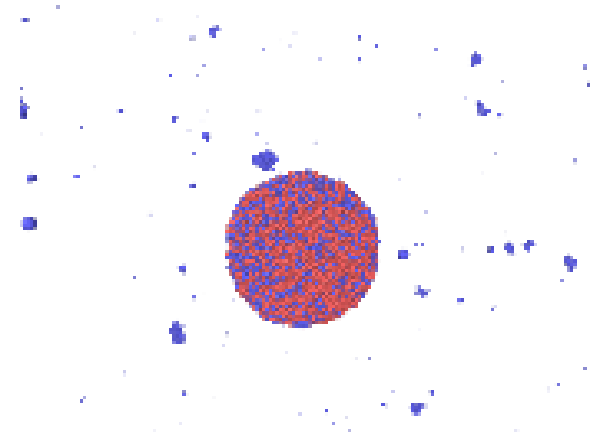
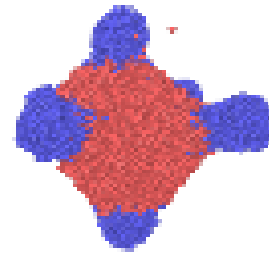
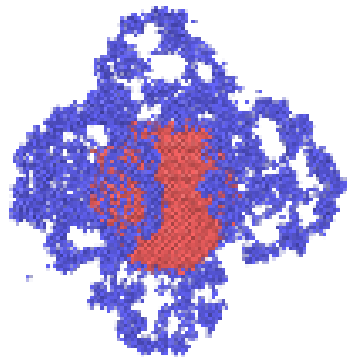


K. Maksimova, PhD thesis Aix-Marseille University, France, 2014

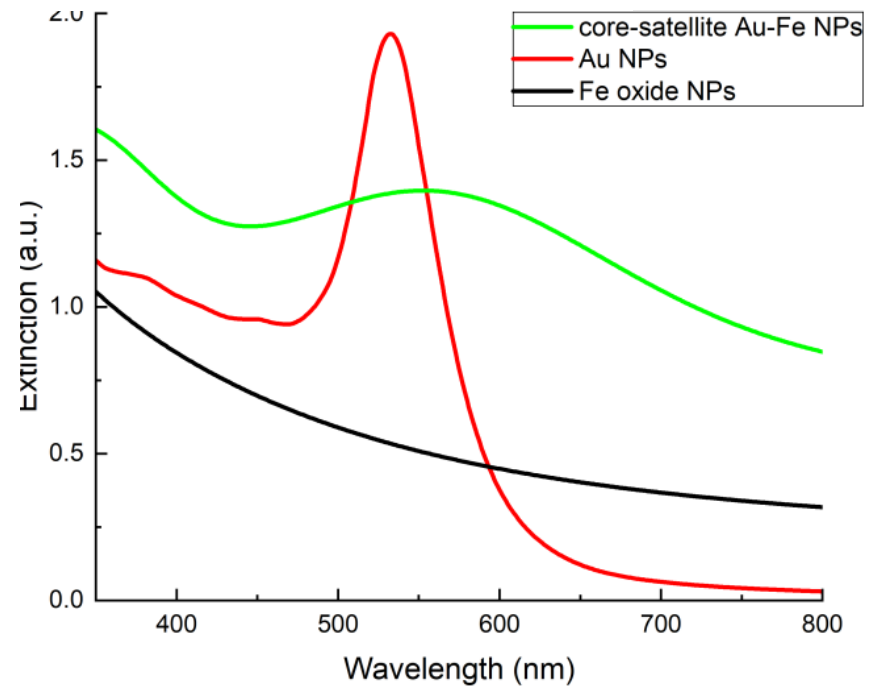
Complex Nano-Objects Formation by Laser Co-Ablation



:STEM image of nanostructures, obtained by mixing of negatively charged laser-ablated Au NPs and positively charged laser-ablated Fe oxide NPs. Right: Calculated extinction spectra of bare Au NPs (red line), Fe oxide NPs (black line) and core-satellite Au-Fe NPs (green line).



Raspberry –like, core-shells or alloys



Laser is a very powerful and versatile tool suitable not only for laser ablation but also for nanoparticle synthesis for optics, catalysis, cancer treatment, solar cells, sensors, anti-bacterial applications, etc.

- The main involved processes include laser absorption, electronic excitation/relaxation, lattice heating and cooling.
- Particle size, composition, geometry, atomic masses, binding energies, excess energy, environment, heating/cooling protocol are important.

Namely, MD simulations of fast NP heating have shown :

- (i) When different nanoparticles interact with a laser they may either fragment, sinter or mix depending on their sizes and heating/cooling rate. To reach alloying without fragmentation NP should not be over-heated.
- (ii) Laser can help creating complex multi-material nano-objects with promising optical, catalytical and plasmono-magnetic properties.

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Thank you for your attention!

tatiana.itina@univ-st-etienne.fr