



Numerical simulation of laser interactions with surfaces and nanoparticles

T E Itina

► To cite this version:

T E Itina. Numerical simulation of laser interactions with surfaces and nanoparticles: Numerical simulation of laser interactions with surfaces and nanoparticles. 31st ANNUAL INTERNATIONAL LASER PHYSICS WORKSHOP (July 3-7, 2023), LPHYS'23, Seminar 5: Nonlinear Optics & Spectroscopy, Institute of Physics, London, UK; <https://www.lasphys.com/workshops/lasphys23/>, Jul 2023, ONLINE (Virtual), France. ujm-04183678

HAL Id: ujm-04183678

<https://ujm.hal.science/ujm-04183678>

Submitted on 25 Sep 2023

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

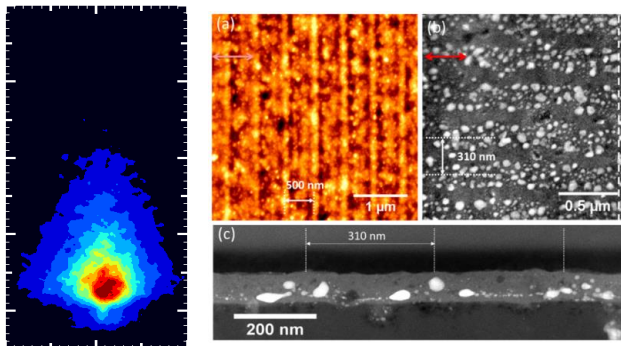
L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Numerical simulation of laser interactions with surfaces and nanoparticles

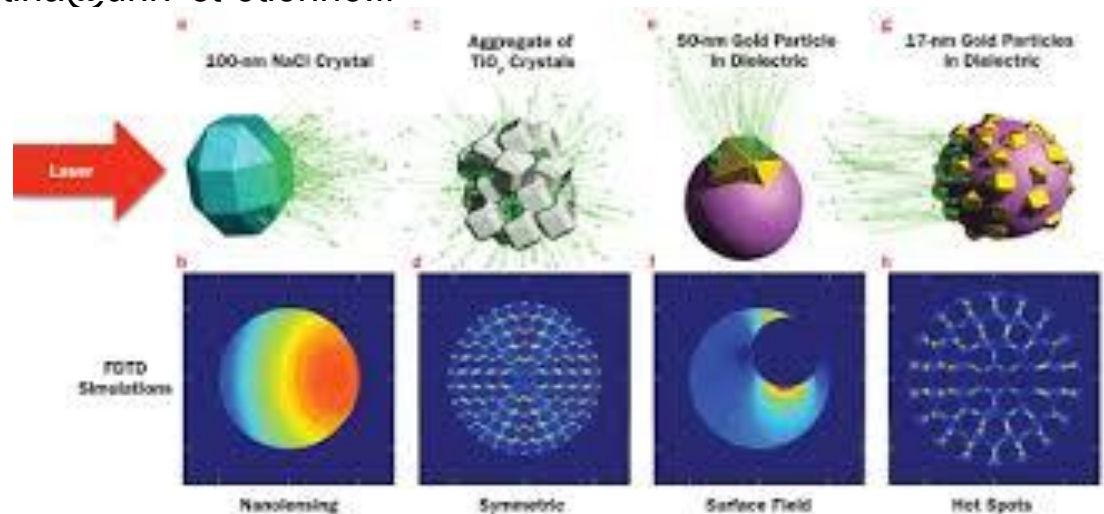
Tatiana E. ITINA

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

tatiana.itina@univ-st-etienne.fr



experiments : LP3, LabHC, ITMO

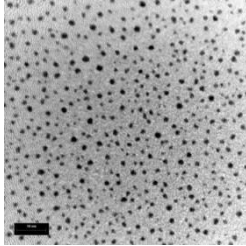
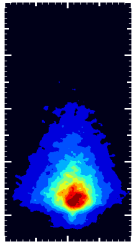


https://www.photonics.com/Articles/Nanoparticles_Probing_the_Plasma_Threshold/a57306

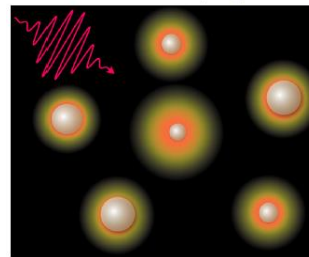
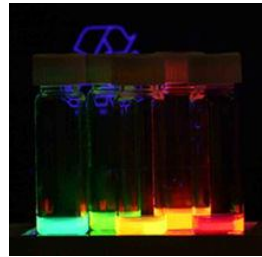
From laser plume to nanoparticles and nanostructures

Main research directions

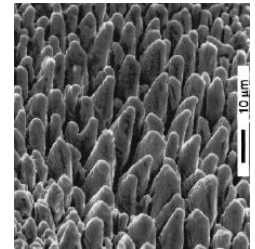
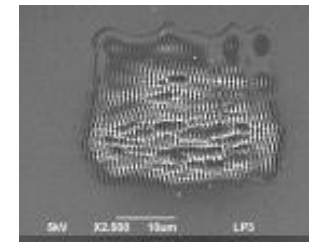
- Laser-induced formation and modification of nanoparticles, monohybrids and nanostructures: modeling vs experiments**



Pulsed laser interactions

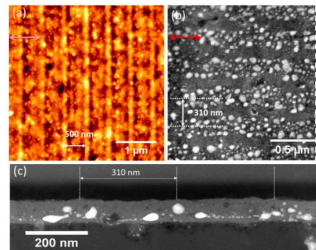


Laser ablation/fragmentation

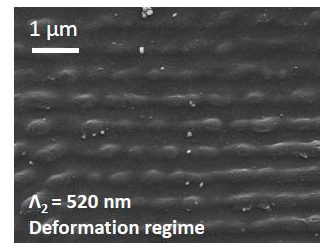


Laser-induced surface/volume structures

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



Nanoparticles inside

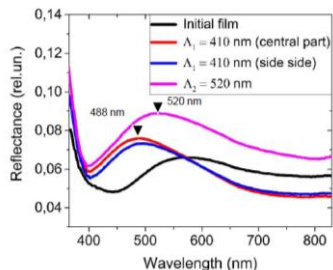


Nanoparticles on the surface



Hierarchical surface structures

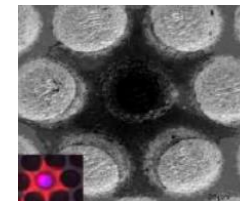
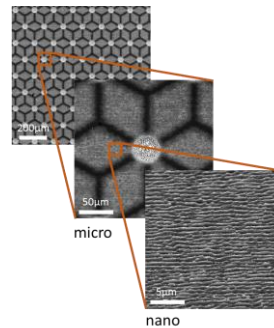
- Properties and applications of the obtained materials: optical properties, wettability, cells and bacterial adhesion/repulsion**



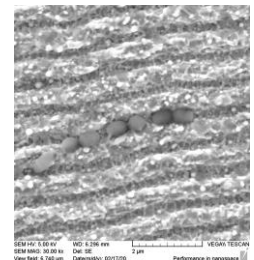
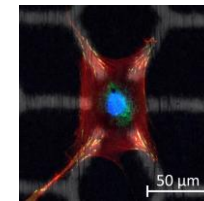
Optical spectra



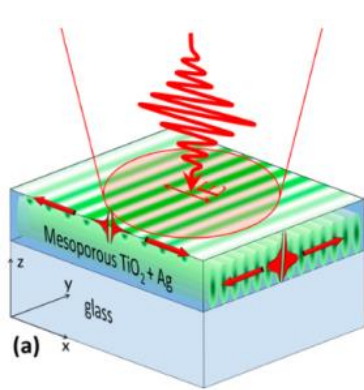
Wettability



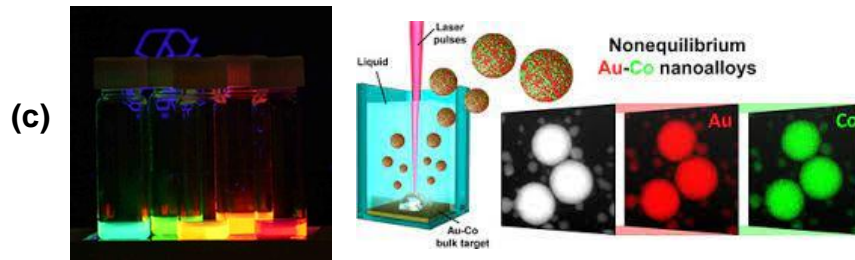
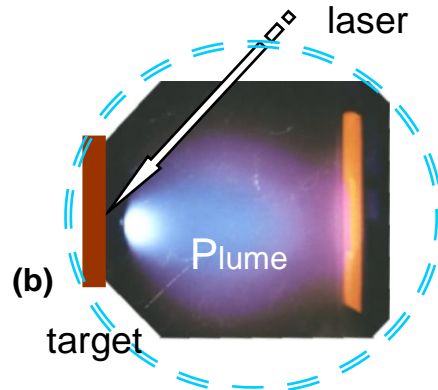
cell and bacteria adhesion



Laser Interactions



In gas or in vacuum with different geometry



In liquids or in the presence of a colloids

Laser interaction commonly involve:

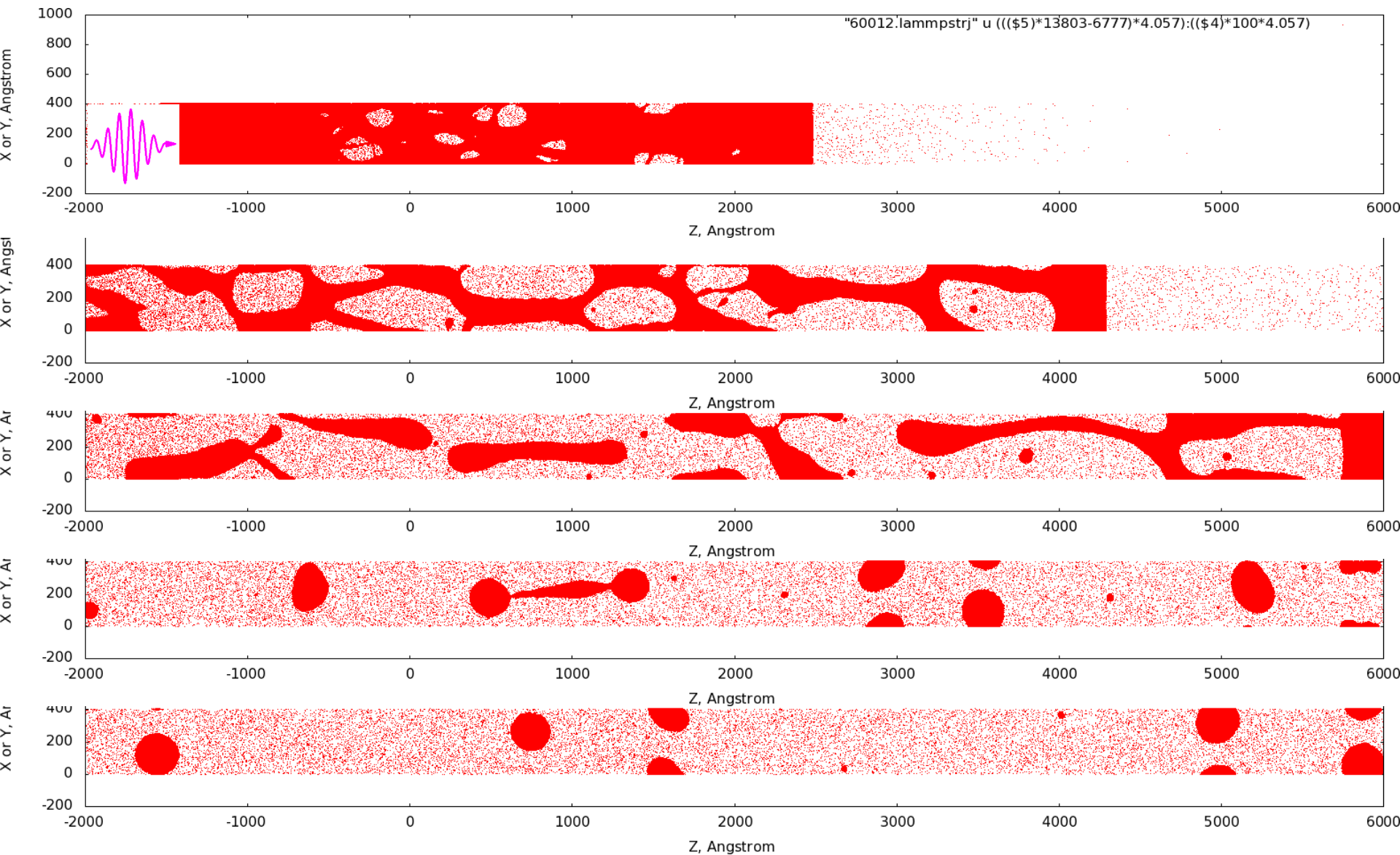
- Energy propagation, electronic excitation, light scattering, reflection and absorption
- Electron-phonon relaxation, heat diffusion, pressure wave propagation, rarefaction and tensile stress, phase transitions, mechanical fragmentation
- Material removal (ablation), plasma plume expansion, reactions, 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**



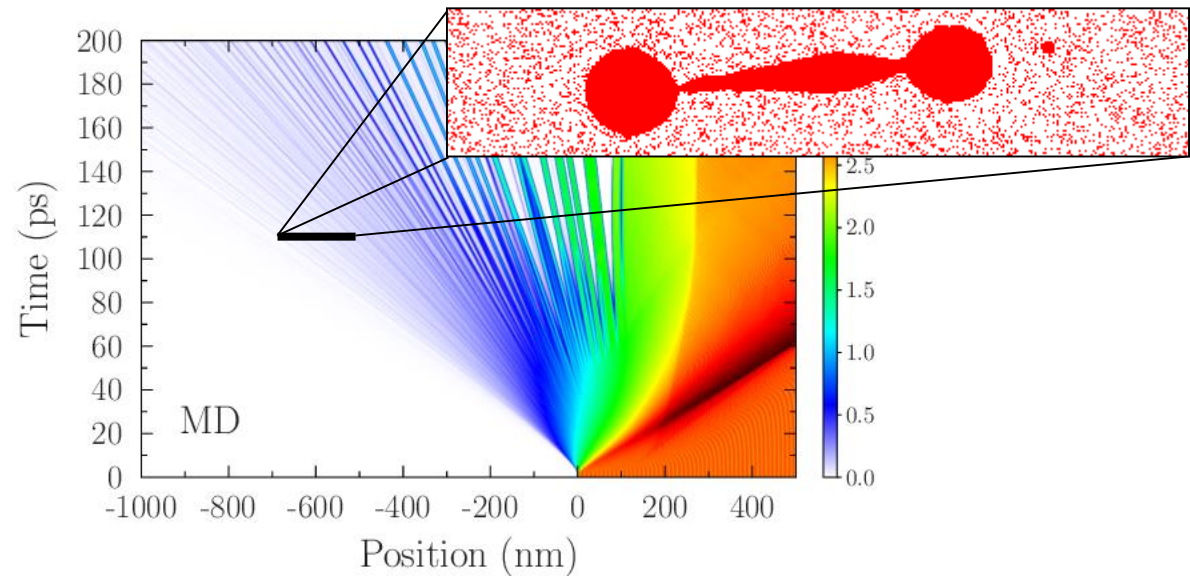
Ablation & Nanoparticles (10M atoms, $F=1 \text{ J/cm}^2$, Al)



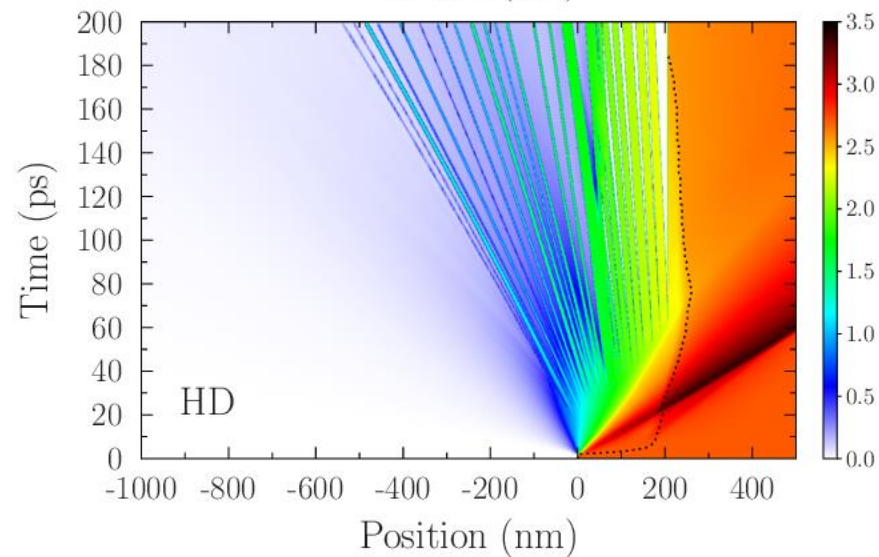
Density

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

TTM-MD

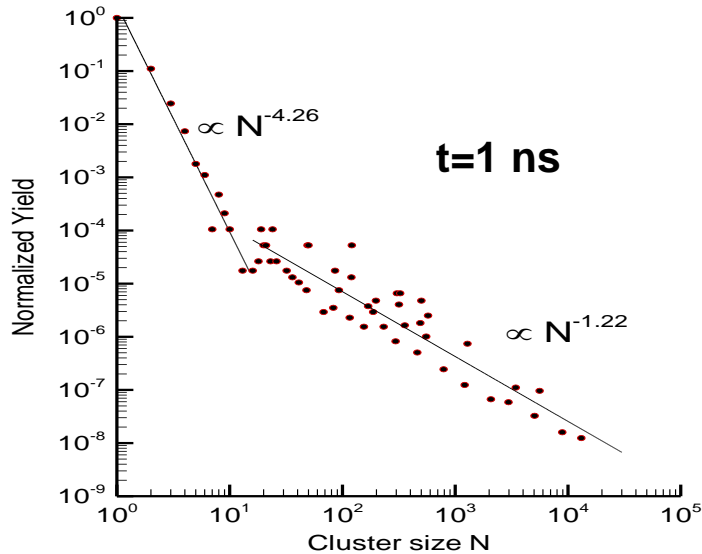


Hydrodynamics

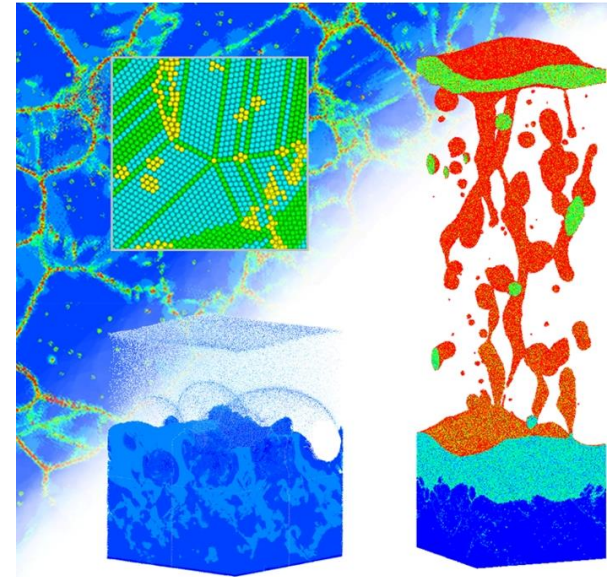
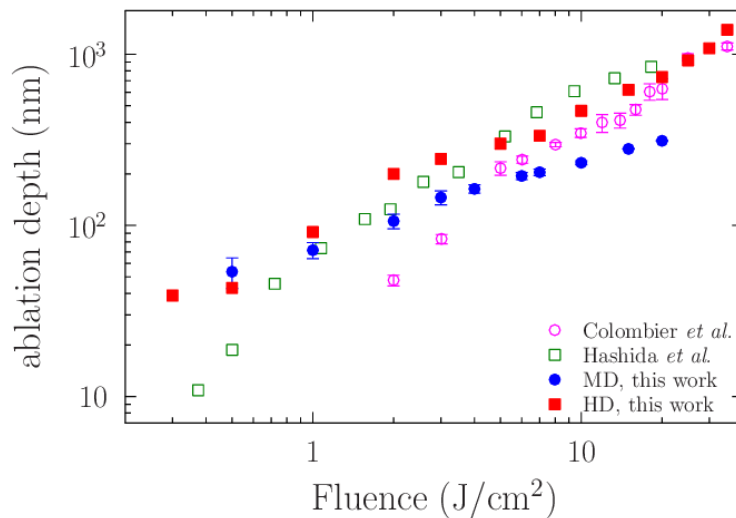


Molecular Dynamics Simulations

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



$\tau = 15$ ps, $F \sim 2$ Fth, 40×10 nm, $t = 1$ ns

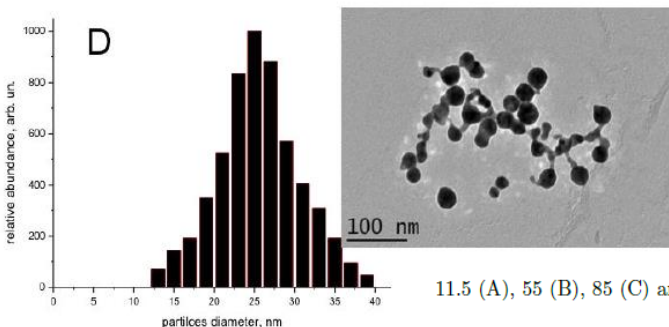
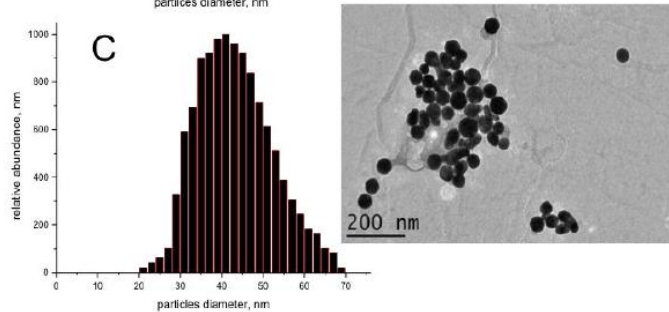
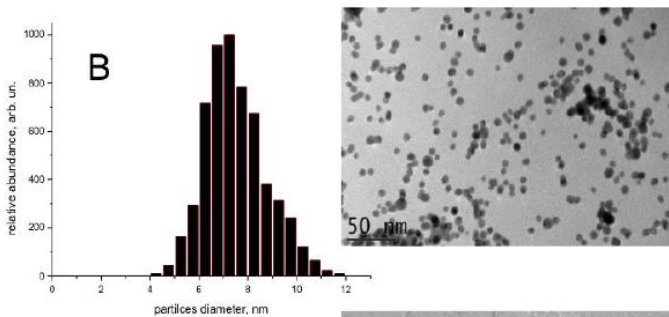
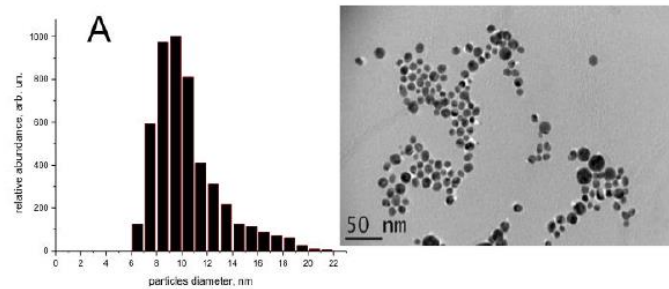


Collaboration with L.V. Zhigilei et al. (Virginia State University, USA)

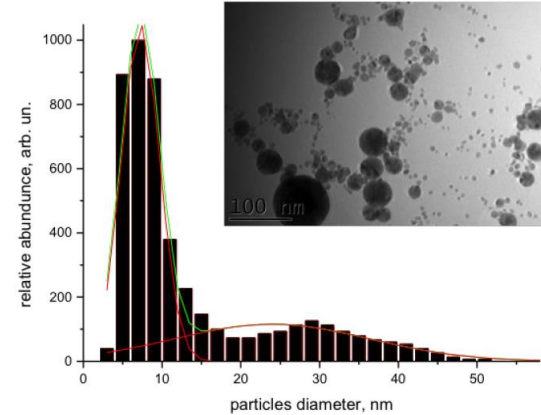
Practically all the molten material is ablated

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

Non-linear Effects in fs Laser Interactions with Au NPs



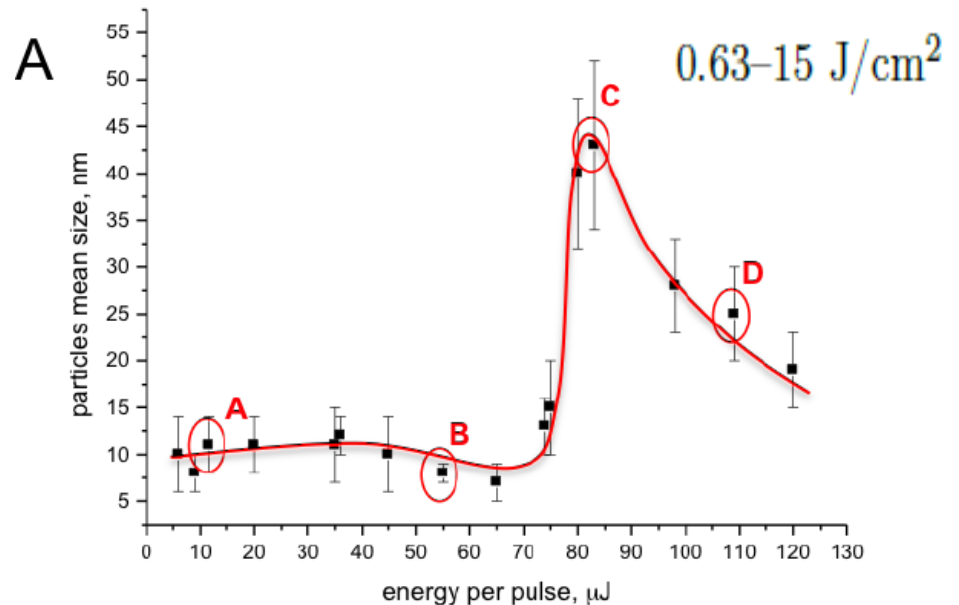
11.5 (A), 55 (B), 85 (C) and 109 (D) μJ



*Upon ablation
1064 nm*

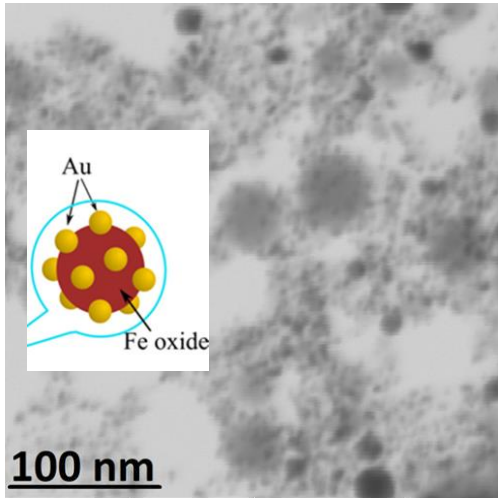
*Additional
fragmentation*

Role of laser energy: non-linear dependency

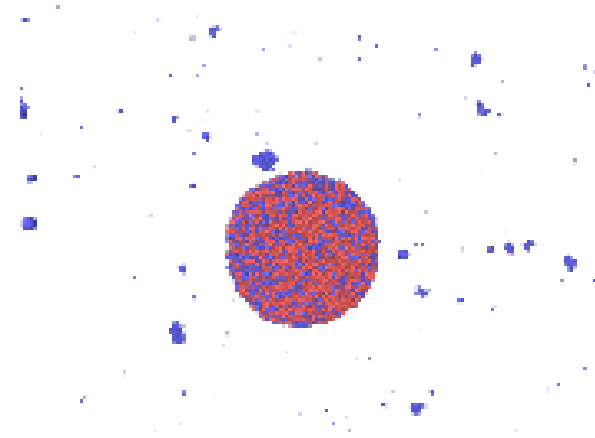
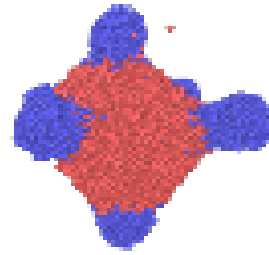
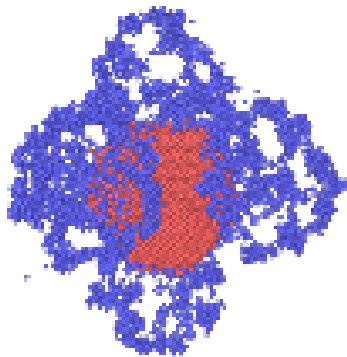


K. Maksimova, PhD thesis Aix-Marseille University, France, 2014

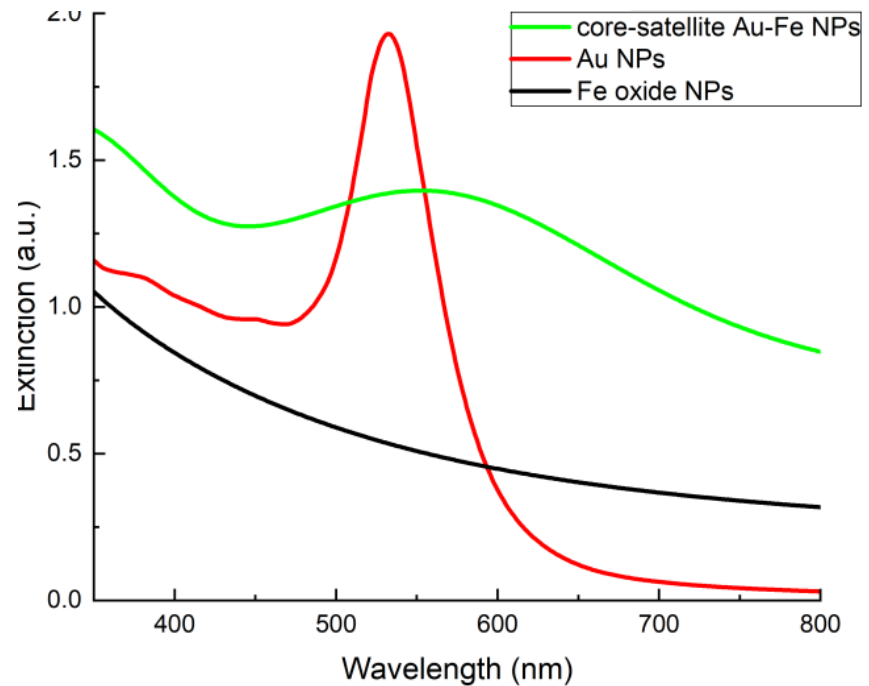
Complex Nano-Objects Formation by Laser Co-Ablation



: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.

Thanks to:

*PhD students and collaborators
PHC (Campus France)
ARQUS project
CNRS and UJM for funds*

Thank you for your attention!

tatiana.itina@univ-st-etienne.fr