FIELD EMISSION PHOTOCATHODE ARRAY (FEA) AND DIELECTRIC LASER ACCELERATOR (DLA)

DESIGN INVOLVING AB INITIO SIMULATIONS

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Introduction

Next generations of high energy light source and electron colliders need compact and efficient processus of initial particle sourcing ; that idea has been already described [1]. Standard photocathodes with powerful RF guns deliver Mev beams, which are accelerated to Gev (light sources) and more (colliders) thanks to cavities, and guided with electron optics. However, to overcome the performances of the couple photo-cathode/RFgun, a completely different concept is proposed : a low energy Field Emitting Array (FEA), running in transient photo-field mode, associated with multistages of Laser Dielectric Accelerators (DLAs).

The figures 1, **standard sources**, and 2, **Laser Dielectric Laser driven**, illustrate these two differents approaches :

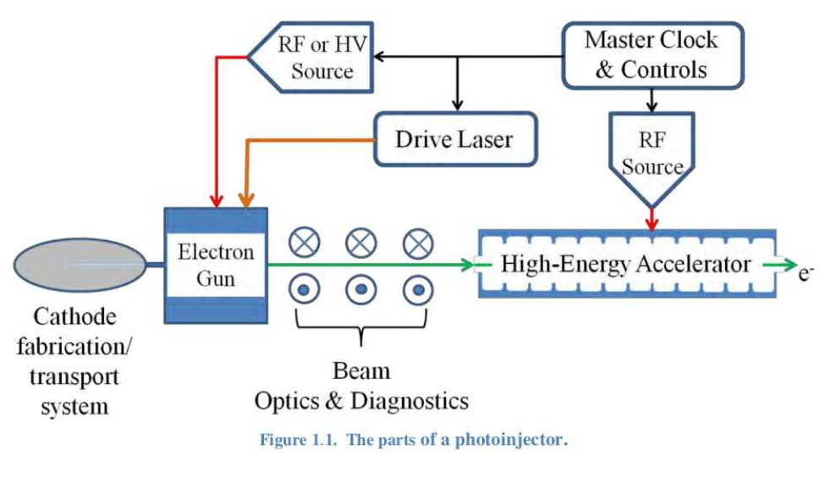
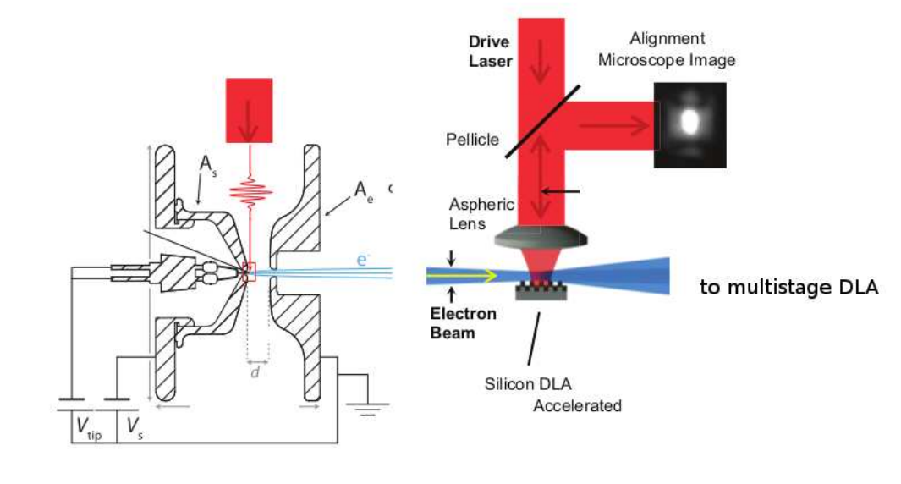


Figure 1 – Standard photocathode and RFgun, from [4]



From KJ Leedle From J England

Figure 2 – new source mixing the principles from [2] and [3]

The **Laser Dielectric Laser driven** of figure 2 lay upon two critical components :

1. A low emittance photocathode with Field Emitting Array of tips (FEA)
2. A serial multistage amplifier(s) -named Dielectric accelerators- which raise the electron energy from keV to MeV and more

The aim is to understand the FEA interaction with electric pulses and laser. In standard simulations, the codes don't take account the surface physics. It is however of primary importance to describe their **energy and momentum distribution** in order to access to electron dynamics.
ab initio simulations could help us to improve our knowledge of the electron behaviour near the surface in vacuum at ambient temperature (10^{-6} to $10^{-8} Torr$). Much work has been done in the past, upon metallic and semi-conductor **plane** photo-cathodes. A promising way will consist to study FEA emission and develop an engineering guide based on solid state physics rules.

I nanostructured photo-cathodes

1. Choice of FEAs

We propose to benchmark two candidates for the ideal FEA photofield performances (fig 3 and fig 4) :

1. « Spindt like » metallic cathodes, tips arrays made in Tungsten, on a Ni support,
2. Monolayer Carbon Nanotubes, also in array, on a (monolayer) graphen, which is put down a Ni support.

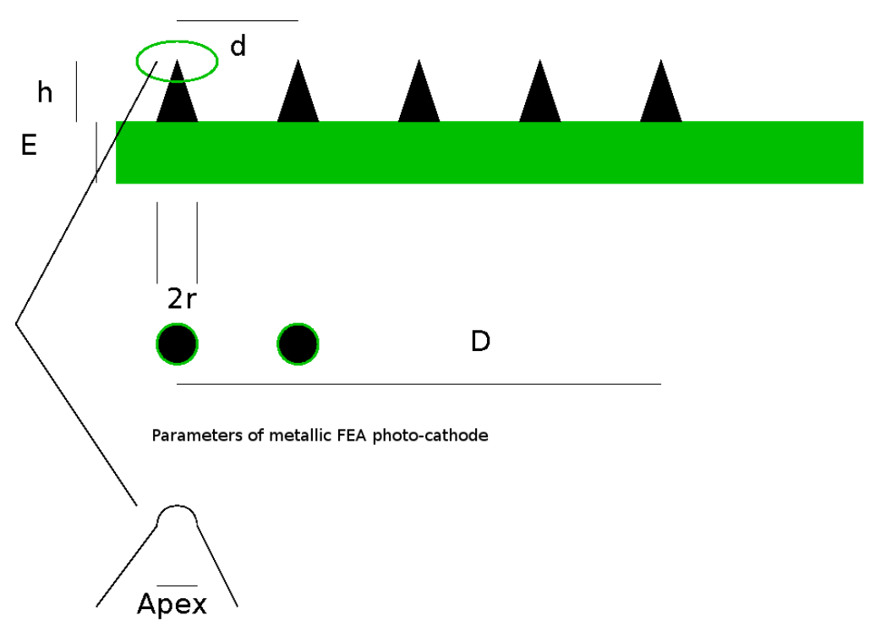


Figure 3 – Spindt FEA

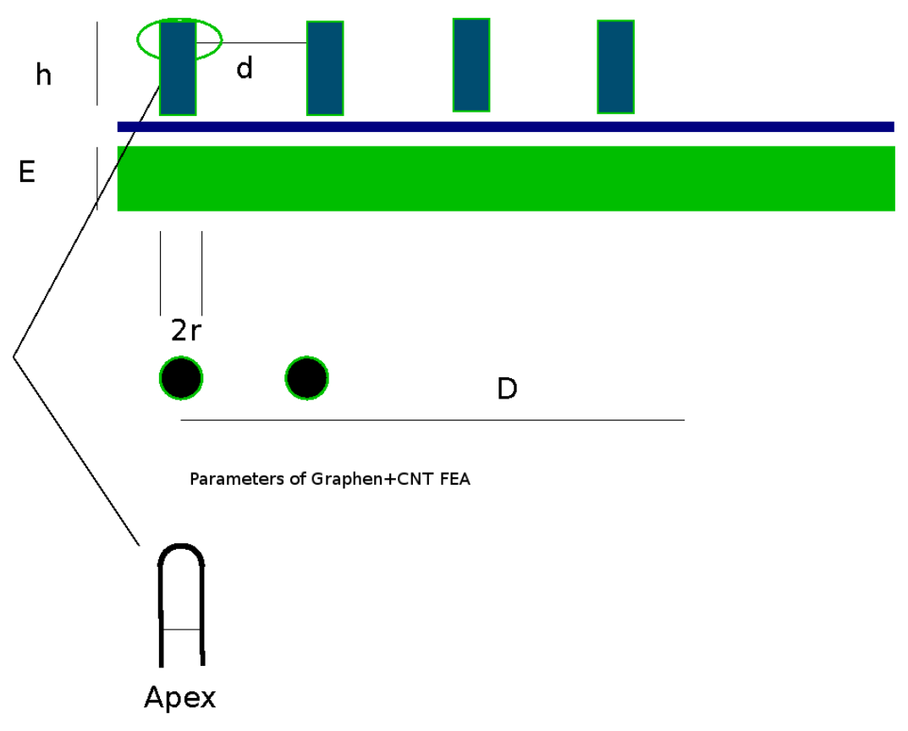
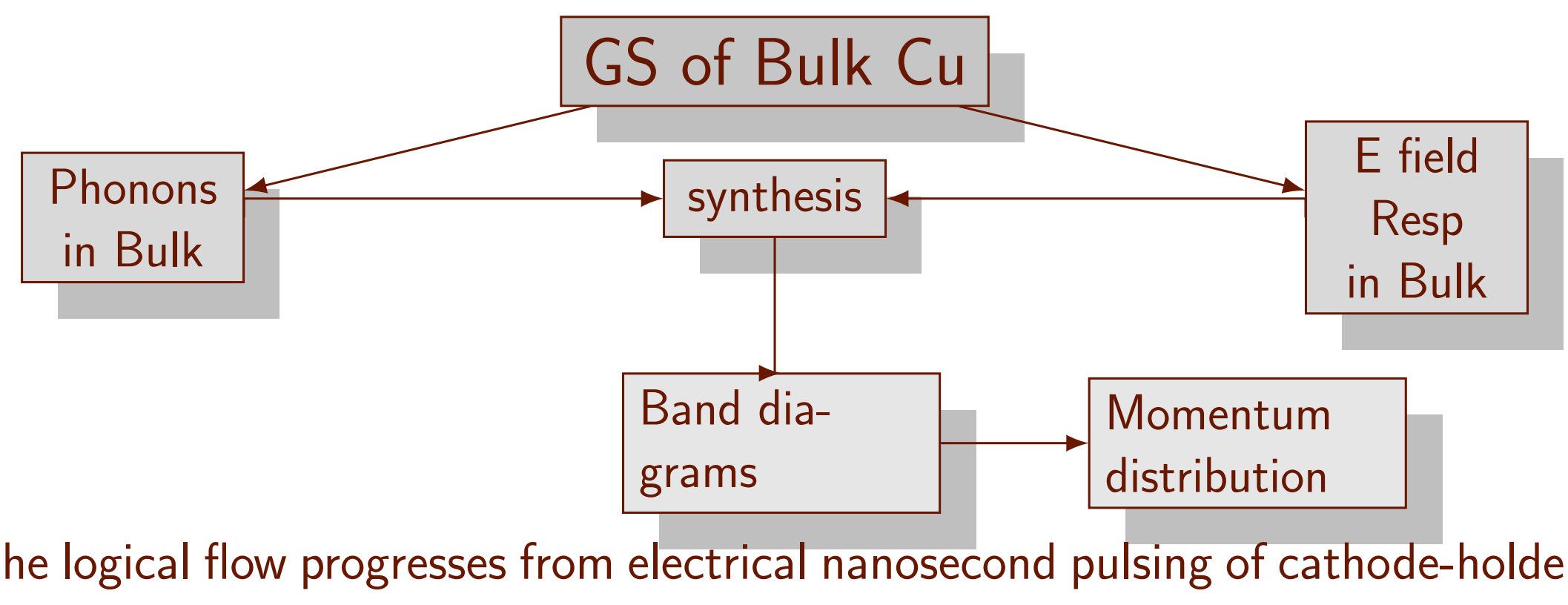


Figure 4 – Monolayer CNT on graphen

Typical dimensions : $1\mu m$ for h, $10\mu m$ for d, 10 to 30nm for metallic apex, 5 nm approximately for CNT apex, Ni interface is connected to a copper cathode holder.

2. Logical steps for Abinit simulations


GS of Bulk Cu

Phonons in Bulk

synthesis

E field Resp in Bulk

Band diagrams

Momentum distribution

The logical flow progresses from electrical nanosecond pulsing of cathode-holder to the transport inside individual tips, and finally in vacuum emission. [a]. A bibliographical study [b] concluded to

1. low influence of pulsed Electrical field inside Cu bulk,
2. notable influence from phonons
3. a low influence of copper metallurgy

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[a] laser interaction description planned in future steps. The cathode-holder will be modeled by single Cu crystal near Cu-Ni interface in [111] direction, ie Miller indexes of CC lattice of Cu so the normal to the surface is oriented to Ni. Also, « Bulk » means the Cu crystal of cathode-holder

[b] to be published

II First simulations with Abinit

1.Ground State on bulk copper

A serial version of Abinit by debian packet was installed on a single machine [a], and also a compiled parallel version for future work. That last result is reported by [**?**] for two single machines, tuned with throttling. Installation of those version has been asked to Lal central machines.
The GS of copper are reputed not to exactly converge, as simple metals [**?**] but are not too far from free electron approximation citation [**?**]. I started from tutorial with AlAs [b], and modified the script. Those I finally choosed, with a simple LDA approximation [c] are :

1. reduced lattice, with 3x11.78 meshes, nband 4, ixc 7, tsmear 0.08
2. ecut 100, nstep 40, tolvrs 1e-8

The simulations lasts 18 minutes, and result is $NSTEP = 16, ETOT = -142.49154214614Ha, \delta E = 2.984E - 08Ha,$ (density residual)$residm = 3.957E - 10vres2 = 2.051E - 09$ So $residm < tolvrs$. results from GW method are to be compared.

2.Dynamic matrix responses

Following again tutorial, I tried to compute the entire response simulation. For the moment, only frozen phonon at $q = 0$ is disponible. The code included automatically 10 band, I did not ascertained if d-band are really included. The results are in course.

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[a] Dell Intel(R) Core(TM) i3-3220 CPU 3.30GHz

[b] some parameters also modified to adapt to a metal, like occpt, diemac, . . .

[c] here also question of pseudo potentials is not seen in-depth, it is planned to choose them

3.Vacuum emission and laser interaction (planned)

Emission probably happens predominatly for a layer at some nm from the surface. Next step will be to modelize the interface Cu-Ni, (Ni thickness $\sim 500\mu m$ suggesting a bulk behaviour). The Cu-Ni bounding will depend on the nature of its link.
The next step is to simulate the tip-vacuum transition. In a 1D formulation, the Fowler-Nordheim(-Forbes) theory [**?**], [**?**], applied to plane cathode, gives us the current density given the electric field F :

$$J \sim \frac{e^3F^2}{4\pi h\phi} exp^{-\frac{4\sqrt{(2m_e)}\phi^{\frac{3}{2}}}{3\hbar eF} v(y)} \quad (1)$$

e : electron charge, v(y) : Nordheim function, ϕ : work function of the material, and $y = e^{\frac{3}{2}}\sqrt{(\frac{\frac{F}{4\pi\epsilon_0}}{\phi}}$: the Nordheim parameter.
No microscopic indication is given, ie starting momentum, energy dispersion, localization, ... First studies tried to link the velocities to electric field chart, considering a perfect conductor surface. The figures 8 and 9 hereafter show how delicate may be that hypothesis Modeling *ab initio* the near atomix layers of the apex is probably mandatory.

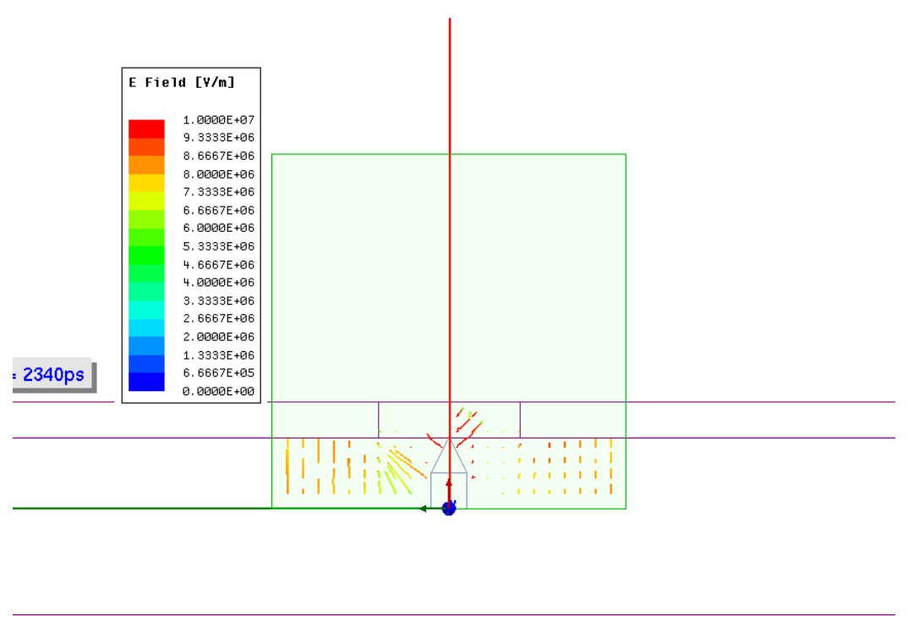

Figure 5 – hfss electromagnetic simulation of an individual tip, perfect conductor

J. Appl. Phys. **115**, 094506 (2014)

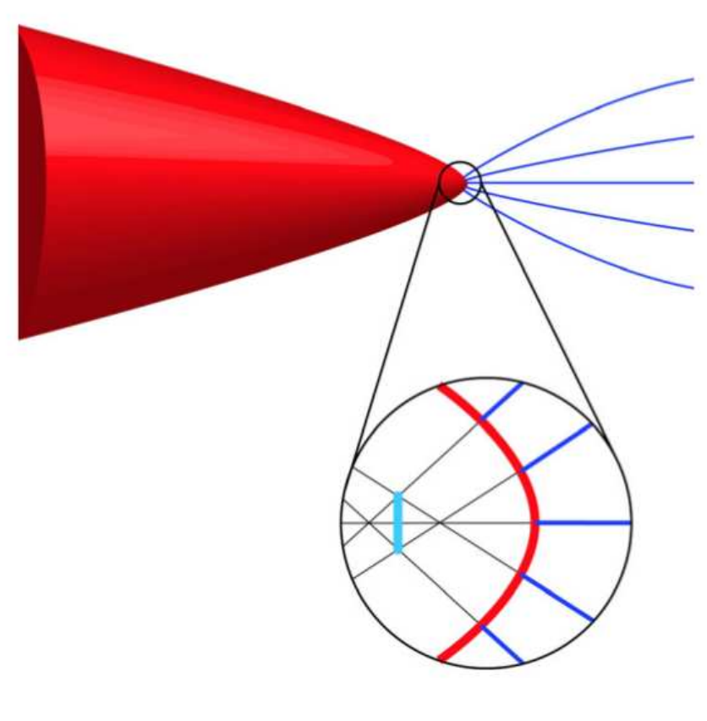

Figure 6 – Simulation of more complete model for an individual tip, from []

[a]

Finally, the laser interaction may be qualitatively described by the 3-step process, figure 7 [b].

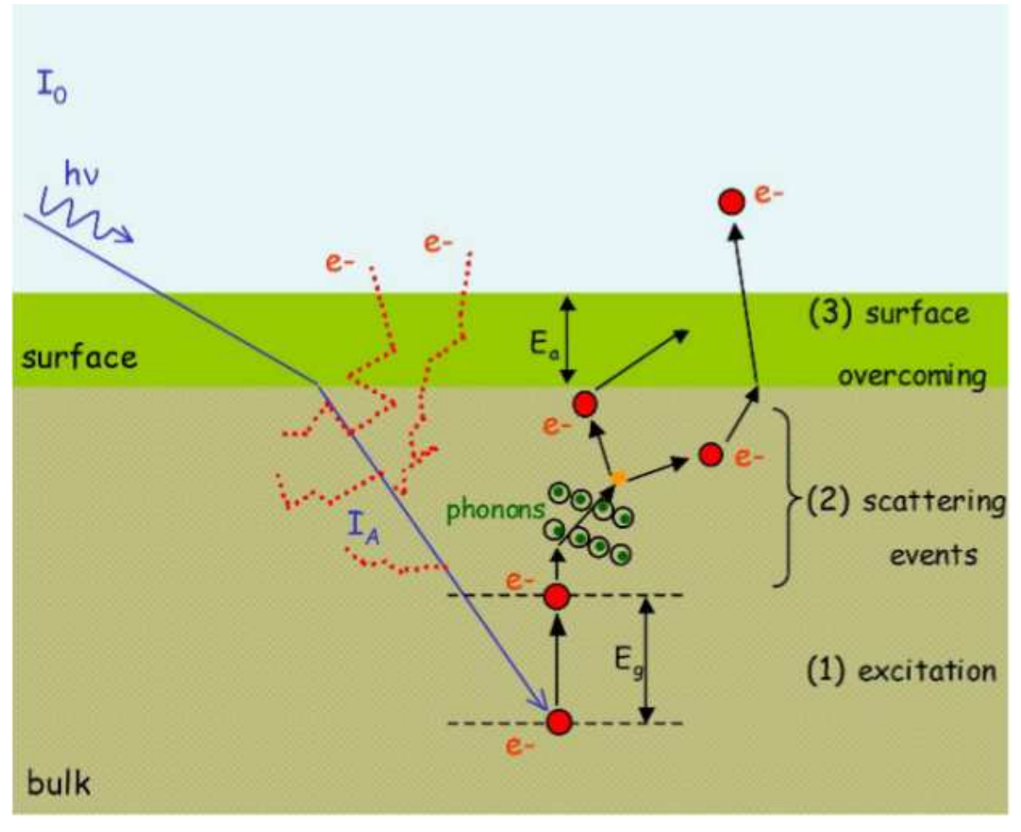

Figure 7 – 3-step description, from [**?**]

Before any analysis, the band structure should be determined. So finally, the bunch physiognomy at immediate proximity of the surface, will at less, depend on :

1. surface states,
2. band structure in time domain,
3. crystal orientation,
4. macroscopic **and** microscopic electric responses inside the tips

Electric macrocopic field between cathode and anode determines the bunch evolution, but we consider that these two problem -near and far from surface- can be splitted.

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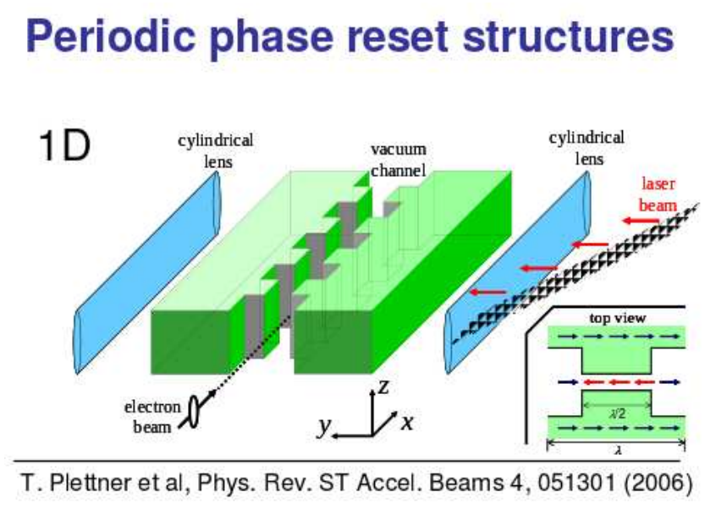
[a] Numerous critisizes came also from experimentalists, regarding the disagreement between their results and FN theory, which is a local one. See for instance [**?**]

[b] according to [**?**], 3-step model is considered now as to be refined to the ideal 1-step model. TDDFT could help to reach that objective

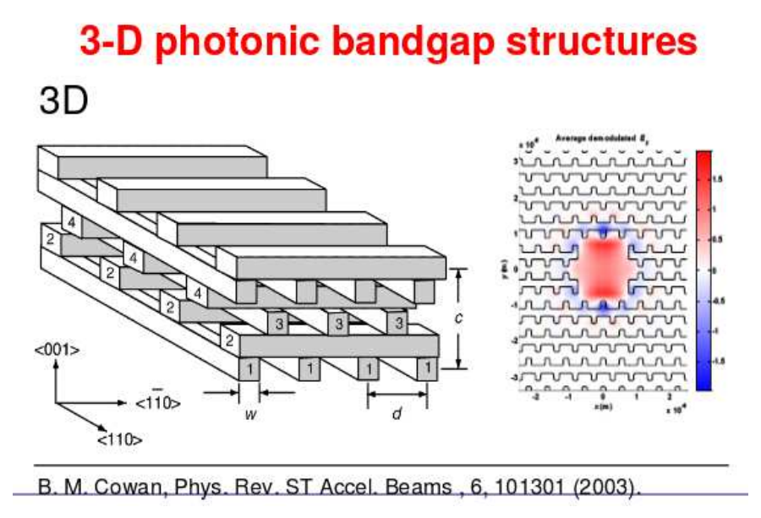
III Laser-matter interaction and DLAs

To illustrate laser-matter coupling, you find here two major schemes, fig 8 and 9 of the today developpements in DLAs arrays [**?**]



T. Plettner et al, Phys. Rev. ST Accel. Beams 4, 051301 (2006)

Figure 8 – DLA made by etched array



B. M. Cowan, Phys. Rev. ST Accel. Beams , 6, 101301 (2003).

Figure 9 – DLA made by 3D photonic array

In the first case, laser radiation goes through the material, with interactions expected during the transmission. In the second case, there is a vacuum path for laser and electron beams.
This (multi)stage should raises the bunch energy, from some tens of keV to some relativistic MeV energy ranges. Demonstrating experiments are in the field and :

1. as was laser-plasma ten years ago, the in-chip accelerator technology is nowaday rapidly expanding,
2. the demonstrated gain is obtained in « interaction distances » of roughly 100μ m, so for multistage, the gain will be impressive.

So the future is closely linked to the issues of **serially assembling DLAs**, and **ascertaining ultrafast electronic or optical synchronism between stages** [**?**].
Furthermore, [**?**], TDDFT could help to evaluate damage threshold of chip crystals [a]. Note that Al203 is considered for future fabrications, owing to its high damage threshold.

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[a] here exemple taken inside SiO_2

IV SUMMARY

1 New compact and performant electron in-chip Dielectric Laser Accelerator (DLA), need a first non-relativistic stage driver, from 0keV to relativistic Mev energy ranges ; the proposed system is a photocathode Field Emitting Array (FEA), combined with a first stage DLA. we feel that the design is linked to abinitio modeling, we started to investigate it thanks to Abinit software.

2 The blocks which should be studied are tied to the photo-cathode and the DLA 1-stage module. For the photo-cathode, we show that a logical approach consists to simulate the electron-phonon and electric response inside bulk of cathode-holder, then to study vacuum emission through tip.

3 The other scope of study concern laser-matter interaction inside the DLA.TDDFT is envisaged to render the photo-field emission. The scope for our appliance, will be a phonon and electric field perturbative approach, because of moderate laser flux and energy, comparatively to bandgap of usual dielectric materials of DLAs

The goal should be to contribute to nano-engineering domain, applied to photo-cathode physics, and design a new family of electron sources

Références

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[2] Johannes Hoffroge and Al. Tip-based source of femtosecond electron pulses at 30 kev. *JOURNAL OF APPLIED PHYSICS 115, 094506*, march 2014.

[3] K LEEDLE and Al. Laser acceleration and deflection of 96.3 kev electrons with a silicon dielectric structure. December 2014.

[4] Rao Triveni and H David Dowell. *An engineering book on photo-injectors*.