Physics-based high-fidelity modeling of high brightness beam injectors

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Introduction: A high brightness particle beam injector is an essential component in the beam line of state-of-the-art accelerator facilities for particle physics, nuclear physics, photon science and material research. Such an injector usually consists of a high brightness electron source embedded in a DC or RF gun followed by post acceleration in a low energy accelerator. In particular, the advent of the photocathode gun [1] leads to a breakthrough in injector for the generation of high-brightness low-emittance electron beams with picosecond to sub-picosecond pulse duration. This advanced technology can substantially improve the beam luminosity for particle colliders as well as enable the development of coherent electron or x-ray probes that can resolve details of dynamic processes on the temporal and spatial scales of an atom.

Owing to the conclusions of many community inputs [2-5] in recent years, DOE recognized the need of next generation photocathode guns in meeting the requirements of high brightness electron/X-ray sources to support the development of future hadron/lepton colliders and frontier material science research. Next generation photocathode guns demand improvement in major metrics, including quantum efficiency (QE), emittance, response time, lifetime, and structural robustness [6]. In addition, high degree of electron polarization is a critical requirement for collider applications, while high charge/current (e.g. ~100mA and >nC/bunch) is needed for electron cooling of hadron beams for colliders. On the other hand, Ultrafast Electron Diffraction/Microscopy (UED/UEM) devices and future hard X-ray Free Electron Lasers (FELs) also critically depend on the development of very low emittance (10s nm - 100s nm) cathodes. Research to enhance photocathode performance has been very active in many accelerator laboratories around the world such as improving semiconductor cathode materials (e.g. CsTe, GaAs, bi-alkali antimonide etc.), nanoscale engineering for the control of electronic structure/stoichiometric of the cathode surface and its protection [7-8], electron amplifier concept for high average power applications [9] and photo-emission or photo-assisted field emission from nanotips [10].

Challenges and suggestions: While semiconductor photocathodes with high QE (~1-10%) in the visible range of laser excitation are promising candidates to replace traditional metallic photocathodes, their performance metrics, i.e., QE, emittance, response time and lifetime are correlated and interdependent. Many photocathodes are operated near emission threshold wavelength (e.g., 532nm for K_2CsSb) in order to achieve low emittance beams whereas photocathode's degradation can adversely impact the emittance evolution in the beam formation process. Moreover, emittance values in semiconductor cathodes observed in experiments in the vicinity of the photoemission threshold are measurably higher compared to predictions by existing models. This is because the carrier transport and emission, hence QE and lifetime, are very sensitive to surface contaminations and stoichiometry, and predictive modeling must include accurate physics processes for the emission and its environment. Therefore, semiconductor cathodes, including both "standard" bulk cathode and other "engineered" cathodes need to be thoroughly evaluated for improvements to fully take advantage of their potentials.

Operating the photocathode in a DC or RF gun represents another complexity where beam formation and acceleration are affected by the driving laser, RF and the space charge and the cathode performance/lifetime impacted by the gun environment from effects such as chemical poisoning, thermal dissociation and ion back bombardment (potentially from the entire volume of the injector). For example, while the photon energy, cathode temperature and ultimately the electron transport/emission processes determine intrinsic emittance of the emitted electrons, the space charge and RF add their corresponding contributions to the final beam emittance [11]. For this reason, laser profile control, cryogenic cathode and high gradient RF

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are attractive paths to improve the beam brightness from the photocathode gun. Furthermore, in novel cathodes with sharp material interfaces, these features usually receive little proper physics treatment and smoothed sharp edges/points are typically used in simulations to obtain finite fields. This traditional treatment is insufficient for electron emission study.

In recent years, understandings of the photocathode performance and lifetime have been greatly facilitated by first-principle or physics-based models. For example, using a model with semi-classical carrier transport in cathode material and detail surface phenomena for emission, the spectral response (QE vs. photon energy), energy distributions of emitted electrons, and response time for a GaAs cathode with negative electron affinity has been simulated with quantitative agreements with experiments [12] without ad-hoc parameterization of the underlying non-equilibrium transport and emission processes. Similar advances are also made for the modeling of diamond amplifier [13] and field emitter experiments [14].

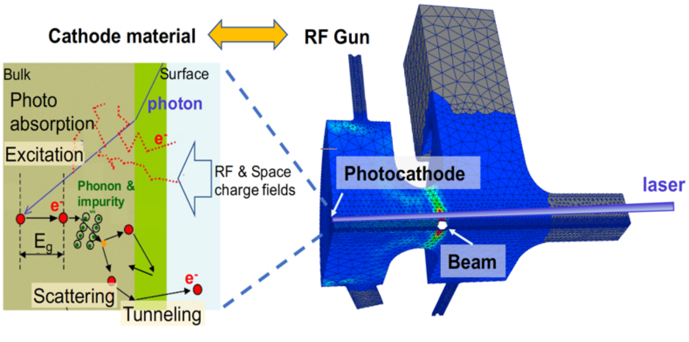

Fig. 1. Schematic of a photogun simulation incorporating detailed emission physics and a high-fidelity multi-physics numerical model.

Despite the needs of and the experimental progress towards the next generation high brightness electron sources, the predictive capability of the performance of novel photocathodes in a gun and the beam properties in the injector is still in its infancy, particularly in the high-current, high-field, Ultra High Vacuum (UHV) environment. Much work is needed to build a validated, high-fidelity, multi-scale, multi-physics model that can be used to design the next generation photo injectors. This model can be developed by leveraging previous efforts in the modeling of different physical aspects of problem at various scales, i.e., through the integration of the electron transport and emission in bulk semiconductor materials and engineered interfaces with state-of-the-art electromagnetic/thermal/structural accelerator cavity modeling tools (Fig. 1). The different time scales of the electron emission and beam forming processes can be bridged via (1) physics-based Monte-Carlo emission model, which takes into account of bulk and surface properties of the cathode and provides an accurate distribution of the electron sources for gun modeling; or (2) adequate integrated electron emission models based on new theoretical analysis and computation methods [15]; or (3) machine learning models trained from accurate simulations. The key properties of the cathode surfaces, e.g., work function, electron affinity, and the impact of adsorption/desorption of contaminant ions should be extracted from detailed Density Functional Theory calculations and in turn used in the modeling of electron emission. These emission models need to be coupled to accurate electromagnetic/thermal/structural calculations (e.g., with proper treatment of nanoscale sharp features) to be fully self-consistent for the prediction of the beam formation process. It also needs to include the interplay between the laser, RF and gun environments with the cathode for assessing the degradation processes. Integration of various code bases with their respective underlying algorithms and data structures on future heterogeneous platforms requires coordinated efforts. Finally, validation with experiments of controlled cathode fabrication and degradation, real-time monitoring (e.g. through multi-wavelength monitoring of QE above to below the emission threshold), will be essential.

Impact: An integrated modeling tool enables high-fidelity end-to-end modeling of high brightness beam photo injectors for the first time. This capability will pave the way and substantially reduce the cost for potential applications in fundamental research, including colliders, hard X-ray FELs and UED/UEMs.

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