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PREDICTING SECONDARY ELECTRON YIELD FROM FIRST PRICIPLES CALCULATIONS

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Currently, the total power, performance and lifetime of high-power RF devices, like vacuum electron devices, RF space systems, and accelerators, are severely limited by a phenomena known as multipactor. This occurs when the electromagnetic field is in resonance with secondary electron emission leading to a runaway avalanche of electrons in the device, resulting in degraded operation and potentially a corona discharge and the destruction of the device. An effective strategy for mitigating multipactor is to use in these devices materials that show a reduced secondary electron yield (SEY), however at present, ideal materials are not known and so currently there is much effort in identifying such low SEY materials. Here we present our efforts, as part of a Michigan State University led Multidisciplinary University Research Initiative (MURI) towards building a model by which the SEY of a material can be predicted based only on the atomic structure of the material, thereby allowing the *in silico* search for effective device materials. Details of this model, in which Density Functional Theory (DFT) is used to calculate the frequency dependent dielectric function of a copper metal surface, which is then used as input to Monte Carlo simulations for secondary electron emission, are presented and compared to experimental results.

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