

**AFRL-RD-PS-
TR-2020-0060**

**AFRL-RD-PS
TR-2020-0060**

IMPROVED ICEPIC SECONDARY ELECTRON EMISSION MODELING

Scott A. Rice, Forrest H. Phillips, and Allycia Gariepy

Applied Research Associates

07 December 2020

FINAL REPORT

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REPORT DOCUMENTATION PAGE				Form Approved OMB No. 0704-0188	
Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing this collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden to Department of Defense, Washington Headquarters Services, Directorate for Information Operations and Reports (0704-0188), 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to any penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number. PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ADDRESS.					
1. REPORT DATE (DD-MM-YYYY) 07-12-2020		2. REPORT TYPE Technical Report		3. DATES COVERED (From - To) 15 NOV 2019 - 30 NOV 2020	
4. TITLE AND SUBTITLE IMPROVED ICEPIC SECONDARY ELECTRON EMISSION MODELING				5a. CONTRACT NUMBER FA9451-20-C-0002	
				5b. GRANT NUMBER	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S) Scott A. Rice, Forrest H. Phillips, and Allycia Gariepy				5d. PROJECT NUMBER	
				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER D0G5	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Applied Research Associates 4942 Dawn Avenue, Suite 220 East Lansing, MI 48823				8. PERFORMING ORGANIZATION REPORT	
9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) AF RESEARCH LABORATORY (DET 8) 3550 ABERDEEN AVE SE, KIRTLAND AFB, NM 87117-5776				10. SPONSOR/MONITOR'S ACRONYM(S)	
				11. SPONSOR/MONITOR'S REPORT NUMBER(S) AFRL-RD-PS-TR-2020-0060	
12. DISTRIBUTION / AVAILABILITY STATEMENT DISTRIBUTION STATEMENT A: Approved for public release. Distribution is unlimited.					
13. SUPPLEMENTARY NOTES Public Release #: AFRL-2021-0471					
14. ABSTRACT This report details the technical results of a year-long effort to improve the secondary electron emission (SEE) model within the AFRL particle-in-cell code ICEPIC, for incident electrons in the range of 10 keV to 500 keV. The simulation code GEANT4 was used to generate SEE statistics across a range of incidence energies and angles using seven typical materials found within high power microwave devices: copper, stainless steel, aluminum, niobium, graphite, aluminum oxide (alumina), and beryllium oxide. A parametric model was defined and demonstrated to fit the available data. Due to the relatively large uncertainty in the available SEE data at high incidence energies, the authors recommend that future work in this area focus on obtaining more data for high-incidence energy electrons, which can then be used to tune and/or refine the model as appropriate.					
15. SUBJECT TERMS PARTICLE IN CELL, PIC, SECONDARY ELECTRON EMISSION, GEANT					
16. SECURITY CLASSIFICATION OF: UNCLASSIFIED			17. LIMITATION OF ABSTRACT UU	18. NUMBER OF PAGES 223	19a. NAME OF RESPONSIBLE PERSON Jason Hammond
a. REPORT Unclassified	b. ABSTRACT Unclassified	c. THIS PAGE Unclassified			19b. TELEPHONE NUMBER (include area code) 505-846-7116

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1.0 SUMMARY

This report details the technical results of a year-long \$247k effort to improve the secondary electron emission (SEE) model within the AFRL particle-in-cell code ICEPIC. Prior to this effort, ICEPIC used an SEE model specialized for electron incident energies up to a few tens of keV. However, the simulation of high-power microwave (HPM) devices with significant electric fields can easily accelerate electrons up to energies on the order of 100 keV or even 1 MeV, necessitating SEE models capable of handling such energy ranges.

A review of the relevant SEE literature revealed a lack of sufficient data to build a general-purpose high incident energy SEE model, so attention was focused on the particle-material interaction code GEANT4. Unfortunately, the available GEANT4 physics models are incapable of generating secondary electrons with emission energies below 10 eV, resulting in an under-estimation of the total secondary electron yield. However, the authors believe that the GEANT4 results adequately capture the qualitative behavior of SEE emission, allowing for the creation of an updated SEE model capable of more faithfully capturing high incident energy behavior, with parameters that can be adjusted as better material data becomes available. The SEE statistics for seven common HPM engineering materials covering both conductors and dielectrics were simulated for incident energies up to 30 MeV, and an updated parametric SEE model was defined and implemented in ICEPIC. This SEE model is backwards compatible with the existing ICEPIC SEE model.

The updated ICEPIC high energy SEE model was evaluated within a parallel plate multipactor scenario, in which a relatively energetic 300 keV electron beam impacts a plate, which produces secondary electrons that seed multipactor. The results are all reasonable, suggesting that the model is behaving as intended.

This report recommends that future work focus on obtaining better-validated SEE data for high incidence energies, before attempting to further refine the ICEPIC SEE model. The least costly way to obtain such data would likely be through modifying or implementing new physics models within GEANT4, in order to lower the allowable generation of secondary electrons with emission energies to 1 eV or below, resulting in more robust SEE data at both low and high incident energies.

2.0 INTRODUCTION

This report details the results of a year-long effort to improve the secondary electron emission (SEE) model within the AFRL particle-in-cell code ICEPIC. Prior to this effort, ICEPIC used an SEE model specialized for electron incident energies up to a few tens of keV. However, the simulation of high-power microwave (HPM) devices with significant electric fields can easily accelerate electrons up to energies on the order of 100 keV or even 1 MeV, necessitating SEE models capable of handling such energy ranges.

This report is organized as follows: Section 3.1 provides the necessary background on SEE in order to understand the larger context of the work documented in this report, and to provide some insight into the limitations of available measured data, and the resulting confidence in theoretical models.

Section 3.2 documents the particle-material interaction code GEANT4, and how it was utilized to generate SEE data due to insufficient measured data above a few tens of keV. As will be shown, the GEANT4 physics models have certain limitations for secondary electrons emitted with low energies, and for incident electrons incident too close to grazing, so some care must be taken with the interpretation of the resulting SEE statistics. However, the authors believe that the GEANT4 results adequately capture the qualitative behavior of SEE emission, allowing for the creation of a more general high incident energy SEE model, with parameters that can be adjusted as better material data becomes available. The SEE statistics for seven common HPM engineering materials covering both conductors and dielectrics were simulated in support of creating this updated SEE model.

Section 4.1 details the updated high energy SEE model which was implemented in ICEPIC. This updated model is in the form of an additive correction to the SEE model that was previously implemented in ICEPIC, which allows for backwards compatibility with existing ICEPIC input files. An optional flag can also be set by the user to modify the emission energy spectra (EES) to more closely match the GEANT4 data at high incident energies.

Section 4.2 provides an evaluation of the updated ICEPIC high energy SEE model in various parallel-plate multipactor scenarios, in which the seed electrons for the multipactor (a relatively low-energy phenomenon) are generated via secondary electrons from an incident high-energy beam consisting of 300 keV electrons. Most of the results can be anticipated based on basic parallel plate multipactor theory, but some unanticipated difference in multipactor initiation time is observed when the optional high-energy emission spectra modification is employed.

Section 5.0 provides a summary of the overall conclusions, followed by section 6.0 which provides a brief discussion of recommendations for future work in this area. The main recommendations revolve around the limitations in underlying data, both measured and available from GEANT4, and how overcoming these limitations can result in a more robust high energy ICEPIC SEE model.

3.0 METHODS, ASSUMPTIONS, AND PROCEDURES

3.1 Background on Secondary Electron Emission

3.1.1 Introduction

There are two characteristic curves (or surfaces) that are frequently used to quantify SEE. The first is the secondary electron yield (SEY) $\delta(E, \theta)$, defined as the ratio of the number of electrons leaving the surface of the material to the number of electrons incident on the material, as a function of incidence energy E and incidence angle θ . The second characteristic curve is the energy emission spectrum (EES) of the secondary electrons $d\delta/dE_{\text{emission}}$ vs E_{emission} , where E_{emission} is the secondary electron emission energy.

There have been various attempts to phenomenologically, analytically and/or computationally model secondary electron emission over the preceding century. Section 3.1 provides a background on prior work, in order to place this report into a larger context. Due to the multitude of investigations into SEE over the years, entire books could be written just summarizing prior work, which is obviously beyond the scope of this present effort. Instead, we will attempt to fairly represent the current state of knowledge and ignorance of SEE. Also complicating any rigorous summary of SEE is the realization that the primary literature unfortunately reveals much conflicting experimental data. Within section 3.1, we first consider experimental data in Section 3.1.2, theoretical models in Section 3.1.3, and then modelling and simulation in Section 3.1.4. We conclude section 3.1 with a short summary in Section 3.1.7.

At the outset of this section, we also note that the literature is not always clear or consistent on what is considered a secondary electron. Within this report, unless specified otherwise, we consider a secondary electron to be any electron emitted from material, subsequent to an impact by an incident (primary) electron. Some authors make a distinction between “secondary electrons” and “backscattered electrons”, with an arbitrary energy boundary of 50 eV emission energy separating these two populations. Some authors instead make a distinction between “true secondary” electrons, “scattered” or “rediffused” electrons, and “reflected” or “backscattered” electrons, depending on the underlying emission mechanism or EES distribution for each population of electrons; the historical ICEPIC SEE model uses this approach when determining secondary electron emission energies. Care must be taken when reviewing the primary literature to understand what specifically an author intends to convey, and sometimes unfortunately educated guesses must be made based upon the available context in the particular work, or the historical period in which the author wrote.

3.1.2 Experimental results

Secondary electron yield for a material, δ , is defined as the ratio of the number of electrons leaving the surface of the material to the number of electrons incident on the material, but typically measured as a ratio of currents, e.g. [1,2]:

$$\delta = \frac{I_{SE}}{I_P} = 1 - \frac{I_T}{I_P} \quad (1)$$

Equation 1: Definition of Secondary Electron Yield

where I_{SE} is the secondary electron current leaving the sample, I_P is the primary current impinging on the sample, and $I_T = I_P - I_{SE}$ is the total current measured by an ammeter connected to the sample. A typical experimental schematic to measure these quantities can be seen in Figure 1. Such measurements would typically be carried out within an ultra-high vacuum (UHV) chamber to minimize error.

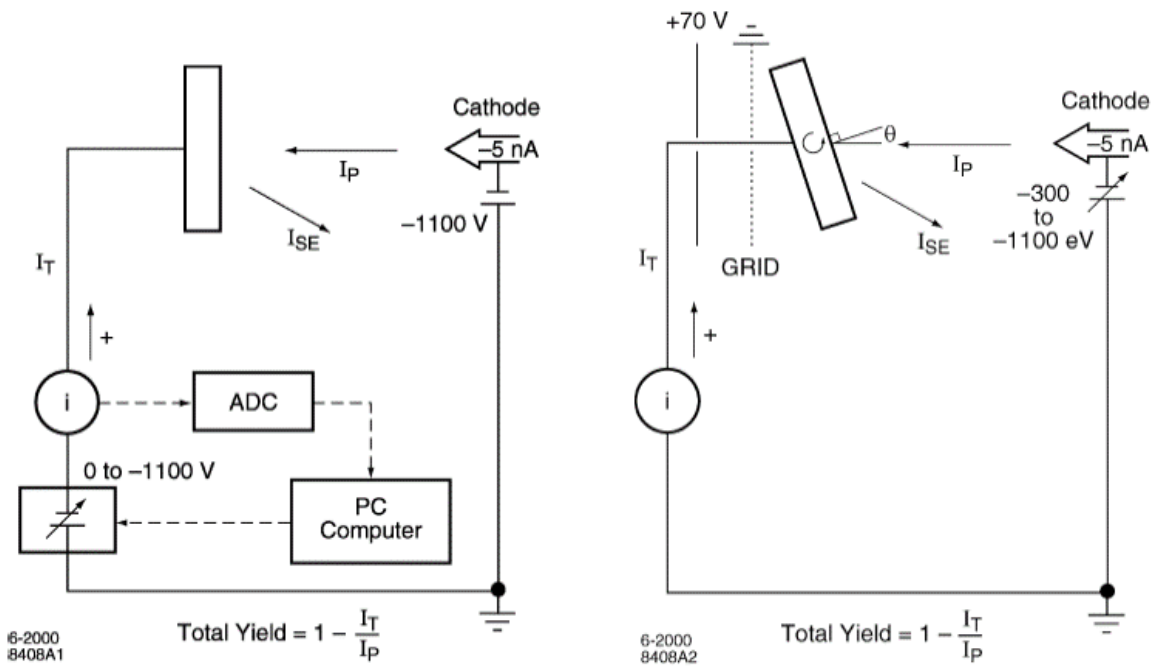


Figure 1: Typical SEY Measurement Setup (left), and with Modification for Angular Dependence Measurements (right). Source: Kirby and King 2001 [2]

In 1995, David Joy first published the most comprehensive collection of measured SEY data [3] known to the authors, with data sources going back to as early as the 1930s. The database's most recently published update was in 2008 [4], and contains data from 137 experimental sources and tabulates secondary electron yield, backscattering yield, X-ray ionization cross sections, and electron stopping powers for both elements and chemical compounds. Joy states that his aim is purely to gather data in one place, and Joy intentionally does not include data that is "the result of interpolation, extrapolation, or curve fitting" [4]. No effort was made by Joy to evaluate the accuracy or precision of the data. A significant limitation of Joy's database is that the vast

majority of the data sets contain no information about how the sample was processed prior to and during SEY measurement, which can significantly influence measured SEY as can be seen in Figure 2 for various aluminum SEY curves. Another limitation of the data within Joy's database is the relative sparsity of data for electrons with incident energies above a few tens of keV.

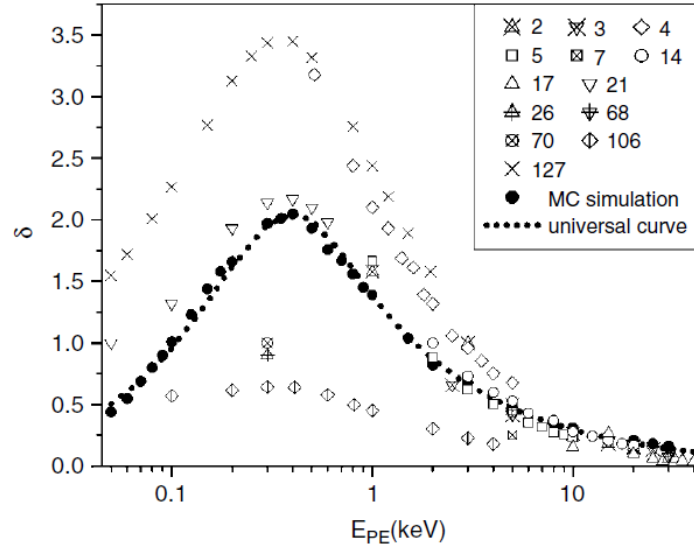


Figure 2: Example of Data Variability in SEY for Aluminum, Legend Numbers Refer to Different References from the Joy Database. Source: Lin and Joy 2005 [5]

Detailed studies have shown that a number of factors can affect the secondary electron yield of a material, including:

- Surface/Bulk contaminants [1,6-11],
- The electron dosing effect [1,2,6,12,13],
- Surface temperature [9,10,14],
- Surface texture/roughness [6,13-17], and
- Surface/Material thickness [7,11,18].

These are not all independent of each other, for example electron dosing or heating a sample can reduce surface contaminants, or the process of cleaning the surface of a sample can change its surface texture [16]. However, it is useful to separately focus on each of these factors in the following discussion.

When pure materials such as copper and aluminum are exposed to air, oxides can develop on the surface and various atmospheric gases can be adsorbed at the surface. The presence of these additional materials influences the SEY, since the SEY becomes the aggregate SEY of the

surface materials instead of the SEY of the desired pure material. A 2015 study by Cimino et al [8] tested two differently-sourced copper samples, both as received and after a thorough cleaning via argon ion sputtering. The samples as received, after a quick wash with ethanol and deionized water, had significantly different secondary electron yields from each other, but converged to nearly identical yield curves after argon ion sputtering removed nearly all of the surface contaminants, as shown in Figure 3; Cimino et al identified their plotted copper sample sources as oxygen-free high thermal conductivity (OFHC) and Large Hadron Collider (LHC), the particulars of which are not pertinent for the present discussion.

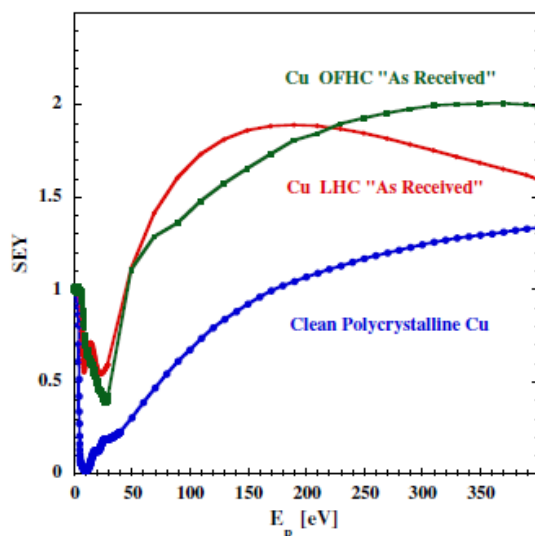


Figure 3: Surface Contaminants Resulted in Significantly Different SEY Curves for Two Differently-Sourced Copper Samples (Red and Green Curves), which Converged to the Blue Curve After Argon Ion Sputtering. Source: Cimino et al 2015 [8]

In a similar fashion, differences in trace materials introduced during the manufacturing process can also affect the secondary electron yield of a material. A 2005 study by Le Pimpec et al [1] tested different types of technical aluminum and found a variation in secondary electron yield maximum between three different samples: Al 1100 ($\geq 99\%$ Al by weight, with 0.2-0.5% Cu and possible impurities of Mn, Zn, Si and Fe), Al 6063 (98.9% Al, 0.45-0.9% Mg, 0.2-0.6% Si, same trace impurities as Al 1100), and a heavily-oxidized piece of Al 6063 retired from the SLAC Low Energy Ring (LER) beam chamber. In addition to the effects of trace materials and their effect upon SEY, this study also illustrated the effects of both electron dosing and the complex surface chemistry which can influence SEY. Electron dosing, similar to argon ion sputtering, is a means of removing surface contaminants from a sample undergoing SEY measurement.

See Figure 4 for the plots from le Pimpec et al which show the maximum SEY for the three different aluminum samples as a function of electron dosing. In these curves, Le Pimpec et al

believe that the high-dose rise in secondary electron yield was from decomposing adsorbed carbon dioxide and carbon monoxide, and the formation of new aluminum oxide, the presence of which was confirmed via x-ray photoelectron spectroscopy. A similar decrease in SEY vs. electron dosing was demonstrated for copper by Baglin et al in [12].

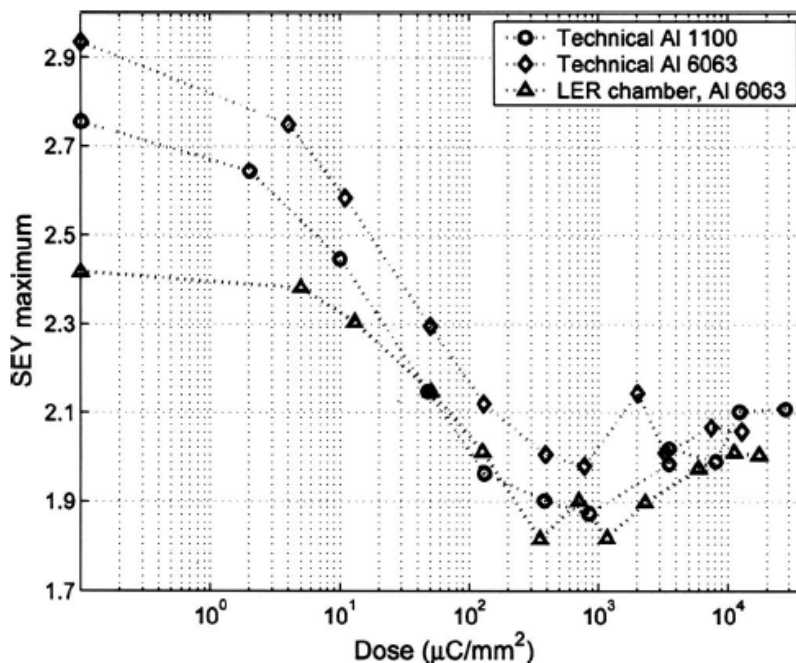


Figure 4: Aluminum Maximum SEY vs. Prior Electron Dose. Source: Le Pimpec et al 2005 [1]

The temperature dependence of secondary electron yield has been studied by Hu et al [10] for temperatures above room temperature. Hu et al report that for copper, the maximum secondary electron yield increases with increasing sample temperature, and that the full-width half-max (FWHM) of the secondary electron energy spectrum decreases with increasing sample temperature as shown in Figure 5. To explain these trends, Hu et al propose that heating the samples causes thermal desorption of gases, including adsorbed argon from the argon sputter cleaning; Hu et al also suggest a possible smoothing of surface morphology at higher temperatures. Another study by Balcon et al [14] found a similar increase in secondary electron yield with increasing temperature in alkali silicate glass, an insulator, when measured at 23°C

and 80°C. Balcon et al propose that this effect is due to an increase of conductivity in their insulator, making it easier for charge carriers to flow to the surface of the material.

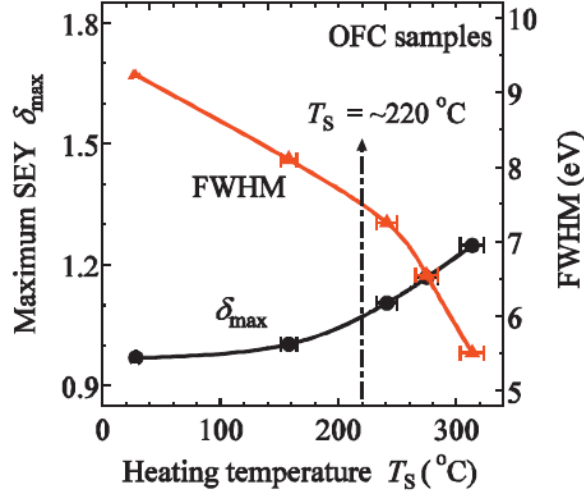


Figure 5: Variations in Maximum SEY (Red) and FWHM of Secondary Electron EES for Ion-Cleaned Copper Samples. Source: Hu et al 2014 [10]

3.1.3 Semi-empirical models

As far as the authors are aware, a rigorous theoretical SEE treatment which can accurately predict real-world SEY curves does not exist, but semi-empirical models do provide insight into some of the underlying physics. Seiler introduced one such semi-empirical model of secondary electron yield in a 1983 paper [19], which assumes that the secondary electron yield has the following form:

$$\delta(E_{PE}) = \int n(x, E_{PE}) f(x) dx \quad (2)$$

Equation 2: Semi-Empirical SEY Model

where $n(x, E_{PE})$ is the number of secondary electrons produced at material depth x by primary electrons with energy E_{PE} , and $f(x)$ is the probability that a secondary electron produced at depth x will reach the surface. Generally, $n(x, E_{PE})$ is assumed to have the form $n(x, E_{PE}) = -\frac{1}{\varepsilon} \frac{dE}{dx}$ where ε is the energy needed to produce a secondary electron, and $\frac{dE}{dx}$ is the rate of energy dissipation within the material. It is commonly assumed that $f(x) = Be^{-x/\lambda}$, where $B < 1$ and λ is the effective secondary electron escape depth.

In the 1983 Seiler paper, many simplifying assumptions were made, including that the energy dissipation rate is constant for a given primary electron energy: $\frac{dE}{dx} = -\frac{E_{PE}}{R}$, where R is the

penetration depth of the incident electron, which depends on the incident electron's energy and the density of the material. Since then, refinements have been made to this model, including different models for the penetration depth and energy dissipation rate [5,20-26]. There have also been parameter fitting studies where the semi-empirical model is applied to aggregated data [5] or newly taken data [26] for a single element, to obtain the best fit for that particular element, and repeated over many elements. The Seiler model and its descendants only models the secondary electron yield, and not the energy or angular distributions of the emitted secondary electrons, which does present a limitation if such models are used as part of a larger SEE model.

Balcon et al also note that surface roughness is a factor when measuring secondary electron yield. From the semi-empirical model, it is clear that increasing the angle of incidence of an incoming electron will increase secondary electron yield, as any secondary electrons produced will have a shorter distance to travel to escape the material surface. Measurements show this to be true, e.g. [1,2,27,28]. However, with a rough surface each electron of an incident electron beam will strike at a different angle, washing out the usual increase of secondary electron yield with angle of incidence, see Figure 6.

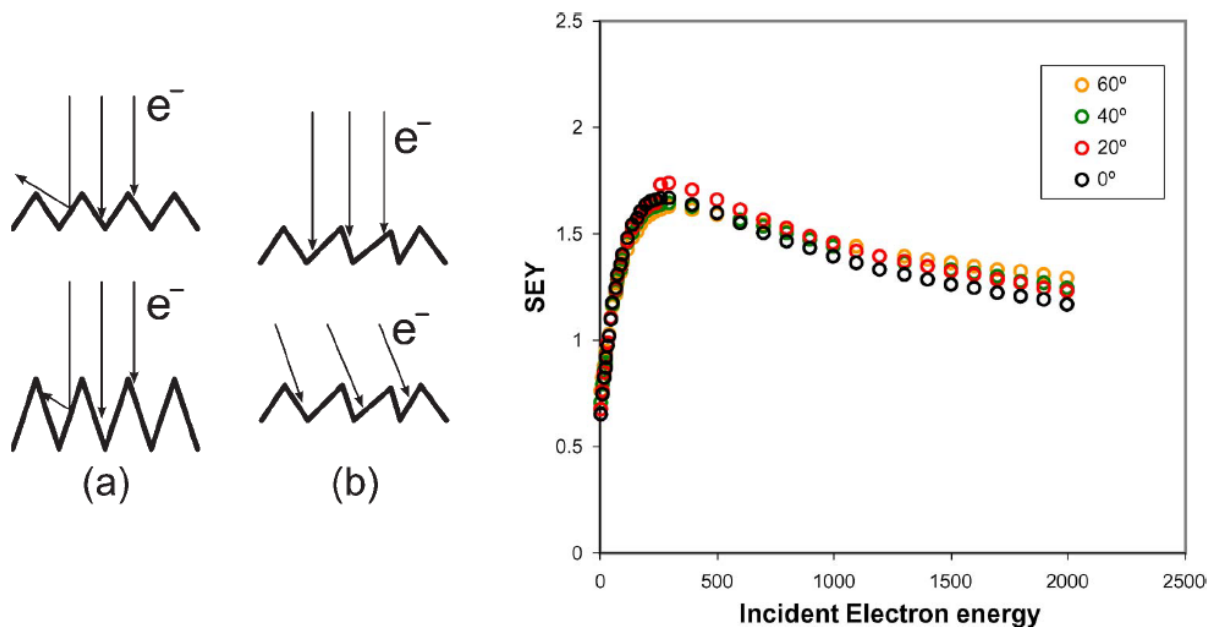


Figure 6: Effects of Surface Roughness on SEY. Geometrical Considerations (left) and SEY of a Rough Chromium surface at Several Angles of Primary Electron Beam Incidence (right). Source: Balcon et al 2012 [14]

Finally, the secondary electron yield of a thin film will increase with increasing film thickness as long as the film thickness is less than the maximum escape length [7,11,18]. Again, this is easily

illustrated with the semi-empirical model, since primary electrons have more material to travel through and generate more electrons. Similarly, adding low yield thin films to the surfaces of bulk materials is a common way to reduce secondary electron emission in the particle accelerator community, which often seeks to suppress multipactor in beam lines to maintain beam integrity[1,2,6,8,29].

3.1.4 Modeling and simulation

The authors are aware of two main parametric models frequently utilized for practical incorporation of SEE within plasma simulation codes. The first, preferred by the microwave device community, is a phenomenological model by Vaughan [30-31] that aims to model the “universal curve” of secondary electron emission that is seen when normalizing the plot of secondary electron yield versus primary electron energy. The second, preferred by the particle accelerator community, is a probabilistic model developed by Furman and Pivi [32] that is applied to a specific material, in contrast to the “universal curve”.

The semi-empirical models discussed in the previous section can also be used for SEE incorporation with plasma simulation codes, but would likely result in slower execution time due to the need to numerically evaluate an integral for each incident electron, instead of a rapid function call to a parametric model. Similarly, there are also other models that borrow strategies from radiative transfer theory [33] or use Monte Carlo codes [34] with differential scattering cross sections [35-39]. The radiative transfer method of Aoufi and Damamme [33] is specifically designed to model insulators, and may be of limited interest for the case of conductors. These more complicated methods, while potentially allowing for more accurate modelling of the underlying SEE physics than simple parametric models, are not considered to be practical for large-scale plasma simulation due to the computational costs, and as such are not considered further in this report for such purposes. However, we will rely upon the Monte Carlo particle-material interaction code GEANT4 to generate SEE statistics upon which we fit a parametric model, as will be discussed in Sections 3.2 and 4.1.

3.1.5 Vaughan Model

The Vaughan SEY model proposes a “universal” curve that can approximately represent the secondary electron yield for various materials when the appropriate model parameters are selected. Vaughan's SEY model requires only about 10 parameters, and using Vaughan's suggested values for some of the less critical parameters leaves only 4 parameters to characterize any given material. One important feature of Vaughan's model is that the SEY is set to zero below a certain threshold impact energy, which Vaughan proposes to be at 12.5 eV. This model provides a good fit to the data around the peak of secondary electron yield, but underestimates the secondary electron yield in the low-energy regime near or below the threshold impact energy, as well as in the high-energy regime $E \gtrsim 3E_{max}$, where E is the incidence energy and E_{max} is the incidence energy which maximizes the SEY. An important limitation of Vaughan's model is that it only specifies an SEY curve, and not the energy and angular distribution for the emitted

electrons, both of which would also need to be specified if this model is to be used in numerical simulations.

A 2017 paper by Ludwick et al [40] attempts to improve upon Vaughan's model by doubling the number of free parameters, which is accomplished by separately fitting Vaughan's model below and above E_{max} . This model can improve upon Vaughan's fit to measured data, at the expense of more parameters. As with the limitation with Vaughan's model, Ludwick's model only specifies SEY, and not the secondary electron emission energies or angles.

3.1.6 Furman and Pivi model

Furman and Pivi [32] provide a model which describes secondary electron emission using a probabilistic approach that is closely linked with the emission kinematics of the secondary electrons. There are approximately 45 parameters per material used in this model, with some allowance for more or fewer parameters in order to capture or neglect features in the secondary electron emission.

The Furman model considers secondary electrons as emerging from three underlying categories (or species): true secondaries, rediffused electrons, and elastic electrons. While such categories are not strictly true from a quantum mechanics viewpoint, this conceptual framework allows for simplifying assumptions in the secondary electron emission model. Within this framework, elastic electrons are incident electrons that have been scattered off the surface with nearly the same energy as the incident electron, and tend to show up as a cluster in the emission energy spectra. Rediffused electrons are electrons that entered the material, interacted with atoms inside the material and shed some energy, and then reemerged from the material with reduced energy. True secondary electrons are electrons that have been liberated from the material due to energy deposited by the incident electron as it traverses the material. ICEPIC makes similar distinctions, but with different names; elastic electrons are called reflected electrons and rediffused electrons are called scattered electrons.

Each of these secondary electron types have different emitted energy spectra. The true secondaries have a Maxwell-Boltzmann velocity distribution with temperature typically between 2 and 4 eV. The rediffused electrons have an almost uniform distribution but with a slight positive slope with incident energy. The elastic electrons have a Gaussian-like distribution with a peak at the incident energy and a width that varies with incident energy and angle. The integral of the total emitted energy spectrum at a particular incident energy and angle give the SEY at that energy and angle.

3.1.7 Section Summary

In section 3.1 we provided a brief overview of the present state of SEE experimental data and associated modelling efforts. The vast majority of prior SEE work has focused on incident electron energies up to a few tens of keV, resulting in insufficient measured data to reliably form a general SEE model at incident energies on the order of 100 keV – 1 MeV, which we desire for

ICEPIC. It is for these reasons that we turn our attention to generating the necessary SEE data, as will be explained in section 3.2.

3.2 Modelling SEE in GEANT4

3.2.1 Introduction

Section 3.2 documents the use of GEANT4 to characterize SEE, in particular the SEY and EES as a function of incident energy. Section 3.2.2 briefly introduces high energy physics (HEP) concepts as a foundation to understand GEANT4. Section 3.2.3 describes how GEANT4 uses HEP principles to track particles in materials. Section 3.2.5 outlines the HEP interactions of greatest importance to SEE. Section 3.2.6 briefly covers the physics models available in GEANT4 for these interactions. Section 3.2.7 describes the simulation scenario employed in this report to generate SEE data, and Section 3.2.8 explains how SEE distributions are created using the results of the simulations. Section 3.2.9 compares selected SEY curves across three successive GEANT4 releases from 2017 through 2019, in order to assess consistency and code maturity. We then conclude in Section 3.2.10 by summarizing the GEANT4 SEE modelling effort.

Unless otherwise noted, all GEANT4 results in this report were produced using version 10.05 patch 1. Version 10.05 was released in December 2018 and was the most up-to-date version available at the commencement of this work. A more recent version 10.06 patch 3 has since become available, which was only used for some minor checking of code self-consistency as discussed in Section 3.2.9.

3.2.2 A Brief Introduction to High Energy Physics

GEANT4 was made by high energy physicists for simulating detectors used in HEP. This section aims to introduce the reader to the terminology of HEP and GEANT4.

The goal of HEP is to describe fundamental particles and their interactions. This is commonly done using the Standard Model (SM). There are 17 fundamental particles in the SM: 6 quarks, 6 leptons, 4 force carriers, and 1 mass generator. These particles interact with each other via four forces: the electromagnetic force, the weak force, the strong force, and gravity (which is not included in the SM and will not be discussed further). The three forces the SM does include are each mediated by one or two of the force carriers.

The electromagnetic force deals with electrically charged particles interacting with each other and is mediated by the photon. The electrically charged particles are the quarks, three of the leptons (including the electron), and one of the two weak force carriers. The portion of the SM that describes how these electrically charged particles interact with the photon, and with each other through the photon, is Quantum Electrodynamics (QED). Within GEANT4, electromagnetic interactions are synonymous with QED particle interactions.

The strong force deals with colored particles interacting with each other and is mediated by the gluon. The colored particles are the quarks and the gluon. A hadron is any non-fundamental

particle made up of quarks, such as protons and neutrons, and hadronic matter is then any matter made up of hadrons. The portion of the SM that describes how colored particles interact with the gluon, and with each other through the gluon, is Quantum Chromodynamics (QCD). Within GEANT4, hadronic interactions are synonymous with QCD particle interactions.

The weak force deals with particles that have weak isospin interacting with each other and is mediated by the W and Z bosons. All particles except the photon and gluon have weak isospin. There is not a special name for the portion of the SM that describes weak force interactions.

Finally, particles that have mass (all the particles except the photon and gluon) will interact with the Higgs boson, which is the mass generator. The fundamental particles get their masses by interacting with the Higgs boson.

The different interactions that come from the SM can be coupled together to create physical processes. While there are technically infinitely many physical processes, there are a finite number that overwhelmingly occur in nature, which GEANT4 uses to simulate particles interacting with matter.

The probabilities of particles interacting to yield a physical process are specified as interaction cross-sections. Classically, these cross-sections may be visualized as 2D cross-section projections of a 3D objects interacting with each other. However, in quantum mechanics, the interpretation is more complicated due to particle locations being represented as a wave function density instead of an object with clear boundaries, as well as the involvement of forces operating over a distance. Interaction cross-sections can be given for binary interactions involving only two fundamental particles, or for more complicated scenarios involving a particle interacting with a group of other particles (such as an atom).

We also note that when considering secondary electron emission, the inbound particle is an electron, but any physically permissible particles may appear in the GEANT4 simulation, and these additional particles may affect the overall secondary electron emission. For example, consider that an incident electron traversing a material could experience Moller-Bhabha scattering (electron scattering off electron), Bremsstrahlung radiation (electron interacts with nucleus and emits a photon), and Coulomb scattering (electron interacts with nucleus). In the case of Bremsstrahlung radiation, it is then possible for the emitted photon to interact with a nearby atom and eject an electron via the photoelectric effect. Compton scattering also allows for the possibility of a photon to interact with an atom and produce a scattered photon of different energy; this scattered photon could then produce a yet different energy electron via the photoelectric effect. The net effect of all possible secondary electron production events yields the overall secondary electron emission.

3.2.3 GEANT4 Particle Tracking

GEANT4 uses the physical processes from HEP to create Monte Carlo simulations of particles interacting with matter [41]. As a particle travels through a material it has some probability of interacting with the particles that make up the material, as represented by different interaction cross-sections. These interactions can result in the original particle deviating from its trajectory, the excitation of particles in the material, or even the creation of new particles. The physically permissible interactions that can occur depend on the type of particle traversing the material and its energy, as well as the material properties.

Before considering the effects of particle interactions, GEANT4 first numerically integrates the Lorentz force equation to determine the hypothetical particle trajectory in the absence of interactions. GEANT4 then uses the interaction cross-sections of various physical processes to randomly determine how far the particle actually moves during each step of the simulation [42]. It does this by calculating the mean free path for each type of interaction (using the interaction cross sections), and then uses Monte Carlo techniques to determine a set of distances travelled before interaction for each potential physical process; the physical process corresponding to the shortest distance is then chosen, or the particle exits the material if no interaction occurs in a small enough distance. The benefit of parametrizing a material using interaction mean free paths is that GEANT4 does not need to explicitly model each particle constituting the material, but rather treat interactions probabilistically.

In addition to the stochastic simulation of interactions as described above based on mean free path, two other interaction situations can arise within GEANT4 simulations. The first of these situations are interactions that can occur for particles at rest with respect to a material. Instead of these interactions occurring after a random distance, these interactions occur after a random time. The second of these situations involve interactions that can change the energy of a particle, and therefore modify the trajectory as computed from the Lorentz force equation, but do not produce new particles.

3.2.4 Production Thresholds & Range Cuts

Absent further constraints, the GEANT4 particle tracking would default to tracking electrically charged particles until they decay or lose all of their kinetic energy [41]. However, for various purposes it is necessary to limit certain interaction processes based on energy or distances.

- Example performance purpose: If it is known that a particle will not make it out of its current medium (and will not produce more particles due to energy limitations), then it is more efficient to deposit the energy of the particle into the medium instead of tracking it. GEANT4 refers to these early terminations as range cuts.
- Example physical purpose: Due to some processes, it is required that the tracking of certain particles (mainly photons, electrons, and positrons) be cut short to avoid infrared divergence, which allows for the generation of an infinite number of photons or electrons

with infinitesimally small energies. GEANT4 refers to these early terminations as production thresholds.

- Example modeling limitation: Some GEANT4 models, including those involving physical processes that we expect would contribute most to SEE, are not validated or accurate down to interaction energies of 0 eV. This means that if a particle is produced below the lower limit of validity, any interactions it undergoes that use these models will produce inaccurate results.

For these reasons, there are cuts and thresholds which limit the energy of particles generated in GEANT4 simulations. If a proposed particle from an interaction does not meet or exceed the relevant threshold, its energy is simply deposited into the material it is currently in, without any further physical effects. A production threshold matching the lower limits of the tested models (10, 100, or 1000 eV) was chosen for these studies. In addition, a range cut of 1 nm was chosen so that these lower limits in energy could be reached.

3.2.5 Relevant Particle Interactions & Processes

GEANT4 is capable of simulating a wide range of particle interactions, but for the incident particles in this study (electrons with a rest mass of 0.511 MeV), and at the kinetic energies considered in this study (up to a few tens of MeV at most), the energetically allowable processes that contribute to secondary electron emission are ionization (Moller-Bhabha scattering), Coulomb scattering, Bremsstrahlung radiation, the photoelectric effect, and Compton scattering. All of these interactions are electromagnetic processes involving electrically charged particles interacting with each other and the photon.

Ionization within GEANT4 is the process in which an electron interacts with an atom and ejects one of the atom's electrons from an atomic orbital into the continuum. If the released electron has a sufficiently high energy, it is often called a delta-ray. In terms of fundamental processes, this is represented as Moller (electron-electron) or Bhabha (electron-positron) scattering.

Coulomb scattering is the scattering of a charged particle by a Coulomb potential. In GEANT4 this usually takes the form of a free particle interacting with an atom's nucleus. The underlying physical interaction being modelled is elastic, meaning any energy lost by the particle is transferred to the nucleus. Within our simulations, this transferred energy is simply deposited in the material without further physical effects.

Bremsstrahlung radiation occurs when an electron or positron radiates a photon via interacting with a nucleus. This occurs due to the acceleration or deceleration of the charged particle, and the subsequent radiation of a photon. This effect may contribute to secondary electrons if the radiated photon then interacts with an atom via the photoelectric effect, resulting in an electron emission.

The photoelectric effect occurs when a photon interacts with an atom and ejects one of the atom's electrons from an atomic orbital into the continuum. The photon is absorbed in this process.

Compton scattering is similar to the photoelectric effect in that an incident photon ejects an electron, except that the photon only loses some energy instead of being absorbed. The photon can then continue through the material.

3.2.6 GEANT4 Interaction Models and Physics Lists

In order to produce quantitative results, the interaction processes must have mathematical models defined. GEANT4 allows for considerable user flexibility to select various pre-defined models, depending on factors such as accuracy, computational cost, and energy ranges of validity; users can also define their own models if needed. Even though GEANT4 users can individually define or select desired models for each of the many physical processes, in practice it is more convenient to use pre-defined GEANT4 physics lists [43]. These lists are tailored for the specific needs of different GEANT4 user communities, and allow for standardized comparisons among results generated by different users.

Physics lists are composed of two parts: a portion specifying which hadronic models are used, and a portion specifying which electromagnetic models are used. Due to energetic considerations, hadronic processes are unlikely to occur in the SEE simulations, and are unlikely to change the results of the simulation. The QGSP_BERT hadronic processes list was somewhat arbitrarily selected because it is one of the most recommended lists in the GEANT4 documentation.

For the electromagnetics portion of the physics list, there are four popular options: the default models, as well as the Penelope models [44], Low Energy Livermore models [45], and DNA models [46]. Among the default models there are several variations, but all variations use models targeting energies between 1 keV and 100 TeV. The Penelope and Livermore models build upon one of the variations of the default models (the opt3 variation from reference [43]), and target different energies: 100 eV – 6 GeV for Penelope models, and 10 eV – 100 GeV for Low Energy Livermore models. The DNA models support energies as low as 2 eV, but are only validated for water and DNA materials, and as such are not relevant to this study.

Among the widely recognized electromagnetics physics lists which are validated for materials of engineering interest, the Low Energy Livermore models are the most applicable for the production of secondary electrons which in the real-world can span energies between 0 eV and the incident electron energy.

3.2.6.1 The Default Models

In this section we briefly discuss the GEANT4 default models of particular importance to SEE, in order to better understand the relevant GEANT4 physical processes, and also to better understand what the alternative Penelope and Livermore models do differently.

The default ionization model [47] treats ionization in one of two ways depending on the maximum energy transferable to a free electron: continuous energy loss if the maximum transferable energy is less than the production threshold of electrons, or the explicit production

of delta-rays if the maximum transferable energy is above the production threshold. In the case of continuous energy loss, the electrons produced via ionization are not inserted into the simulation, but rather are simply treated as energy deposited into the ionized material and subtracted from the energy of the incident electron. If the maximum transferable energy of an incoming electron exceeds the production threshold, then a delta-ray can be produced.

GEANT4 includes Coulomb scattering in two processes: multiple scattering [48] and single scattering [49]. Since these two models fulfill different purposes, the GEANT4 physics lists treat them separately. The formulation for multiple scattering can be found in reference [48] and the formulation for single scattering can be found in reference [49].

GEANT4's default model for Bremsstrahlung radiation [50] is similar to the ionization model in that below a certain energy threshold an incident electron undergoes continuous energy loss instead of explicitly producing a photon, while above that energy threshold a photon is inserted into the simulation.

GEANT4's default model for the photoelectric effect [51] uses atomic shell information to produce electrons. If the energy of the photon is greater than a shell's energy, then a photoelectron (free electron) can be produced. GEANT4 picks the closest available atomic shell. The energy used to create the photoelectron is then subtracted from the photon and its trajectory modified.

GEANT4's default Compton Scattering model [52] is actually two models used in combination. The first model is valid above 10 keV and ignores atomic shell effects. The second model includes atomic shell effects and extends the energy range down to 1 keV, at the expense of more computational cost.

Due to the Default models being accurate down to interaction energies of 1 keV, a low energy threshold cut of 1 keV was used for all Default model simulations considered in this study; this means that no secondary electrons with kinetic energies less than 1 keV could be considered with these particular models.

3.2.6.2 The Penelope Models

The Penelope models [44] were developed specifically for Monte-Carlo simulation with extra attention placed on relatively low energy physics [53], as compared to the MeV-to-TeV range of energies typically encountered in modern particle accelerators. With respect to the interaction models being particularly relevant to SEE, there are Penelope models available for ionization [54], Bremsstrahlung radiation [55], the photoelectric effect [56], and Compton scattering [57]. Unfortunately, there is no Penelope model for Coulomb scattering. The Penelope models are considered accurate down to energies of 100 eV

Due to the Penelope models being accurate down to interaction energies of 100 eV, a low energy threshold cut of 100 eV was used for all Penelope model simulations considered in this study;

this means that no secondary electrons with kinetic energies less than 100 eV could be considered with these particular models.

3.2.6.3 The Low Energy Livermore Models

The Low Energy Livermore models [45,58] (often referred to as simply the Livermore models) make direct use of atomic shell cross section data [59-63], in order to more accurately model low energy interactions than in the default or Penelope models. With respect to the interactions being particularly relevant to SEE, there are Livermore models available for the following processes: ionization [64], Bremsstrahlung radiation [65], the photoelectric effect [66], and Compton scattering [67]. Unfortunately, there is no Livermore model for Coulomb scattering.

Due to the Livermore models being accurate down to interaction energies of 10 eV, a low energy threshold cut of 10 eV was used for all Default model simulations considered in this study; this means that no secondary electrons with kinetic energies less than 10 eV could be considered with these particular models. Note also that this 10 eV threshold cut is lower than the standardized 100 eV threshold cut commonly used by other GEANT4 users with the Livermore models.

3.2.6.4 GEANT4 Model Validation

GEANT4 takes two approaches to validating its physics models [68]. At high energies where data is not available, simulation results are compared to theory predictions. At low energies where data is available, simulations are compared directly to relevant datasets. Since GEANT4 includes hundreds of different models, this validation is beyond the ability of any single person. There is a Testing and Quality Assurance Working Group [69] that validates GEANT4 weekly.

In an effort to assess GEANT4 repeatability among point releases, which should ideally change little if the code results are indeed valid (reasonably representing reality), the authors of this report compared the predicted SEY for three successive point releases of GEANT4, specifically 10.04, 10.05, and 10.06, as will be discussed in Section 3.2.9. Unfortunately, those results do show significant differences, which present some unresolved questions about the validity of the GEANT4 models.

3.2.7 Secondary Electron Simulation

With GEANT4 described, we are now in a position to consider the simulation of GEANT4 SEE data. A simulation volume was defined to consist of a cube with sides of length 0.5m centered at the origin, which is desired to be treated as a vacuum. GEANT4 does not come with a pre-defined vacuum material, so a vacuum was represented as a material (G4Material type) with an atomic number of 1, an atomic mass of 1.00784g, and density of 0, which GEANT4 will reset to the minimum allowable density of $1\text{e-}25\text{ g/cm}^3$.

Into this simulation volume was placed a material plate and an electron source, as shown in Figure 7. The material plate is centered at $x = 0\text{ cm}$, $y = 0\text{ cm}$, and $z = 5\text{ cm}$. The plate has equal x- and y-extents of 20 cm, and a z-extent of 5 cm. An electron source is placed on the x-axis, directing electrons towards the middle of the face of the material plate at a specified energy; the

specific location of the electron source along the axis allows for control of the incidence angle θ . For each trial, one electron is emitted from the source, and any electrons emerging from the lower plate face at $z = 2.5$ cm were recorded as a secondary electron. Many trials could thus be run in order to generate secondary electron emission statistics.

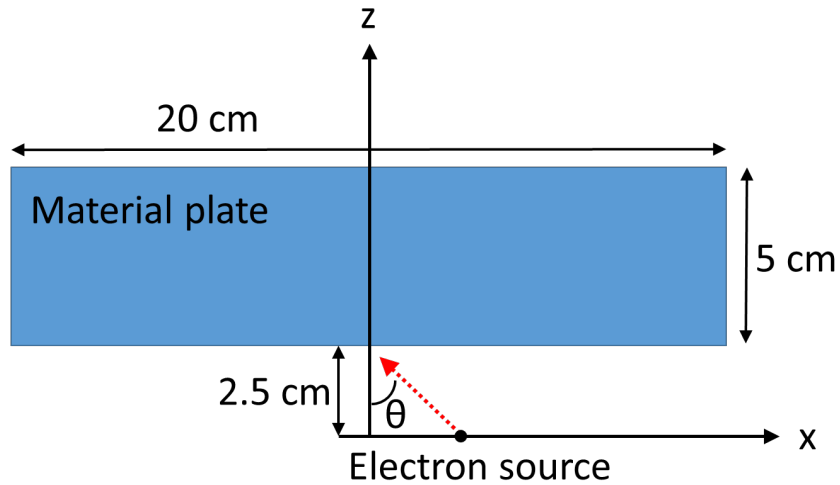


Figure 7: Setup Used to Simulate Secondary Electron Emission.

It is important to note that there is experimental data which show that SEY is dependent on the intensity of the beam (or equivalently, the dose of electrons the surface is getting C/mm^2), as was noted in section 3.1.2. This dose-dependent effect is beyond the capabilities of what we would be able to simulate in GEANT4 using the resources available to us, and is neglected in our analysis.

Secondary electron emission was simulated for incident electrons with energies ranging from 10 eV to 30 MeV in 25 logarithmically spaced points, and with incident angles ranging from 0 to 80 degrees in steps of 20 degrees. For each incident (energy, angle) pair, 10,000 trials were run for each of the three GEANT4 electromagnetics physics lists (default, Penelope, and Livermore) described above in Section 3.2.6. The secondary electron yield is then calculated as the total number of secondary electrons recorded divided by the number of incident electrons (10,000). The emission energy and angle for each secondary electron was also recorded in order to characterize the emission spectra.

A common assumption for secondary electrons is that regardless of the incident angle of the primary electrons, the secondary electrons follow a $\cos(\theta)$ angular emission spectrum, where θ is measured normal to the emission surface. This is not strictly true due to some bias towards a forward scattering direction (analogous to a ball bouncing obliquely from a surface), but when the surface roughness at the atomic scale is considered, there is not a well-defined forward scattering direction. The GEANT4 results did show a moderate bias towards the forward

scattering direction for oblique incident directions, but GEANT4 also assumes perfectly smooth surfaces, so the magnitude of this effect is likely over-estimated by GEANT4. ICEPIC currently assumes a $\cos(\theta)$ angular spectrum for true secondary and scattered electrons, and a specular scattering direction for reflected electrons. The authors believed that this was a reasonable choice for the angular emission spectrum, so we focused our efforts on the more significant discrepancies with the SEY curves and emission energy spectrums when comparing GEANT4 results and the historical ICEPIC SEE model.

3.2.8 Evaluation of GEANT4 Physics Lists

In this section we compare SEY curves produced by GEANT4 to SEY curves produced by the Vaughan [30,31] and Furman [32] models discussed in Section 3.1.4. For these comparisons, we limit ourselves to only copper and stainless steel, due to Furman's paper only providing appropriate model parameters for these two materials. For the SEY curves produced by GEANT4, we examine results generated with the three different physics list options discussed in Section 3.2.6, specifically the default, Penelope, and Livermore models.

The copper and stainless steel distributions from GEANT4 were respectively created using GEANT4's pre-defined G4_Cu and G4_STAINLESS-STEEL materials [70], the latter material defined to be 74% iron, 18% chromium, and 8% nickel. The Furman copper curves were created using the parameters defined in his paper, which Furman determined by fitting his model parameters to 25 different copper experiments; the Furman stainless steel parameters were determined by fitting his model to a single measured dataset of type 304 stainless steel. Type 304 stainless steel has a minimum of 18% chromium and 8% nickel, although the exact elemental proportions are not precisely specified beyond that. The Vaughan SEY distributions were created using parameters that recreate the Furman distributions near the peak at normal incidence.

The resulting copper SEY curves can be seen in Figure 8 through Figure 12 respectively for incident angles of 0°, 20°, 40°, 60°, and 80°. For an incident angle of 80° (Figure 12), we note that the GEANT4 results with all physics lists show a constant SEY coefficient of unity across all incident energies examined, with all incident electrons reflected elastically. This likely represents an intrinsic limitation to the GEANT4 physics models; no further investigation into GEANT4 incident angles approaching grazing was undertaken. For the remaining incident angles from 0° to 60°, it is evident the GEANT4 Livermore models shows a significant SEY deficit for incident energies below approximately 1 keV, and the GEANT4 Penelope and default models show a significant SEY deficit for energies below approximately 100 keV. This is due to the low-energy limits of these models and the respective production thresholds of 10, 100, and 1000 eV as described in Section 3.2.4. A significant portion of the EES (shown in Appendix A) is lost because it is below the GEANT4 energy production thresholds, of particular significance is the loss of low-energy secondary electrons which tend to be emitted from a surface following a Maxwell-Boltzmann distribution with a temperature of a few eV.

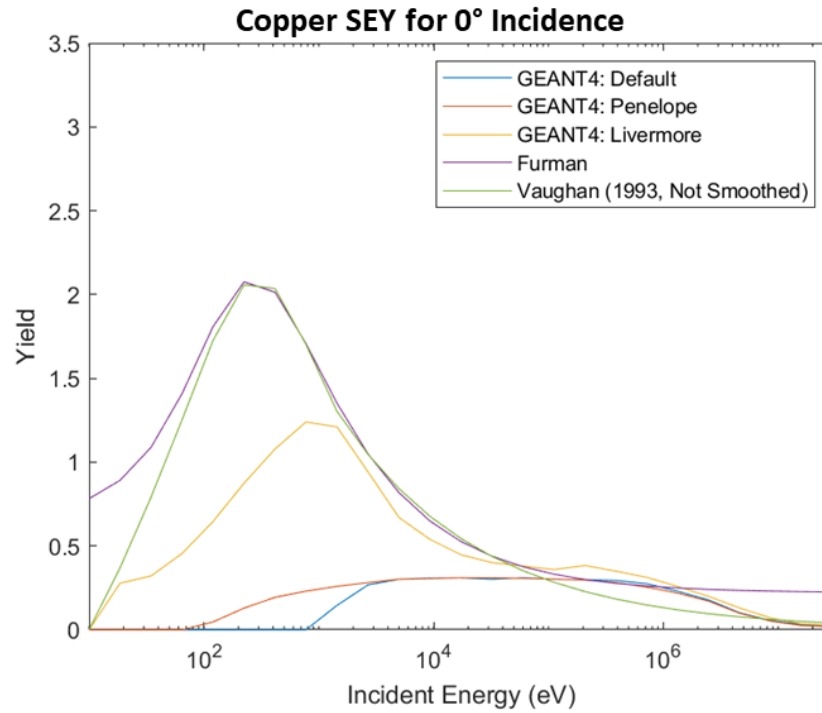


Figure 8: A Comparison of the Copper SEY Curves at 0° Incidence.

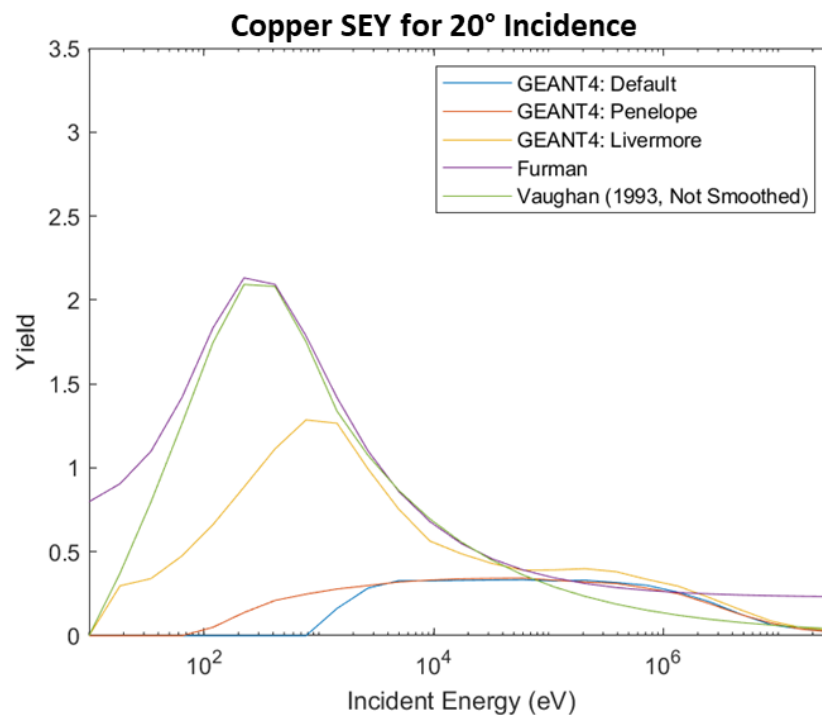


Figure 9: A Comparison of the Copper SEY Curves at 20° Incidence.

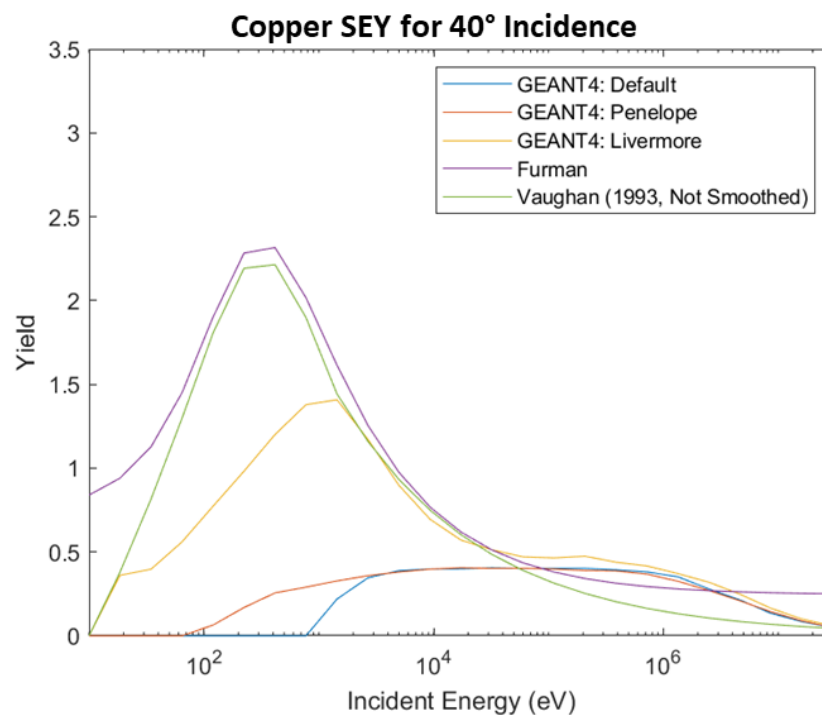


Figure 10: A Comparison of the Copper SEY Curves at 40° Incidence.

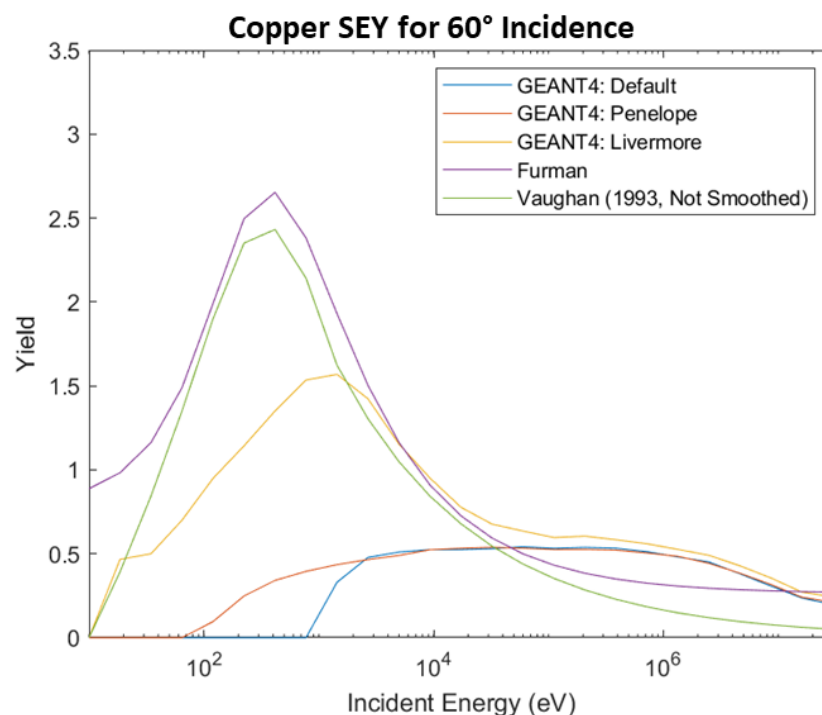


Figure 11: A Comparison of the Copper SEY Curves at 60° Incidence.

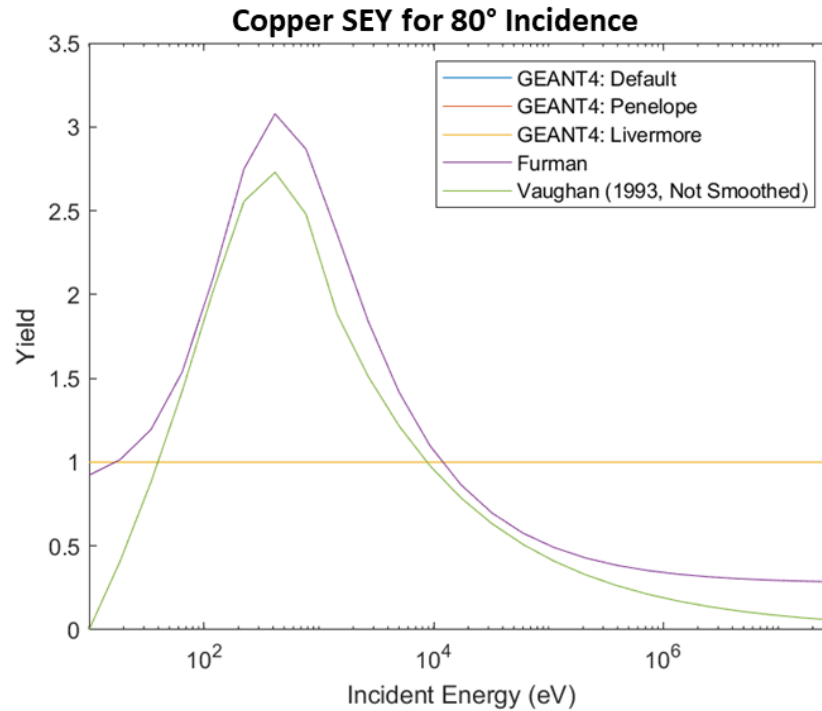


Figure 12: A Comparison of the Copper SEY Curves at 80° Incidence; All GEANT4 Curves Result in a Value of Unity.

The stainless steel SEY curves can be seen in Figure 13 through Figure 17 respectively for incident angles of 0°, 20°, 40°, 60°, and 80°. As with copper, for an incident angle of 80° (Figure 17) we note that all GEANT4 results show a constant SEY coefficient of unity across all incident energies examined, caused by all incident electrons being reflected elastically. Unlike the copper results in which the GEANT4 SEY curves exceed the Furman SEY curves above approximately 100 keV, for stainless steel all the GEANT4 SEY curves are significantly less than the Furman SEY curve across all incident energies and angles except at an incident angle of 80°. We do note that Furman chose his parameters to best fit measured stainless steel SEY data only up to incident energies of 1.1 keV, so his model behavior significantly above this energy may not be valid.

As with the copper results for incident angles from 0° to 60°, the GEANT4 stainless steel SEY curves show that the Livermore models produce a significant SEY increase at low incident energies as compared to the default and Penelope models. This is attributable to the Livermore models able to model interaction energies down to 10 eV, as opposed to 100 eV and 1000 eV respectively for the Penelope and default models.

Based on the SEY curves examined in this section, as well as EES curves in Appendix A, it is clear that the GEANT4 Livermore models are in closer agreement to the Furman and Vaughan

SEY curves than the GEANT4 default or Penelope models, due to the GEANT4 Livermore models being able to better produce low energy secondary electrons subsequent to a high energy incident electron impact. As a result, we have chosen to use the GEANT4 Livermore physics list for the production of all synthetic data we use to produce an updated the ICEPIC secondary electron emission model. Additional emission spectra for Aluminum, Niobium, Graphite, Aluminum Oxide (alumina), and beryllium oxide using the GEANT4 Livermore models can be found in Appendix B; all of these spectra and the associated SEY curves shown in Appendix C will inform the high incident energy SEE model introduced in section 4.1.

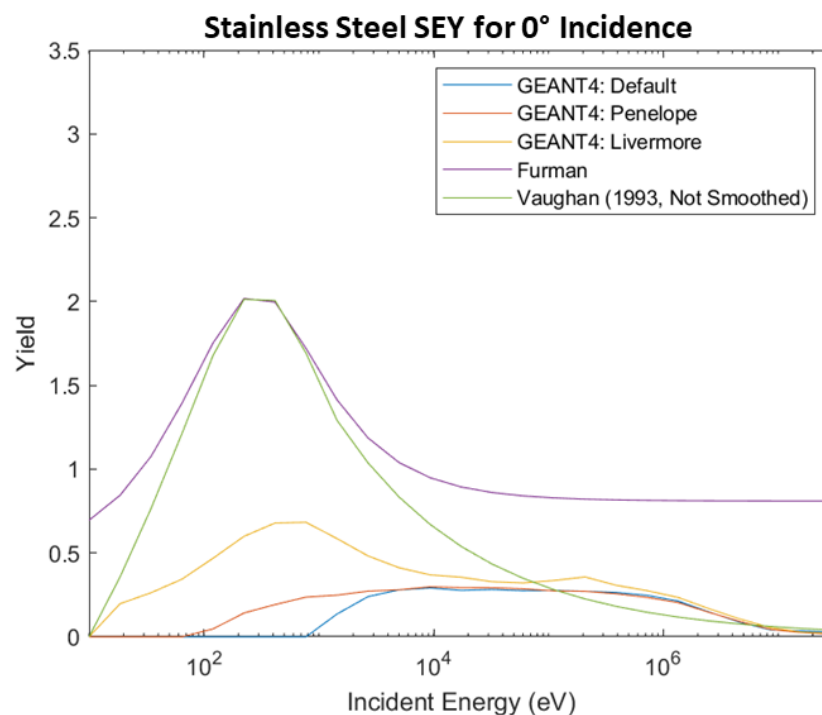


Figure 13: A Comparison of the Stainless Steel SEY Curves at 0° Incidence.

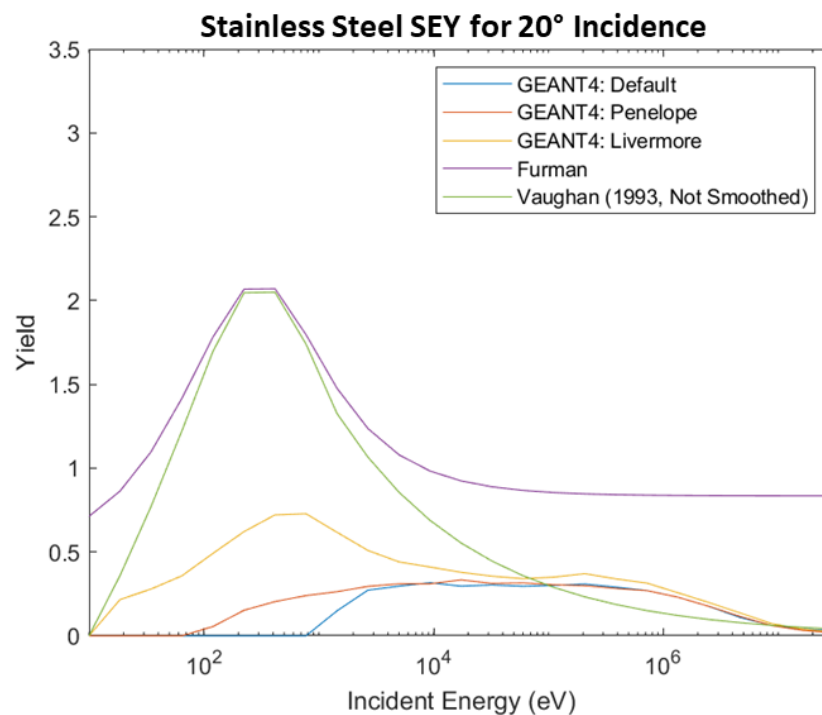


Figure 14: A Comparison of the Stainless Steel SEY Curves at 20° Incidence.

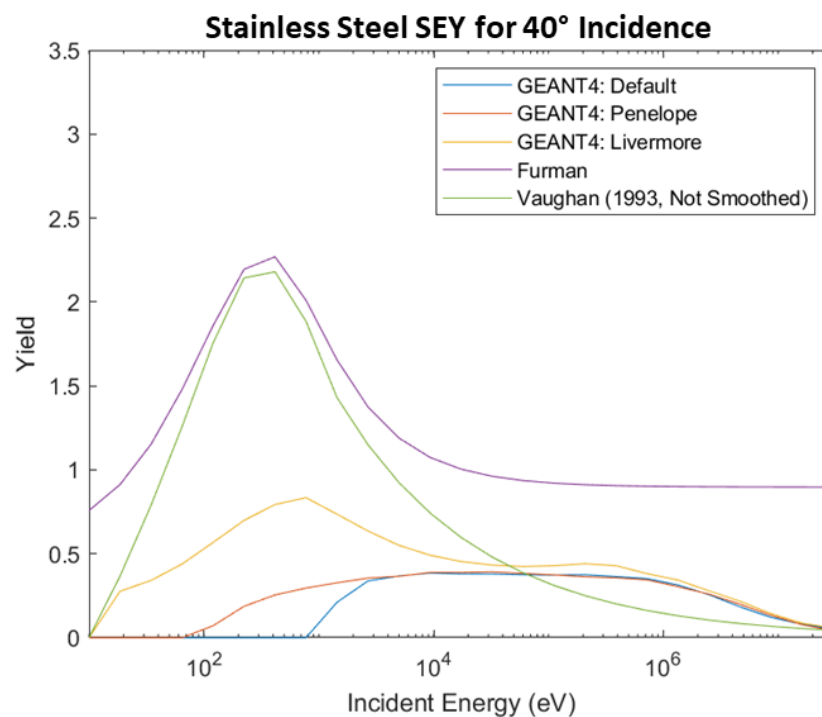


Figure 15: A Comparison of the Stainless Steel SEY Curves at 40° Incidence.

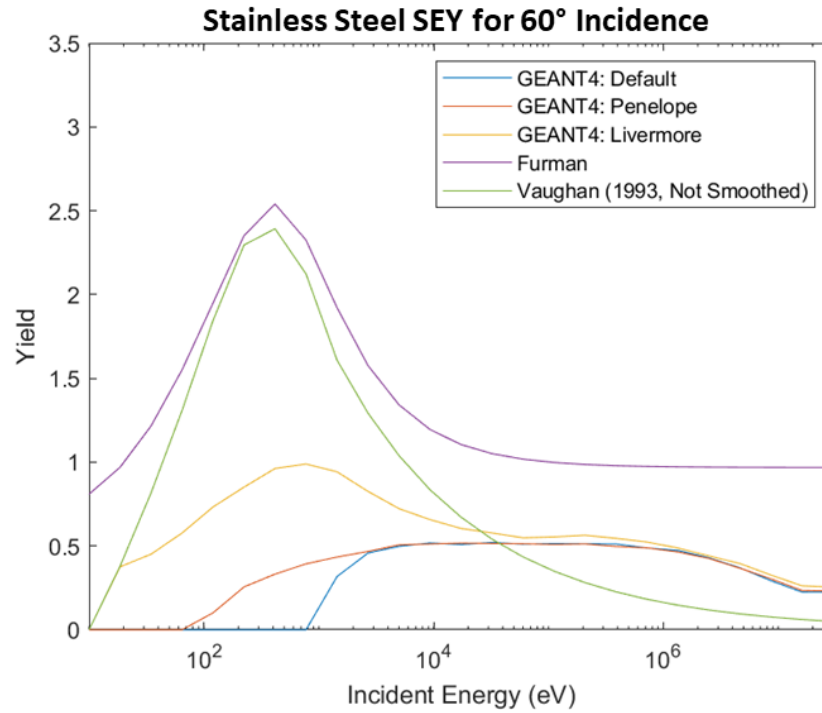


Figure 16: A Comparison of the Stainless Steel SEY Curves at 60° Incidence.

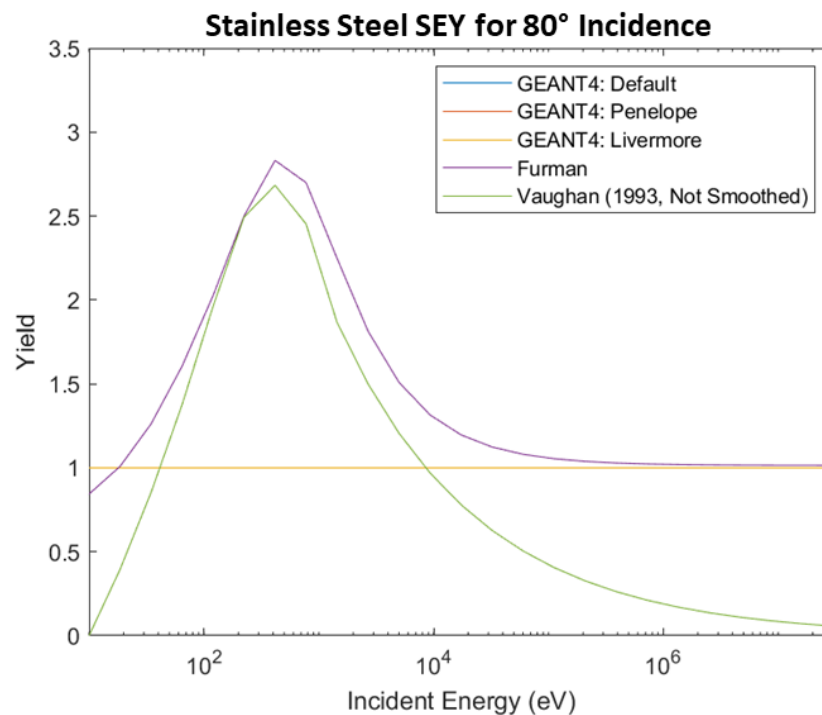


Figure 17: A Comparison of the Stainless Steel SEY Curves at 80° Incidence; All GEANT4 Curves Result in a Value of Unity.

3.2.9 GEANT4 Self-Consistency Between Point Releases

One indirect measure of the GEANT4 SEE prediction uncertainty is a comparison of predicted SEY curves across successive GEANT4 point releases. We then assume that the GEANT4 prediction uncertainty is at least as big as the differences among these results. Comparisons were made between the three most recent successive GEANT4 point releases: 10.04 (released December 2017), 10.05 (released December 2018), and 10.06 (released December 2019).

Figure 18 shows the comparison results for copper using the Livermore models, for both the lowered 10 eV production threshold used to generate the results in this report, as well as the default 100 eV production threshold typically used with this model. Similar comparisons are shown in Figure 19 for graphite, and in Figure 20 for niobium. For all materials we used the GEANT4 built-in material definitions.

The results show non-trivial SEY differences between the three most recent successive GEANT4 point releases 10.04, 10.05, and 10.06, especially between version 10.04 and the subsequent two point releases. This lack of consistency suggests significant uncertainty in the GEANT4 SEY curves. This conclusion may be somewhat concerning for anyone seeking to perfectly characterize SEE behavior from GEANT4 simulations, but it should be noted that among measured SEY data, there are also significant differences which are not all well-understood or able to be well-controlled. Regardless, the authors do believe that the GEANT4 SEY curves provide qualitatively representative results of real-world SEY curves, which are sufficient to develop a more general high incident energy SEE model for computer codes such as ICEPIC.

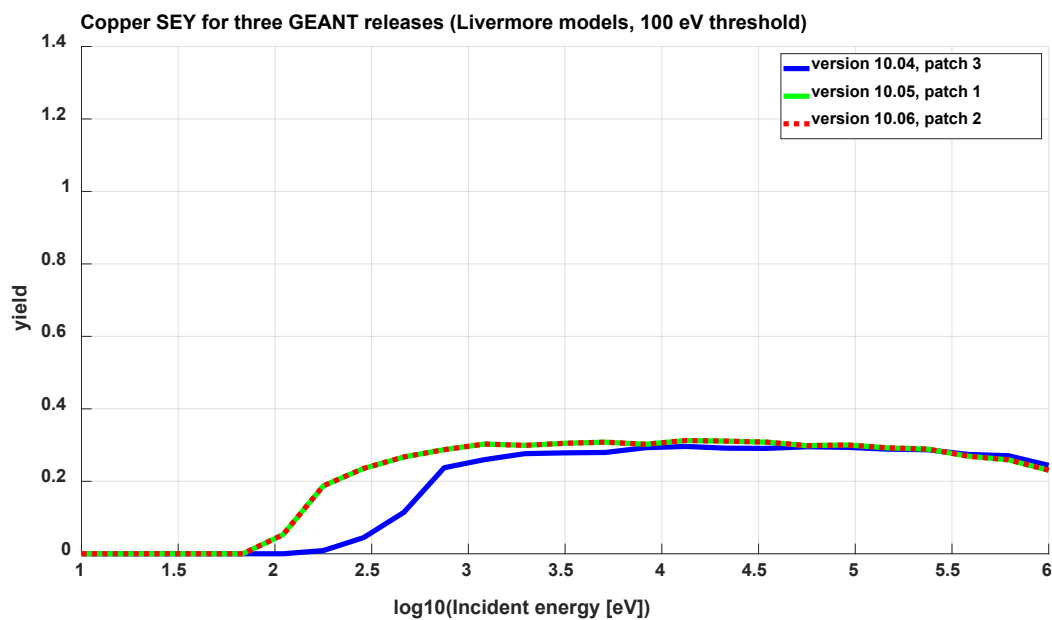
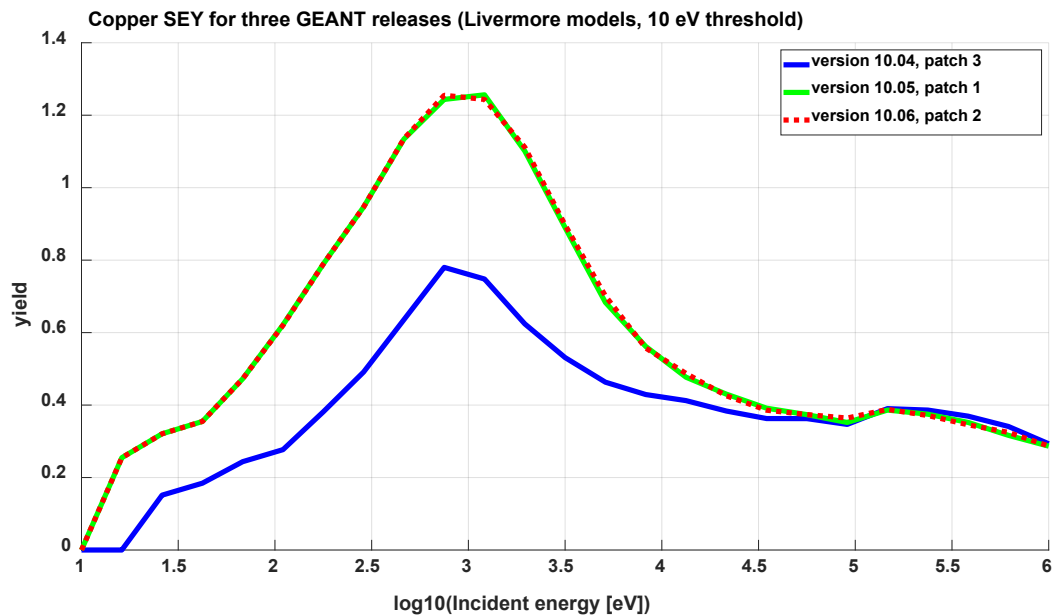


Figure 18: Comparison of Predicted Copper SEY Using Three Consecutive GEANT Point Releases with the Livermore Models: Lowered Production Threshold of 10 eV As Used in this Report (top) and the Typical Default Production Threshold of 100 eV (bottom).

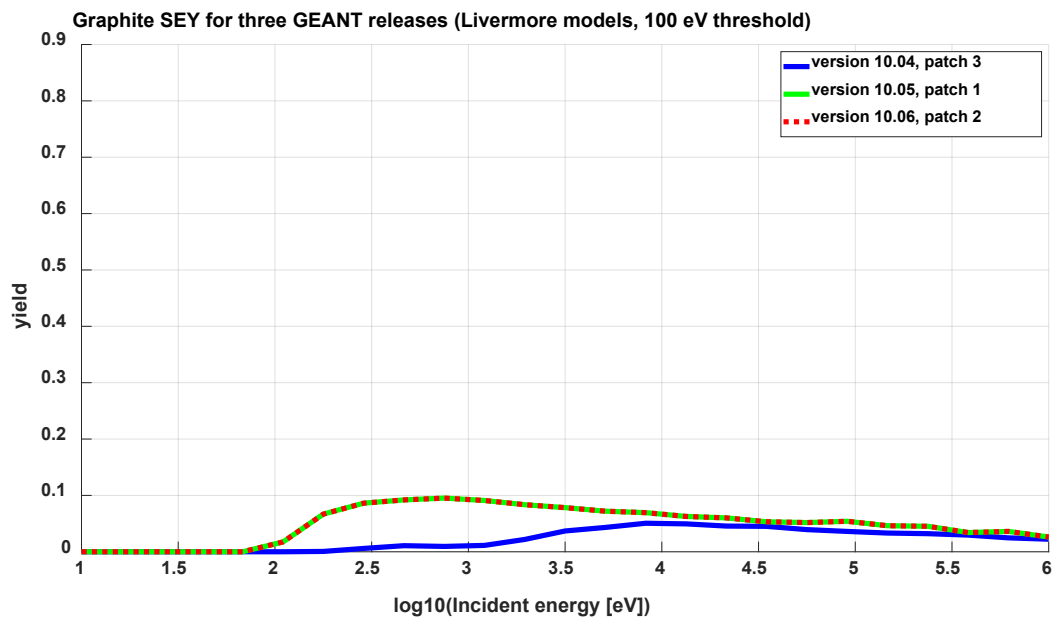
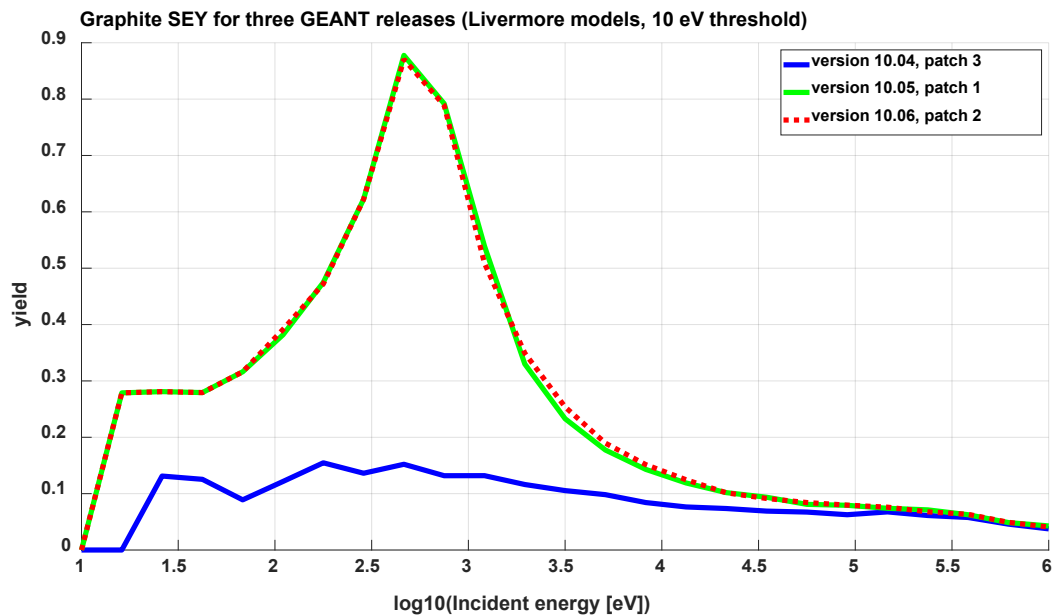


Figure 19: Comparison of Predicted Graphite SEY Using Three Consecutive GEANT Point Releases with the Livermore Models: Lowered Production Threshold of 10 eV As Used in this Report (top) and the Typical Default Production Threshold of 100 eV (bottom).

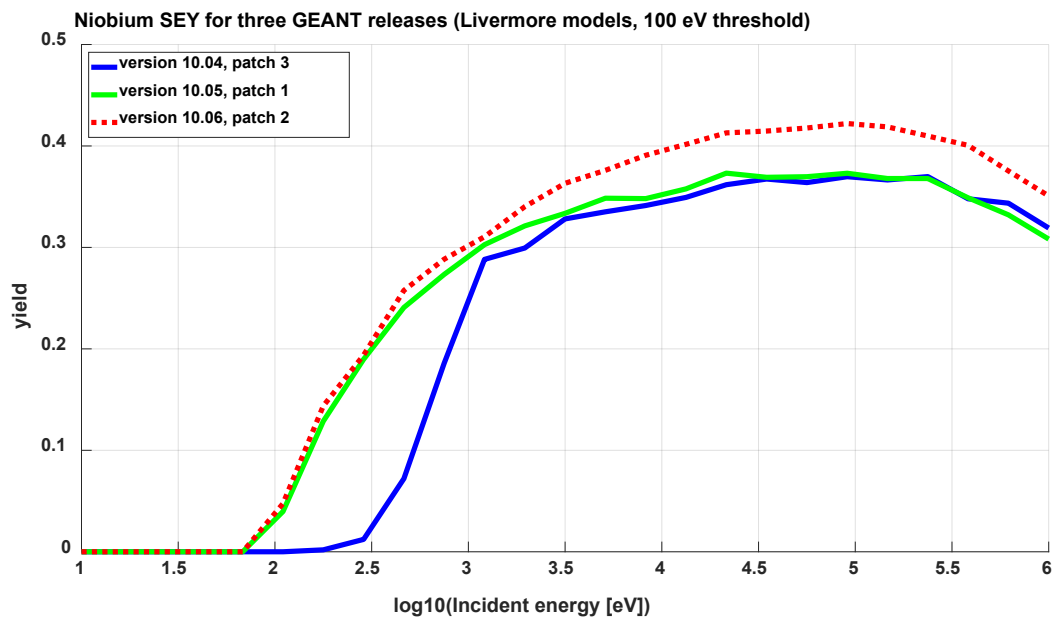
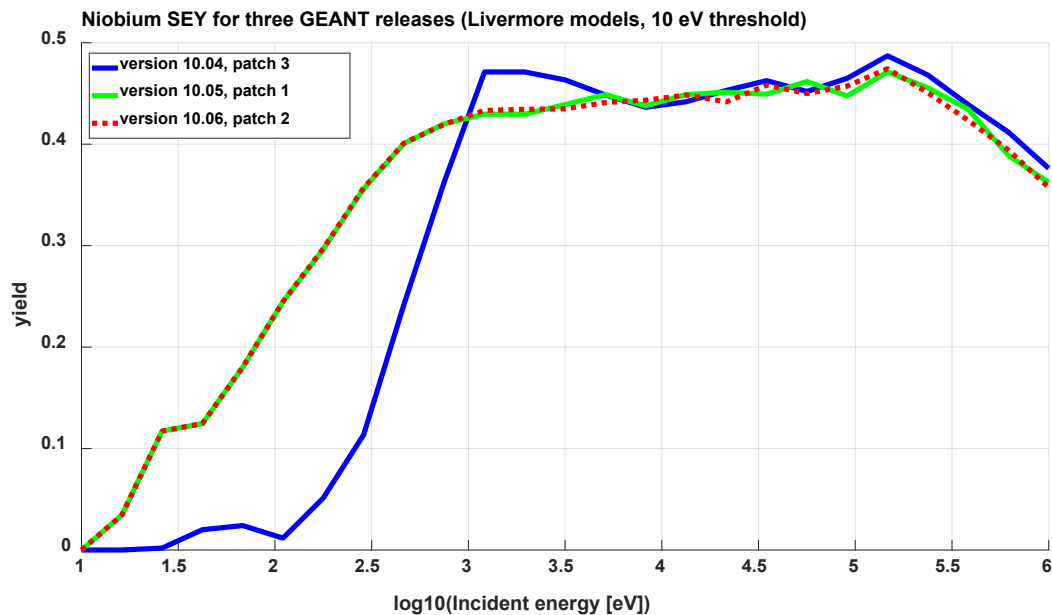


Figure 20: Comparison of Predicted Niobium SEY Using Three Consecutive GEANT Point Releases with the Livermore Models: Lowered Production Threshold of 10 eV As Used in this Report (top) and the Typical Default Production Threshold of 100 eV (bottom).

3.2.10 Section Summary

GEANT4 is a particle simulation toolkit developed by high energy physicists for the purpose of simulating particles interacting with matter and particle detectors. Typically these particles are at energy levels which are orders-of-magnitude greater than the upper limit of ~ 500 keV electron incident energy range for which we seek to extend ICEPIC's secondary electron emission model.

Comparison studies were performed to assess the level of agreement between (1) GEANT4-generated SEY curves, and (2) the SEY curves of Furman and Vaughan which are reasonably well validated for incident energies up to a few keV. Three different GEANT4 models were studied: the default models, the Penelope models, and the Low Energy Livermore models. The Livermore models allow interaction energies down to 10 eV, Penelope models down to 100 eV, and the default models down to 1000 eV. All three models allow interaction energies well above the highest energies considered in this present report.

In order to generate the electron emission statistics in GEANT4, a single electron was launched into materials. This was repeated for 10,000 trials for each incident energy and angle considered. The number and kinematics of any electrons scattered from the surface were then recorded and used to produce SEY and EES distributions. Due to thresholds for minimum interaction energies, all GEANT4 results show an SEY deficit at low incident energies as compared to Vaughan and Furman SEY curves, but the GEANT4 Livermore models were qualitatively the best due to the lowest available interaction energies of 10 eV. However, real-world secondary electrons are commonly produced at energies of a few eV, and are thus still significantly missing in the GEANT4 simulations using the Livermore models.

For large incident angles, GEANT4 perfectly reflects any electrons impacting the plate, regardless of incident energy. This leads to an SEY curve that is then unity for all incident energies, which is inconsistent with the limited measured data available for large off-normal incidence angles.

Despite the above-noted limitations, due to the Livermore models producing the best agreement with the available measured data and the Vaughan and Furman SEY curves for copper and stainless steel, the Livermore models were selected to generate data that was used to define a high-energy SEE model within ICEPIC, as will be discussed in section 4.1.

4.0 RESULTS AND DISCUSSIONS

4.1 Creation of an ICEPIC high-energy SEE model

4.1.1 Introduction

With the generation of secondary electron emission (SEE) statistics via GEANT4 introduced in section 3.2, we now turn our attention towards defining a parametric SEE model for use within ICEPIC, capable of more accurately modelling secondary electrons subsequent to high-energy incident electrons. Section 4.1.2 begins with a background discussion of the historical ICEPIC model. Section 4.1.3 then summarizes the GEANT4 data for seven representative materials drawn from conductors, dielectrics, and carbon (graphite), which demonstrate significantly diverse SEY behavior that we wish to represent in the ICEPIC high-energy SEE modification.

The updated ICEPIC SEY curve is presented in Section 4.1.4, along with the criteria that we believe any suitable model should satisfy, which led to the final model specification. Section 4.1.5 presents parametric fits of the updated ICEPIC SEY model to the GEANT4 data. Section 4.1.6 explains a minor update implemented in the emission energy spectra options available to ICEPIC users. Section 4.1.7 presents some alternative options for updated ICEPIC SEY curves, which are worthy of consideration, but which the authors believe suffer one or more shortcomings as compared to the selected ICEPIC SEE modifications. Section 4.1.8 then provides a summary of the main points covered in section 4.1.

4.1.2 Background

Before the present work, ICEPIC only supported a secondary electron yield (SEY) curve $\delta(E, \theta)$ as specified by Vaughan [30-31], given mathematically by:

$$\delta_{\text{Vaughan}}(E, \theta) = 0 \text{ for } E \leq E_0 \quad (3)$$

$$\delta_{\text{Vaughan}}(E, \theta) = \delta_{\text{max}0} \left(1 + k_{sd} \frac{\theta^2}{2\pi} \right) \begin{cases} (w \exp(1 - w))^{0.56}, & w \leq 1 \\ (w \exp(1 - w))^{0.25}, & 1 < w \leq 3.6 \\ 1.125w^{-0.35}, & w \geq 3.6 \end{cases} \quad (4)$$

$$w = \frac{E - E_0}{E_{\text{max}0} \left(1 + k_{se} \frac{\theta^2}{2\pi} \right) - E_0} \quad (5)$$

Equation 3: Vaughan SEY Mathematical Definition

where E denotes incident energy and θ denotes incident angle as measured from the surface normal. ICEPIC users commonly will need to specify at least $\delta_{\text{max}0}$ and $E_{\text{max}0}$; the remaining parameters can either use the default values as specified in the ICEPIC documentation, or values specified by the user as desired. See Figure 21 for an example Vaughan SEY curve generated using $\delta_{\text{max}0}=2.094$, $E_{\text{max}0}=270.4$ eV to approximate an SEY curve for measured copper found in [32], and all remaining parameters left at the ICEPIC default values.

Also shown for comparison in Figure 21 are SEY curves generated by two other methods for comparison, and measured data taken from Joy’s SEY database [4]. The first comparison curve is generated from the so-called “universal law for secondary electron yield” discussed by Lin in [5], which is based upon theoretical considerations of incident electron energy deposition per unit length within a material, and the probability of a liberated secondary electron escaping back to the surface. We will refer to this curve as the “Lin SEY curve” despite the theoretical basis going back many decades before Lin’s paper. Using the same variable names as in the Vaughan model above, the Lin SEY curve can be written as:

$$\delta_{Lin}(E, \theta = 0) = 1.28 \delta_{max0} \left(\frac{E}{E_{max0}} \right)^{-2/3} \left(1 - \exp \left(-1.614 \left(\frac{E}{E_{max0}} \right)^{5/3} \right) \right) \quad (7)$$

Equation 4: Lin SEY Mathematical Definition

As can be seen in Figure 21, the Lin SEY curve is qualitatively narrower about the SEY peak than the Vaughan curve and available measured data, resulting lower estimated SEY at low and high energies. This is the opposite behavior that we expect is needed in an updated ICEPIC SEY model, based upon an under-prediction of ICEPIC breakdown currents as compared to that seen in physical devices. We thus do not consider Lin’s SEY curve as a valid replacement for Vaughan’s SEY model in ICEPIC.

The second comparison SEY curve in Figure 21 is generated from a secondary electron emission model presented by Furman [32]. We note that the Vaughan and Furman SEY curves tend to be in close agreement over a wide range of incident energies, with the major exception being for relatively low incident energies less than a few tens of eV. As will be noted later, the Furman model is probably not appropriate for ICEPIC based on criteria to be presented in Section 4.1.4, but the Furman low-energy SEY behavior may be more correct than the Vaughan model when default Vaughan parameters are used, which forces the SEY to zero below a threshold incidence energy.

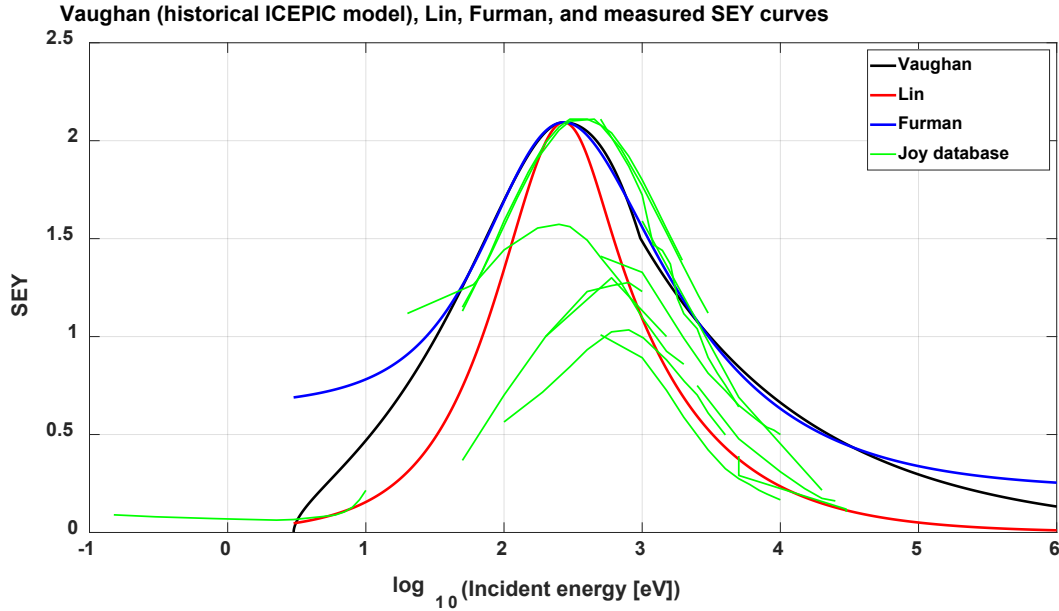


Figure 21: Example Vaughan, Lin, and Furman SEY Curves Generated with $\delta_{\max 0}=2.094$ and $E_{\max 0}=270.4$ eV to Approximate Copper, and Measured Copper SEY Curves from the Joy SEY Database [4].

4.1.3 GEANT4 data

GEANT4 was used to generate SEY and emission spectra for copper, stainless steel, aluminum, niobium, graphite, aluminum oxide, and beryllium oxide. For all materials, simulated data includes incident energies from 10 eV to 30 MeV, with incident angles of 0° , 20° , 40° , and 60° . As noted in section 3.2, GEANT4 is incapable of generating secondary electrons below a 10 eV threshold, and as such GEANT4 results exclude most true secondary electrons which are frequently emitted at less than 10 eV of energy.

We note that true secondary electrons become a relatively smaller portion of the total secondary electron population (consisting of true secondary electrons, reflected electrons, and scattered electrons) as the incident energy increases, and thus we expect GEANT4 results to be valid at sufficiently high incident energies exceeding roughly 10 keV, as can be seen by an examination of the GEANT4 SEY components shown in Appendix D. However, some caution is advised because both the theoretical Lin SEY curve [5] and measured curves shown in [26] for the low-keV range show monotonically decreasing SEY after the SEY peak, which is not observed in the GEANT4 data. Despite this uncertainty with the GEANT4 data, we use it here because the GEANT4 SEY curves qualitatively exhibit behavior representative of real-world SEY curves.

Example GEANT4 curves for seven different materials are shown for 0° incidence and 60° incidence (relative to surface normal) respectively in Figure 22 and Figure 23. Note that most of

the materials have a low-energy peak that can be reasonably approximated with Vaughan's parametric SEY model, but that the high energy portion of some materials do not decrease as in Vaughan's model. We seek to provide a modification to the ICEPIC SEY curve to account for this behavior.

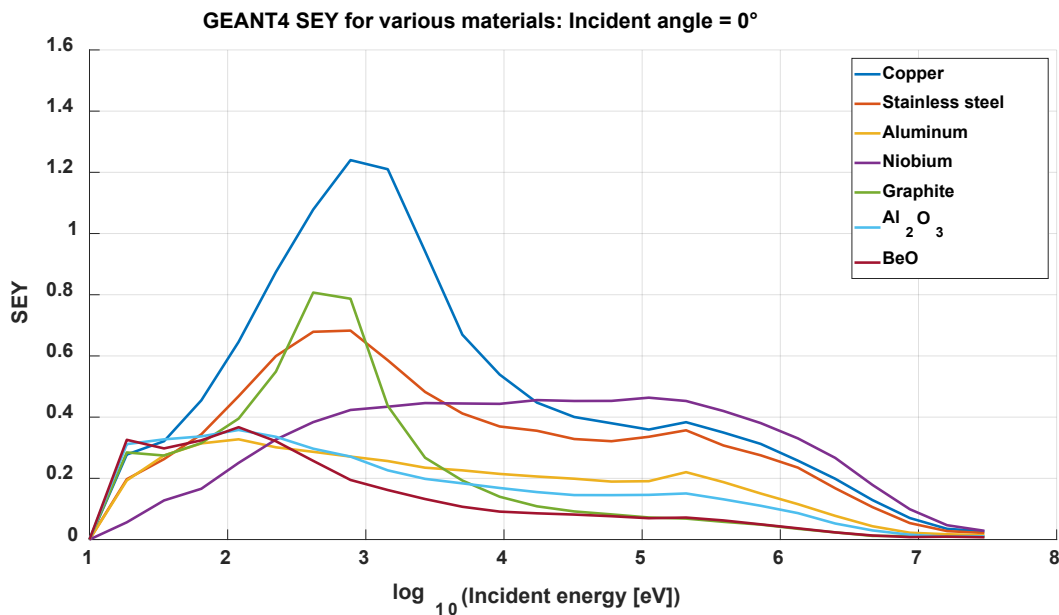


Figure 22: SEY Curves for Various Materials at 0° Incidence Generated with GEANT4.

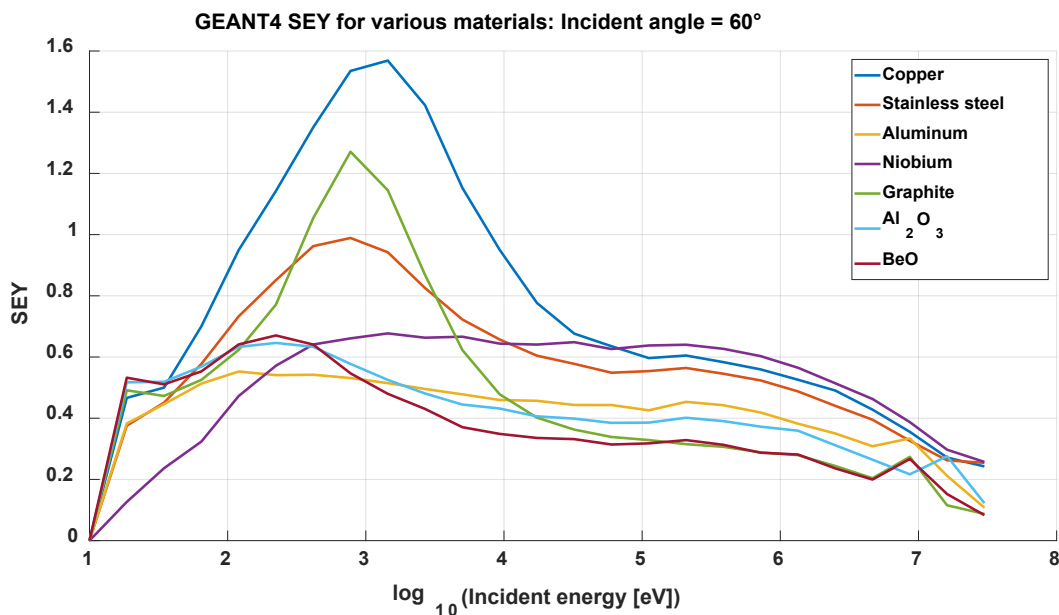


Figure 23: SEY Curves for Various Materials at 60° Incidence Generated with GEANT4.

4.1.4 Proposed SEY modification

For the present SEY modification, we believe that any updates to the ICEPIC model must be guided by the following criteria:

- (1) The updated ICEPIC SEY model must be backwards compatible with the existing SEY model.
- (2) The updated ICEPIC SEY model must not overwhelm users with too many parameters to be specified. Anything more than around 5-10 parameters begins to be cumbersome.
- (3) We are more concerned with defining a model that can qualitatively produce SEY behavior that an ICEPIC user may encounter, even if that behavior does not conform to a theoretical SEY curve such as the Lin curve, or a semi-empirical model such as the Vaughan curve; we want to provide a model which can be tuned as better SEY data becomes available.

The last criterion is due to the significant uncertainty in actual SEY curves for any given material sample, as pointed out in [5] and shown in Figure 24 below.

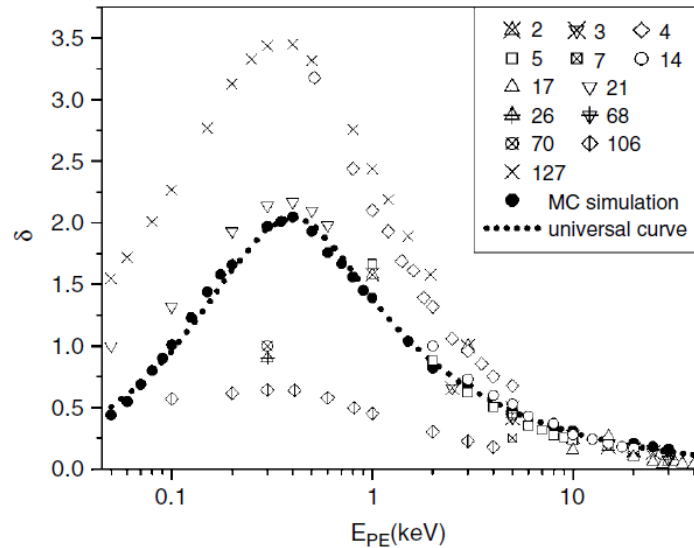


Figure 24: Example of SEY Variability in Measured SEY for Aluminum, Taken from Figure 2 of [5]; Legend Numbers Refer to Different Measured Data Sources in [5].

With these criteria in mind, we propose an additive correction to the current ICEPIC SEY of the form:

$$\delta_{correction}(E, \theta; A(\theta), k(\theta), E_c(\theta), n) = A(\theta) \exp\left(-\left|k(\theta) \cdot \log_{10}\left(E/E_c(\theta)\right)\right|^n\right) \quad (8)$$

where:

$$A(\theta) = A(0) \cdot \left(1 + k_{sd2} \frac{\theta^2}{2\pi}\right) \quad (9)$$

$$E_c(\theta) = E_c(0) \cdot \left(1 + k_{se2} \frac{\theta^2}{2\pi}\right) \quad (10)$$

$$k(\theta) = k(0) \cdot \left(1 + k_{se2} \frac{\theta^2}{2\pi}\right)^{-1} \quad (11)$$

Equation 5: Additive Correction SEY Mathematical Definition

The parameters $A(0)$, $k(0)$, $E_c(0)$ and n must be specified for this additive correction. The parameters k_{se2} and k_{sd2} respectively default to the Vaughan model parameters k_{se} and k_{sd} in Vaughan model equations (4) and (5), but are allowed to be specified to be different if needed by the ICEPIC user. The total SEY would then be given by the summation of $\delta_{vaughan}(E, \theta)$ and $\delta_{correction}(E, \theta)$:

$$\delta_{total}(E, \theta) = \delta_{vaughan}(E, \theta) + \delta_{correction}(E, \theta) \quad (12)$$

Equation 6: Net SEY with Additive Correction

The summation form of equation (12) easily lends itself to backwards compatibility, since defining the default value of correction amplitude $A(0)$ to be zero will result in the Vaughan SEY curve previously implemented in ICEPIC.

Note that $\delta_{correction}(E, \theta)$ can be considered as a modified Gaussian function defined over $\log_{10}\left(E/E_c\right)$, where a value of $n=2$ would correspond to a Gaussian function, and other values of n will adjust the sharpness of transition from the peak to the tails of the function. E_c defines the center of this modified Gaussian function, and the base-10 logarithm is selected over other logarithms to allow for easier mental comparisons of electron incident energies and E_c . The parameter k defines the width of the central lobe of the function. See Figure 25 for example high energy correction curves with notional parameters.

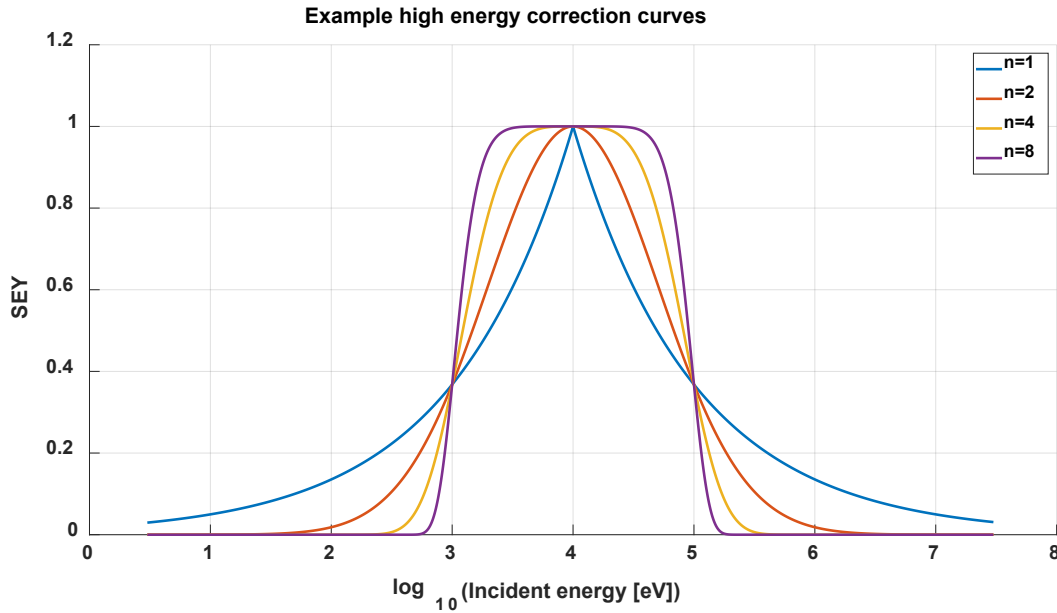


Figure 25: Example High Energy Correction Curves for $E_c=1E4$ eV, $k=1$, and $A=1$.

As noted in Section 4.1.1, Furman [32] has also defined SEY curves. Furman's model was considered and deemed insufficient for the current ICEPIC SEY model extension effort because (1) it is not backwards compatible with the present ICEPIC model, (2) it requires the specification of many dozens of parameters, (3) some combinations of parameters (including those provided in Furman's paper for stainless steel) can result in numerical issues, (4) Furman's model was not validated at the high incidence energies of interest greater than tens of keV, and (5) the variations in measured data can be larger than the differences between Furman's and Vaughan's SEY curves when appropriate model parameters are used. The net result is that Furman's model would likely result in much more challenge for ICEPIC users with uncertain benefit.

4.1.5 SEY model fits to GEANT4 data

4.1.5.1 Normal incidence

We first consider fitting the proposed model of equation (11) to only normal incidence data. Simultaneous model fits to both normal and off-normal incidence is considered in Section 4.1.5.2.

Figure 26 through Figure 32 respectively show the GEANT4 normal incidence SEY data for copper, stainless steel, aluminum, niobium, graphite, aluminum oxide (alumina, Al_2O_3), and beryllium oxide (BeO), along with the proposed model with selections of parameters chosen to match well at normal incidence; any unspecified parameters used the default values as found in ICEPIC. In all cases the proposed model is able to reasonably match the GEANT4 data to much higher fidelity than the Vaughan model can achieve. The model parameters were adjusted manually to achieve reasonable fits to the GEANT4 data. A more sophisticated optimization

approach could be used to optimize the fits as needed. Note that the Niobium SEY curve shown in Figure 29 uses components of the both the Vaughan SEY and correction term, but could be reasonably approximated using just the correction term while setting the Vaughan SEY component to zero.

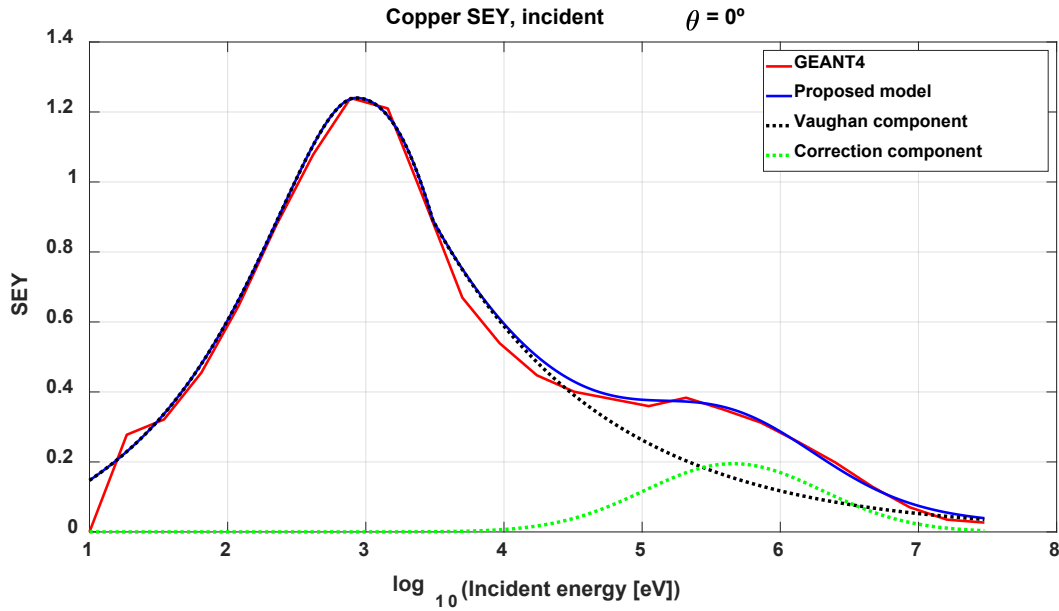


Figure 26: Copper SEY Curves from GEANT4 and Proposed Model in Equation (11):
 $\delta_{\max 0}=1.24$, $E_{\max 0}=850$ eV, $A(0)=0.195$, $E_c(0)=457$ keV, $k(0)=1.1$, and $n=2$.

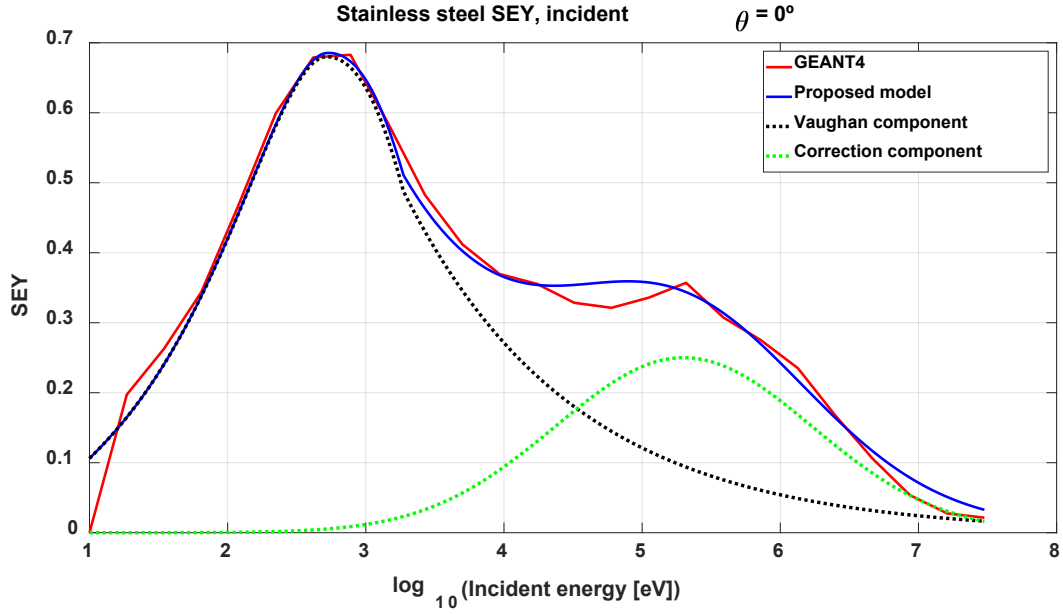


Figure 27: Stainless Steel SEY Curves from GEANT4 and Proposed Model in Equation (11):
 $\delta_{\max 0}=0.68$, $E_{\max 0}=520$ eV, $A(0)=0.25$, $E_c(0)=200$ keV, $k(0)=0.76$, and $n=2$.

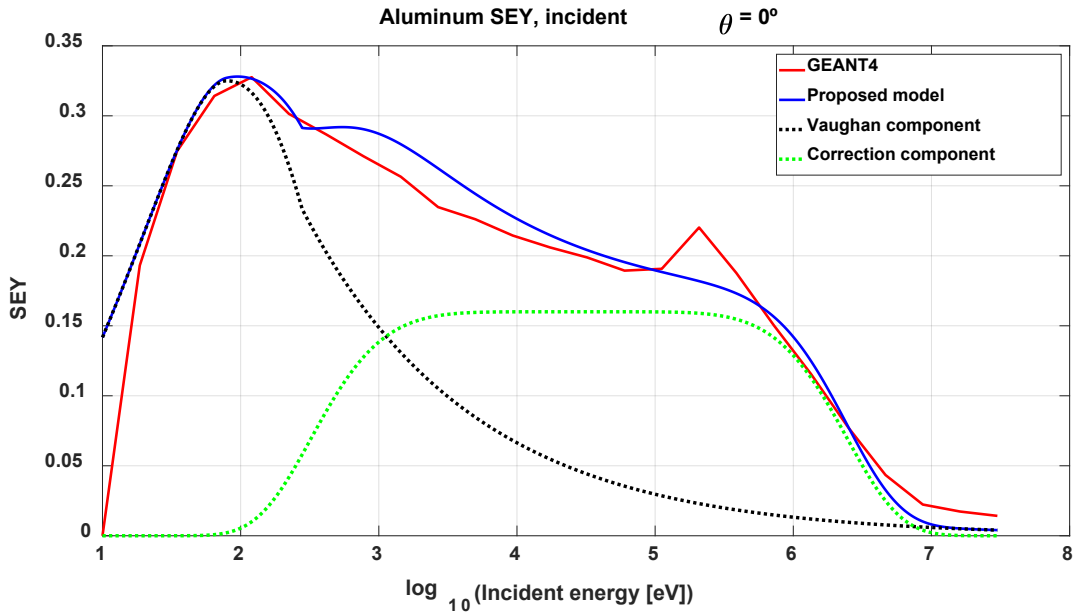


Figure 28: Aluminum SEY Curves from GEANT4 and Proposed Model in Equation (11):
 $\delta_{\max 0}=0.325$, $E_{\max 0}=79.4$ eV, $A(0)=0.16$, $E_0(0)=28.2$ keV, $k(0)=0.50$, and $n=6$.

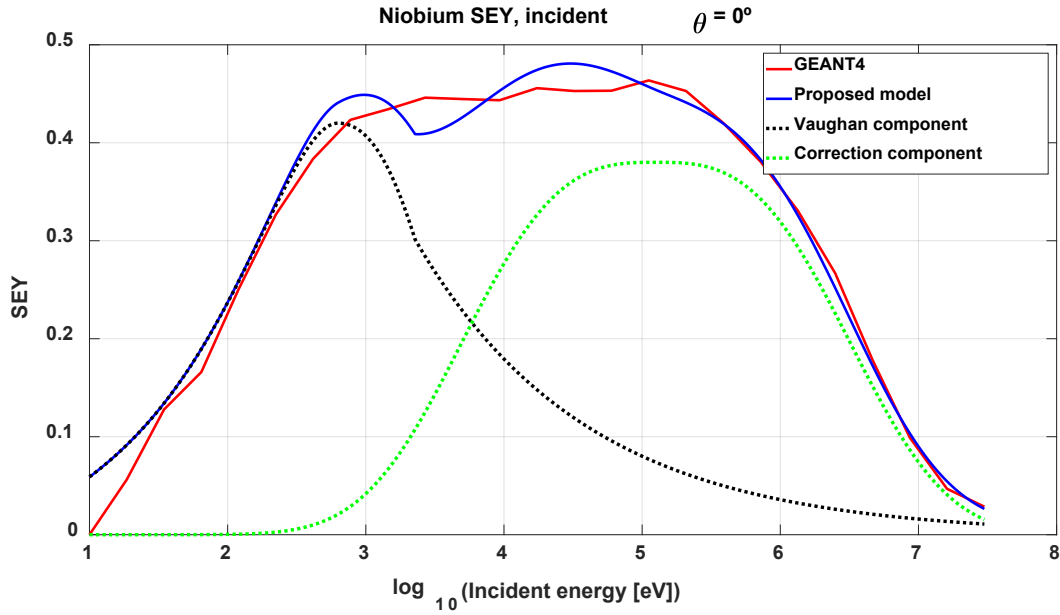


Figure 29: Niobium SEY Curves from GEANT4 and Proposed Model in Equation (11):
 $\delta_{\max 0}=0.42$, $E_{\max 0}=631$ eV, $A(0)=0.38$, $E_c(0)=126$ keV, $k(0)=0.62$, and $n=3$.

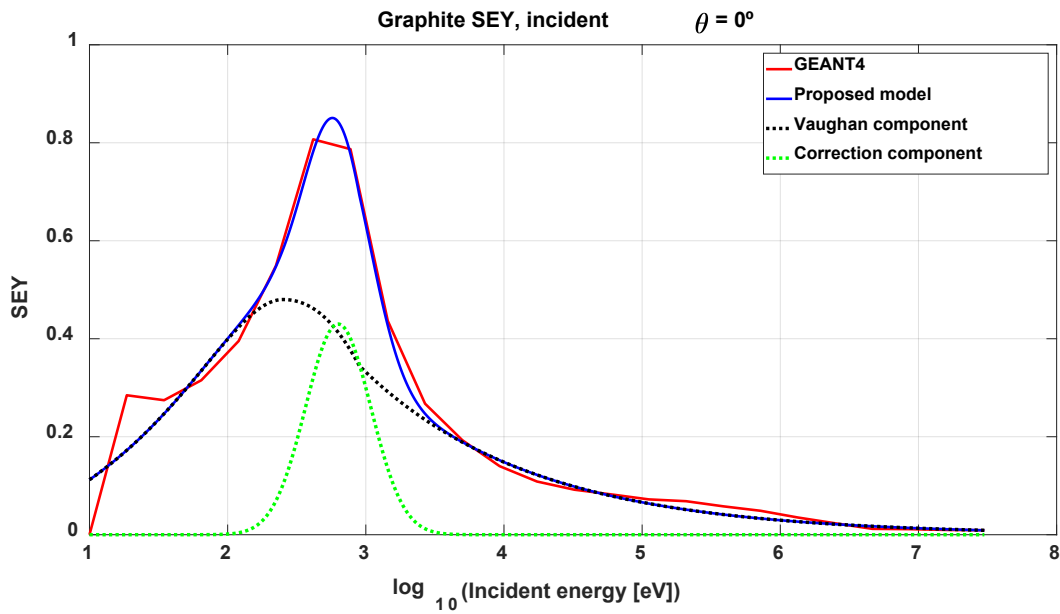


Figure 30: Graphite SEY Curves from GEANT4 and Proposed Model in Equation (11):
 $\delta_{\max 0}=0.48$, $E_{\max 0}=251$ eV, $A(0)=0.43$, $E_c(0)=631$ eV, $k(0)=3$, and $n=2$.

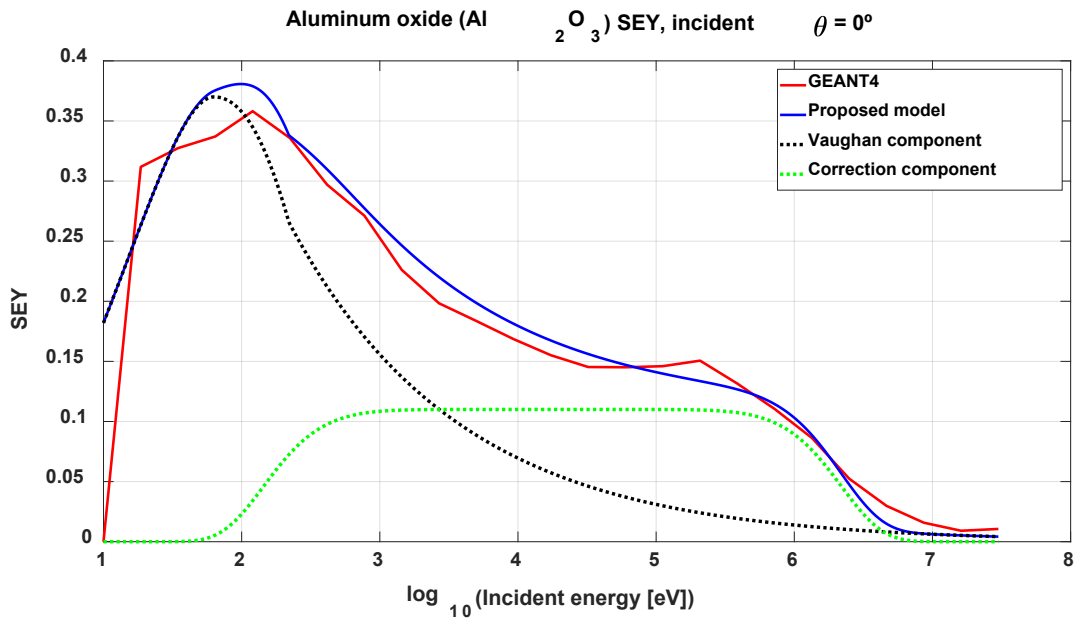


Figure 31: Al_2O_3 SEY Curves from GEANT4 and Proposed Model in Equation (11): $\delta_{\text{max}0}=0.37$, $E_{\text{max}0} = 63.1$ eV, $A(0)=0.11$, $E_c(0)=17.8$ keV, $k(0)=0.47$, and $n=8$.

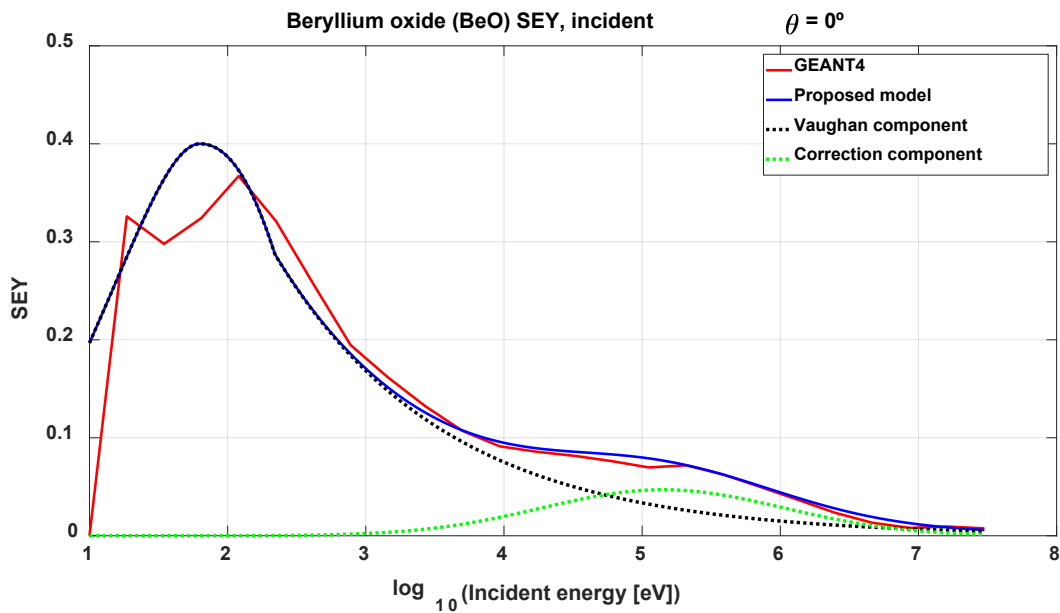


Figure 32: BeO SEY Curves from GEANT4 and Proposed Model in Equation (11): $\delta_{\text{max}0}=0.4$, $E_{\text{max}0} = 63.1$ eV, $A(0)=0.047$, $E_c(0)=141$ keV, $k(0)=0.81$, and $n=2$.

4.1.5.2 Off-normal incidence

The SEY of materials typically grows as the incidence angle θ increases. A similar behavior with θ is also observed for the incidence energy which produces the SEY peak. Vaughan's model accounts for this behavior via the factors $\left(1 + k_{sd} \frac{\theta^2}{2\pi}\right)$ and $\left(1 + k_{se} \frac{\theta^2}{2\pi}\right)$ respectively in equations (4) and (5). Vaughan states that default values of unity for k_{sd} and k_{se} are typical, and values up to approximately 2 would be appropriate for exceptionally smooth, clean, and oxide-free surfaces. GEANT4 SEY curves at increasing incidence angles show that both the low and high energy portions of the SEY curves grow, and both shift along the incident energy axis in the same direction, which suggests use of angle corrections of the same form as Vaughan, specifically $\left(1 + k_{sd2} \frac{\theta^2}{2\pi}\right)$ and $\left(1 + k_{se2} \frac{\theta^2}{2\pi}\right)$ in the high-energy correction parameters as defined in equations (8), (9), and (10). However, the GEANT4 results sometimes show much more significant angle dependence than assumed by Vaughan, at times requiring angle-dependence parameters up to approximately 12. This may be due to the GEANT results assuming a perfectly smooth material boundary down to the atomic scale, which is unlikely to occur for even highly-polished real-world material samples.

For each material, the high energy SEY correction model was simultaneously fit to the GEANT4 data for incidence angles of 0° , 20° , 40° , and 60° . This fit was attempted using the conjugate gradients algorithm applied to minimizing the L2 norm between the model and the GEANT4 data, but this approach was abandoned due to the optimization algorithm only finding local minima. The particular material parameters were instead pre-selected via a Monte Carlo search over a wide range of potential parameter values, and then material parameters were either directly adopted, or manually adjusted to further refine the fit. If a subjectively-assessed satisfactory fit was attainable using identical values for k_{sd} , k_{se} , k_{sd2} , and k_{se2} , then this choice of parameters was selected. However, if an unsatisfactory fit was attainable with this restriction, then k_{sd2} and k_{se2} were independently adjusted. Parameter values are provided along with the SEY curves to be discussed; any unspecified parameters used the default values for the ICEPIC model parameter.

Figure 33 through Figure 39 respectively show the GEANT4 SEY data at for incidence angles of 0° , 20° , 40° , and 60° for copper, stainless steel, aluminum, niobium, graphite, aluminum oxide (alumina, Al_2O_3), and beryllium oxide (BeO), along with the appropriate selections of model parameters to match across the range of incidence angles. We note that the fits at normal incidence are not as good as the normal incidence fits shown in the previous section, which is attributed to the model now needing the best fit the data across the range of incidence angles examined.

An examination of the curves show that the simple additive correction can reasonably well represent the GEANT4 curves for copper (Figure 33), stainless steel (Figure 34), aluminum (Figure 35), niobium (Figure 36), less so for aluminum oxide (Figure 38) and beryllium oxide (Figure 39) and somewhat poorly for graphite (Figure 37). In the case of graphite, the proposed

model struggles to approximate the GEANT4 SEY curve, which appears to significantly deviate from the assumed shape of the Vaughan SEY model for relatively low incident energies up to a few keV. Aluminum, Niobium, and Aluminum Oxide also have SEY curves which significantly deviate from the assumed shape of the Vaughan model, but in ways that can fortunately be captured using the additive correction, resulting in reasonable overall SEY curve approximations.

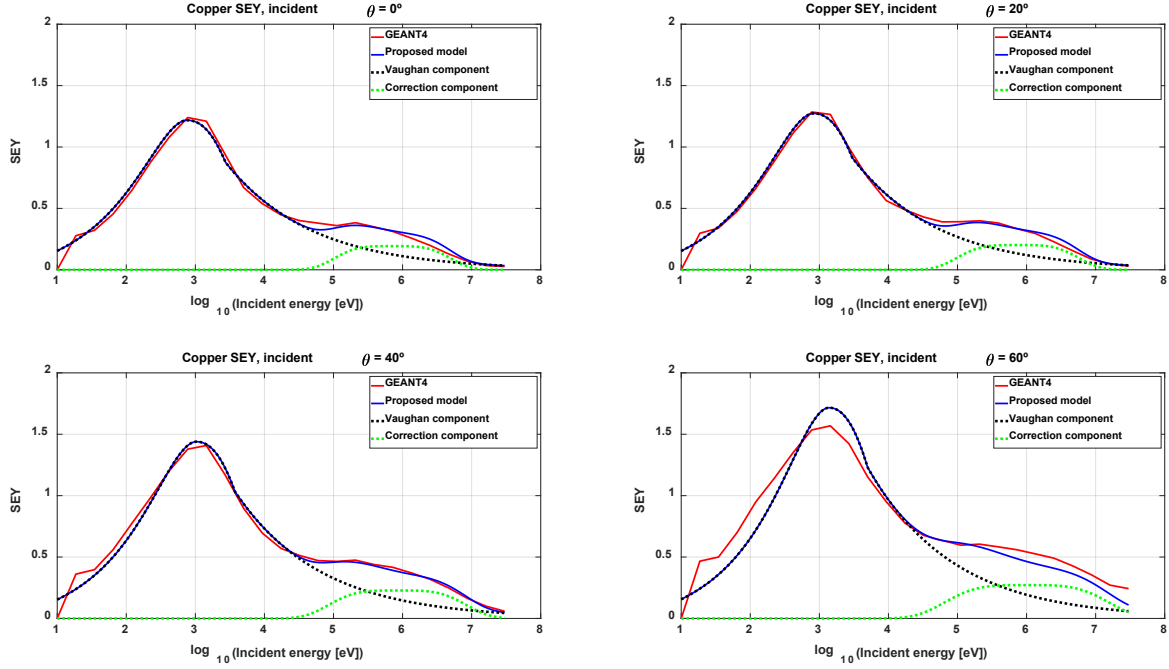


Figure 33: Copper SEY Curves from GEANT4 and Proposed Model in Equation (11), for Incidence Angles $\theta=0^\circ$ (top left), $\theta=20^\circ$ (top right), $\theta=40^\circ$ (bottom left), and $\theta=60^\circ$ (bottom right): $\delta_{\max 0}=1.22$, $E_{\max 0}=761$ eV, $A(0)=0.271$, $E_c(0)=1.007$ MeV, $k(0)=0.775$, $n=3.85$, $k_s=2.34$; k_{se2} and k_{sd2} Set to Same Value as k_s .

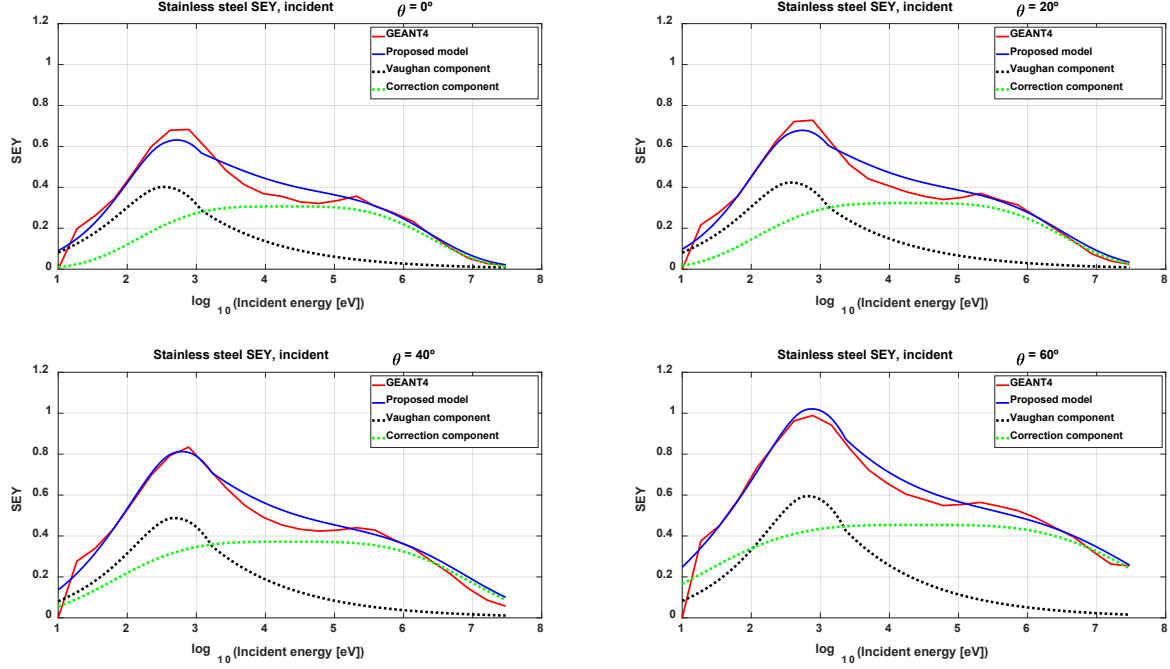


Figure 34: Stainless Steel SEY Curves from GEANT4 and Proposed Model in Equation (11), for Incidence Angles $\theta=0^\circ$ (top left), $\theta=20^\circ$ (top right), $\theta=40^\circ$ (bottom left), and $\theta=60^\circ$ (bottom right). $\delta_{\max 0}=0.402$, $E_{\max 0}=329$ eV, $A(0)=0.454$, $E_c(0)=28.2$ keV, $k(0)=0.291$, $n=3.62$, and $k_s=2.75$; k_{se2} and k_{sd2} Set to Same Value as k_s .

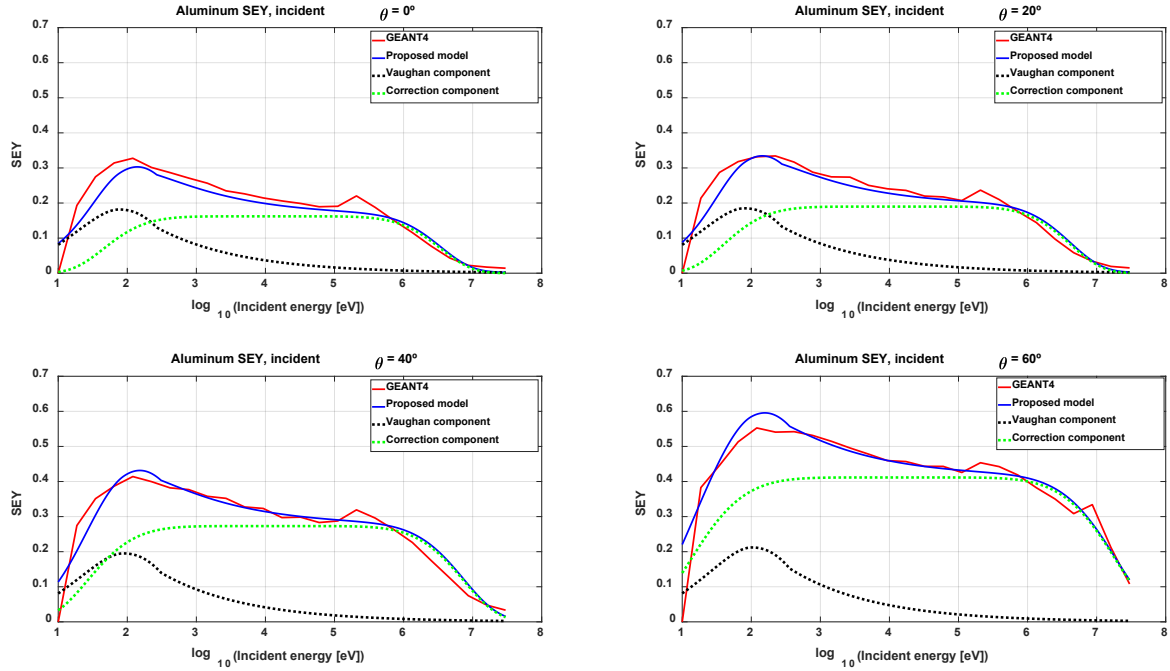


Figure 35: Aluminum SEY Curves from GEANT4 and Proposed Model in Equation (11), for Incidence Angles $\theta=0^\circ$ (top left), $\theta=20^\circ$ (top right), $\theta=40^\circ$ (bottom left), and $\theta=60^\circ$ (bottom right). $\delta_{\max 0}=0.182$, $E_{\max 0}=76.1$ eV, $A(0)=0.412$, $E_c(0)=15.8$ keV, $k(0)=0.316$, $n=6.38$, $k_s=1.984$, $k_{se2}=1.489$, and $k_{sd2}=8.822$.

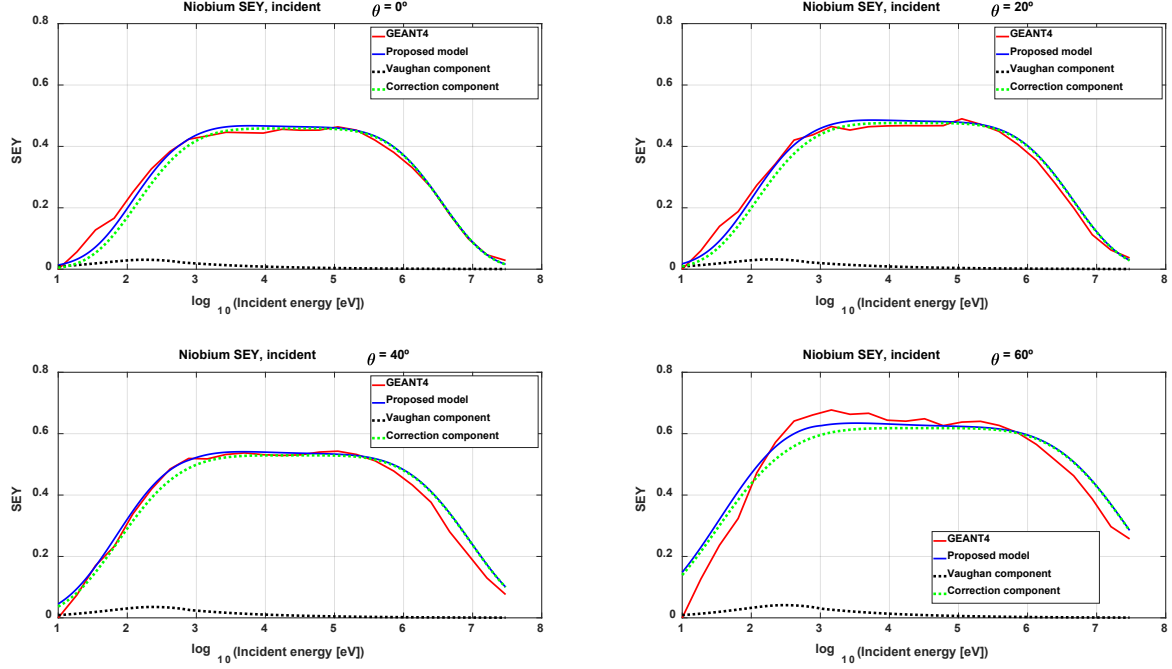


Figure 36: Niobium SEY Curves from GEANT4 and Proposed Model in Equation (11), for Incidence Angles $\theta=0^\circ$ (top left), $\theta=20^\circ$ (top right), $\theta=40^\circ$ (bottom left), and $\theta=60^\circ$ (bottom right). $\delta_{\max 0}=0.0307$, $E_{\max 0}=172$ eV, $A(0)=0.618$, $E_c(0)=30.3$ keV, $k(0)=0.315$, $n=4.32$, and $k_s=2.00$; k_{se2} and k_{sd2} Set to Same Value as k_s .

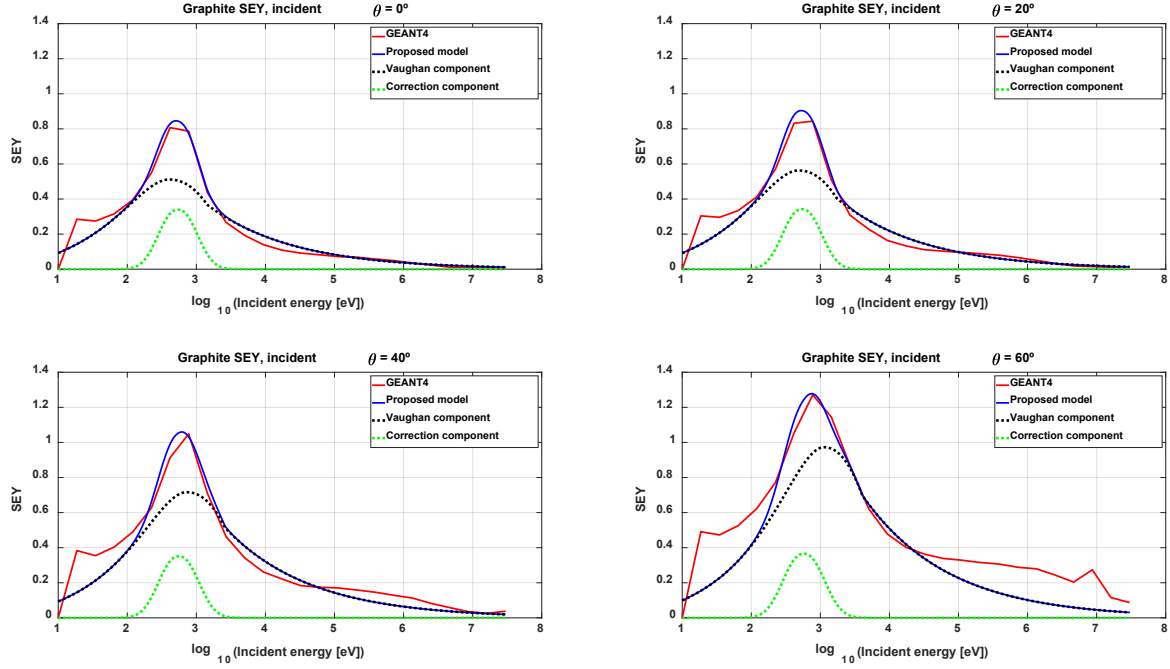


Figure 37: Graphite SEY curves from GEANT4 and Proposed Model in Equation (11), for Incidence Angles $\theta=0^\circ$ (top left), $\theta=20^\circ$ (top right), $\theta=40^\circ$ (bottom left), and $\theta=60^\circ$ (bottom right). $\delta_{\max 0}=0.511$, $E_{\max 0}=401$ eV, $A(0)=0.365$, $E_c(0)=576$ keV, $k(0)=2.54$, $n=2.28$, $k_s=5.17$, $k_{se2}=0.375$, and $k_{sd2}=0.438$.

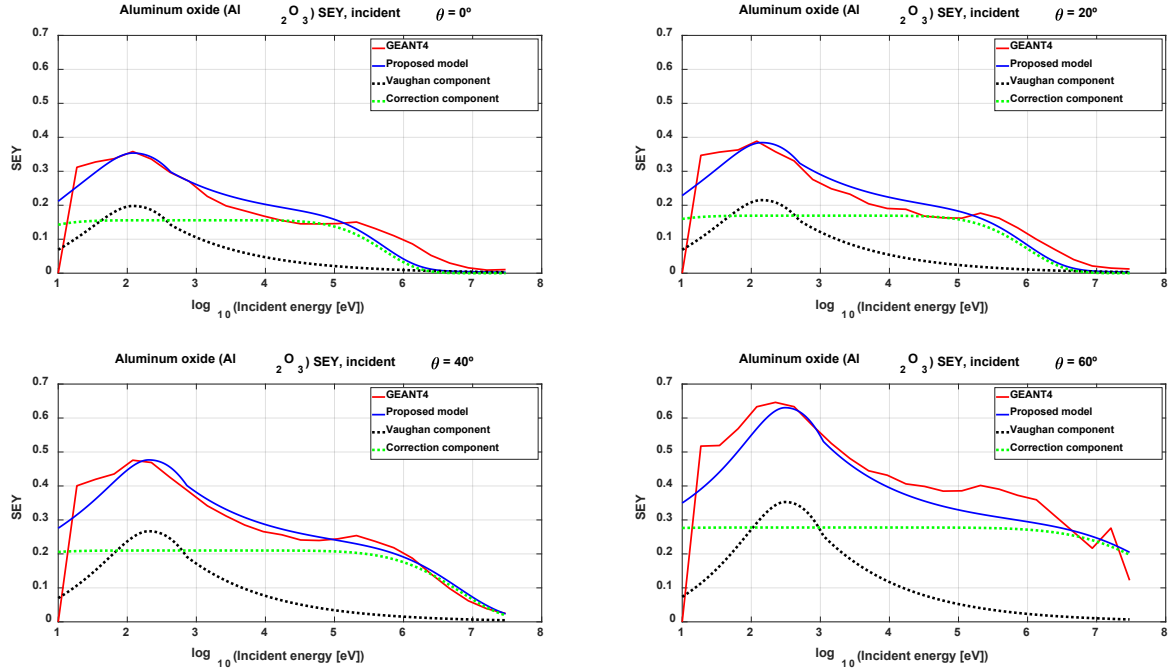


Figure 38: Aluminum Oxide SEY Curves from GEANT4 and Proposed Model in Equation (11), for Incidence Angles $\theta=0^\circ$ (top left), $\theta=20^\circ$ (top right), $\theta=40^\circ$ (bottom left), and $\theta=60^\circ$ (bottom right). $\delta_{\max 0}=0.198$, $E_{\max 0}=120$ eV, $A(0)=0.278$, $E_c(0)=1.56$ keV, $k(0)=0.197$, $n=6.35$, $k_s=4.48$; k_{se2} and k_{sd2} Set to Same Value as k_s .

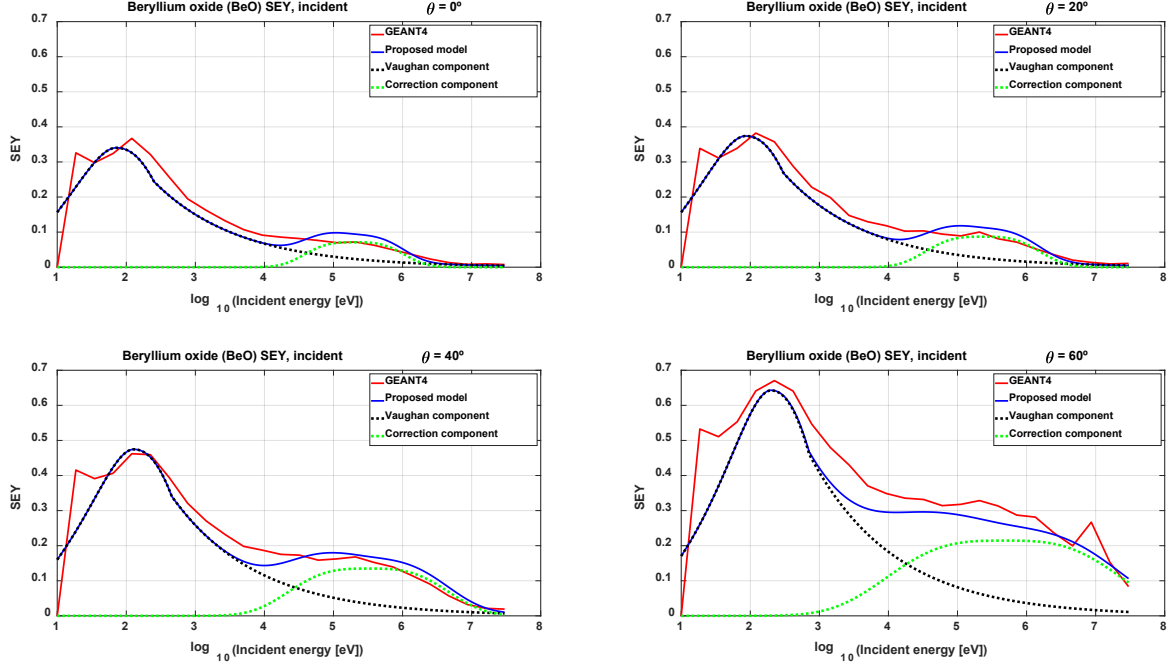


Figure 39: Beryllium Oxide SEY Curves from GEANT4 and Proposed Model in Equation (11), for Incidence Angles $\theta=0^\circ$ (top left), $\theta=20^\circ$ (top right), $\theta=40^\circ$ (bottom left), and $\theta=60^\circ$ (bottom right). $\delta_{\max 0}=0.340$, $E_{\max 0}=71.7$ eV, $A(0)=0.214$, $E_c(0)=472$ keV, $k(0)=0.520$, $n=3.18$, $k_s=5.09$, $k_{se2}=7.75$, and $k_{sd2}=11.6$.

4.1.6 Emission energy spectra

In addition to the yield curve, the energy emission spectrum of secondary electrons needs to be specified. ICEPIC allows the user to specify the fraction of reflected electrons (same energy as incident electrons), scattered electrons (uniform energy between 0 and incidence electrons), and true secondary electrons (Maxwell-Boltzman flux distribution). However, as we approach incidence energies of approximately 10 keV and beyond, the contribution of scattered electrons tends to dominate the contributions from reflected and true secondary electrons. In order to accommodate this, we propose an optional parameter E_{override} , and any incident energies above this values will completely generate scattered electrons, and no true secondary electrons or reflected electrons. The default value of E_{override} is set to infinity within the updated ICEPIC SEE model to ensure backwards compatibility, but can be to a smaller energy as desired by an ICEPIC user.

4.1.7 Alternative options

We believe that the implemented additive correction to the ICEPIC SEY model offers the best balance of simplicity and flexibility to ICEPIC users, but other options may also deserve consideration. In this section we provide three other options to enhance the high energy SEY model in ICEPIC.

4.1.7.1 Ludwick SEY model

The Vaughan SEY $\delta_{vaughan}(E, \theta)$ given in equation (4) has fixed exponents k in the factor $(w \exp(1 - w))^k$, specifically $k = 0.56$ or $k = 0.25$ depending on if the incident energy is below or above the location of the peak in the SEY curve. Ludwick [40] has presented a generalization of the Vaughan SEY curve, in which different exponents k are allowed for the w and $\exp(1 - w)$ factors:

$$\delta_{Ludwick}(E) = \delta_{max0} \cdot w^{k_1} \cdot (\exp(1 - w))^{k_2} \quad (13)$$

Equation 7: Ludwick SEY Mathematical Definition

As with Vaughan, the values of the exponents change depending on if the incident energy is below or above the location of the peak in the SEY curve. Ludwick's modification to the Vaughan model allows for independent control of the rates of SEY increase and decrease on each side of the peak. Such a modification could allow for an increase in high-energy SEY if desired by a user in ICEPIC, and could allow for backwards compatibility by simply setting the default values of k_1 and k_2 to be the Vaughan values. However, the Ludwick SEY model still qualitatively behaves like the Vaughan SEY model (monotonically decreasing after reaching a peak), such that it is unable to capture any second peaks which may appear at higher energies in SEY curves.

Figure 40 shows a comparison of normally-incident copper data simulated with GEANT4, the Ludwick SEY curve with parameters selected for a slow decay of SEY at high energies, and the Vaughan SEY curve. Both the Ludwick and Vaughan SEY curves used values of $\delta_{max0} = 1.25$, $E_{max0} = 850 \text{ eV}$, and the ICEPIC default threshold value $E_0 = 3 \text{ eV}$. Below the SEY peak, both the Vaughan and Ludwick SEY curves used the default Vaughan exponential parameter $k = k_1 = k_2 = 0.56$. Above the SEY peak, the Ludwick model was defined to use $k_1 = -0.25$ and $k_2 = 0$. Note that the sharp transition at the Ludwick SEY peak is due to the need to fit his model across many orders of magnitude of incident energies, which was not the intention of Ludwick's model; his goal was to have a better parametric fit to an SEY curve about the peak and over the range of 0 – 5 keV incidence energies, much less than the tens of MeV span we are attempting to fit in Figure 40.

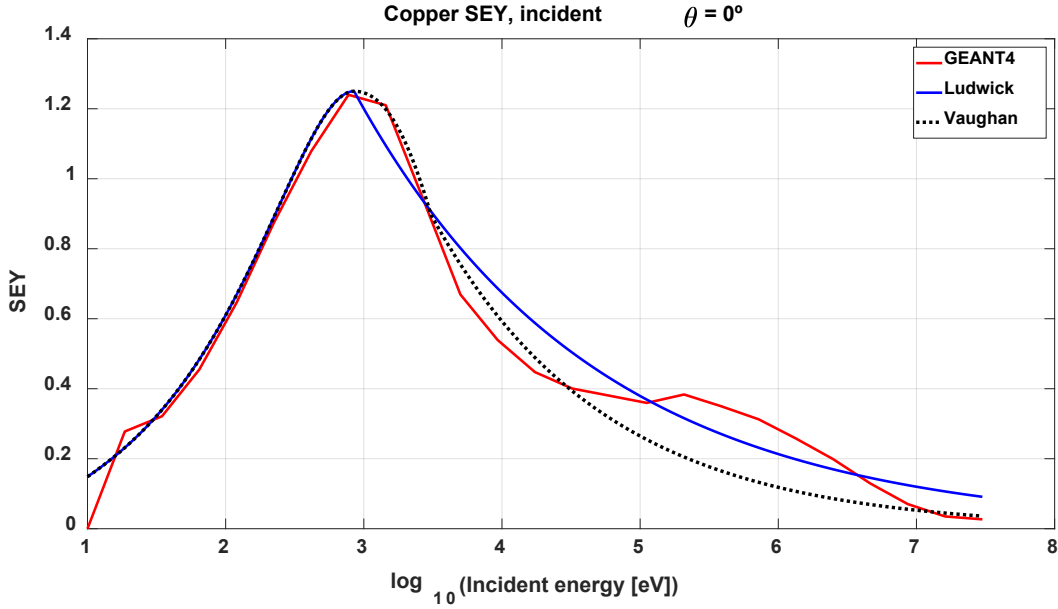


Figure 40: Comparison of GEANT4, Ludwick, and Vaughan SEY Curves for Simulated Copper at Normal Incidence.

4.1.7.2 Vaughan model with adjustable high-energy asymptotic behavior

Examination of equation (4) shows that at high incidence energies, Vaughan's SEY is defined to be $1.125w^{-0.35}$. Adjustment of the exponent from the defined value of -0.35 could allow for a relative increase or decrease in the SEY at high energies, and would be backwards-compatible with the existing ICEPIC code by setting the default value to be as the code currently defines it. Note that this curve will still qualitatively behaves like the Vaughan SEY model (monotonically decreasing after reaching a peak), such that it is unable to capture any second peaks which may appear at higher energies in SEY curves.

Figure 41 shows a comparison of normally-incident copper data simulated with GEANT4, the modified Vaughan SEY curve with the high-energy asymptote changed from the default -0.35 to -0.28, and the default Vaughan SEY curve. Both Vaughan SEY curves used values of $\delta_{max0} = 1.25$, $E_{max0} = 850 \text{ eV}$, and the ICEPIC default threshold value $E_0 = 3 \text{ eV}$.

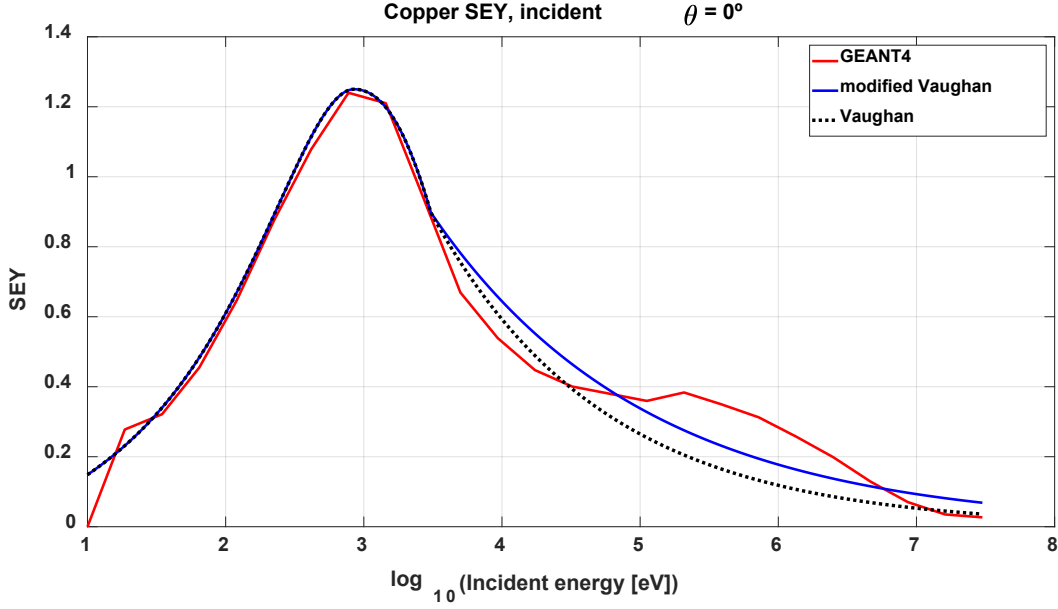


Figure 41: Comparison of GEANT4, Vaughan SEY with a Modified High-Energy Asymptotic Behavior, and Default Vaughan SEY Curves for Simulated Copper at Normal Incidence.

4.1.7.3 More general parametric model

Given enough degrees of freedom, a parametric model could fit any desired data. If a simple additive correction as defined in equation (7) is insufficient for the fidelity desired, another option may be to define a more general parametric model using multiple additive corrections as defined in equation (7), or perhaps polynomials or other basis functions defined on

$\log_{10} \left(E/E_0(\theta) \right)$, for example $\sum_{n=0}^N c_n(\theta) \cdot \left(\log_{10} \left(E/E_0(\theta) \right) \right)^n$ in the case of polynomials. The downside with such parametric approaches is that there is a tendency to lose the connection with the underlying physics; this criticism may also fairly be applied to the presently proposed additive correction, and perhaps even the Vaughan SEY model, which are both based on empirical fits to available data.

4.1.8 Section Summary

Throughout section 4.1, we have discussed the updated high-energy SEE model implemented in ICEPIC. This model is based upon the available GEANT4 data. The selected SEE model takes the form of an additive correction which defaults to being zero, allowing for backwards compatibility with existing ICEPIC input files.

As part of the development of this new model, we presented criteria which guided the ICEPIC SEE model updates, and discussed alternative options to the final SEE model which was selected. We believe that the final model implemented within ICEPIC allows for an optimal combination of fidelity to the available data, flexibility to represent future emission data a user may encounter, and simplicity.

An optional adjustment of the emission spectra is also included in the updated model, in order to allow the SEE model to more closely match GEANT4 emission spectra for incident electrons greater than a few tens of keV. Unfortunately, due to limitations in GEANT4, it is not possible to accurately characterize the relative contribution of low-energy secondary electrons to the overall EES, so some uncertainty remains in the appropriate choice of secondary electron EES. This will be addressed further in the future recommendations covered in section 6.0.

4.2 Evaluation of the ICEPIC high-energy SEE model

4.2.1 Introduction

In section 4.1 we described the updated SEE model for high incident energy electrons which was implemented in ICEPIC. In this section we use this SEE model to generate seed electrons which lead to a parallel-plate multipactor scenario. By varying selected parameters within the high incident energy SEE model, we also can assess the sensitivity of the resulting ICEPIC simulations upon the underlying model parameters.

Section 4.2.2 introduces the baseline parallel-plate multipactor scenario, upon which we will add complexity in Section 4.2.3 by using the $E_{override}$ parameter from Section 4.1.6 to adjust the energy emission spectra. We then proceed to introduce a magnetic field in Section 4.2.4 and jointly adjust the SEY angle sensitivity parameters k_{sd} , k_{se} , k_{sd2} , and k_{se2} from section 4.1. Section 4.2.5 then concludes with a brief summary of the findings. We note that due to the nonlinear dependence of multipactor currents on the above parameters, we tend to focus on trends in the results as parameters change, as opposed to the particular results of a given scenario in isolation, which would not necessarily be translatable to a different ICEPIC simulation scenario.

4.2.2 Parallel-plate multipactor: baseline scenario

For the parallel plate multipactor simulations considered in this evaluation, an ICEPIC vacuum simulation volume of size 80 cm x 80 cm x 10 cm was defined within an (x,y,z)-space, with geometry discretization $ds=0.5$ cm along each dimension. PEC plates of size of 40 cm x 40 cm x 1 cm were introduced into this vacuum, such that there was a 4.5 cm separation between the plate faces participating in the multipactor. An RF potential of 1000 V at a frequency of 83.1 MHz was applied to the top plate relative to the bottom plate; the RF potential magnitude and frequency were chosen to yield a strong multipactor response for the chosen gap distance. A pictorial representation of this simulation arrangement is shown in Figure 42. For all results generated in this evaluation, 30 RF periods were simulated using time steps dt equal to half the

Courant time step: $dt = ds/(c \cdot 2\sqrt{3})$, where c is the speed of light. A macroparticle weight of $1E6$ was used for all electrons (beam and secondary) in these simulations.

A high energy beam composed of electrons with 300 keV kinetic energy and a current of 5 mA is emitted in a narrow beam from the center of the top plate along the $-z$ direction (ie. in a direction normal to this plate). Upon impact with the lower plate, this high energy beam will generate secondary electrons which can then seed multipactor. The average number of secondary particles (all non-beam particles) present during the final RF period of the simulation was recorded, allowing us to assess the sensitivity of the high incident energy SEE model on the resulting ICEPIC simulation.

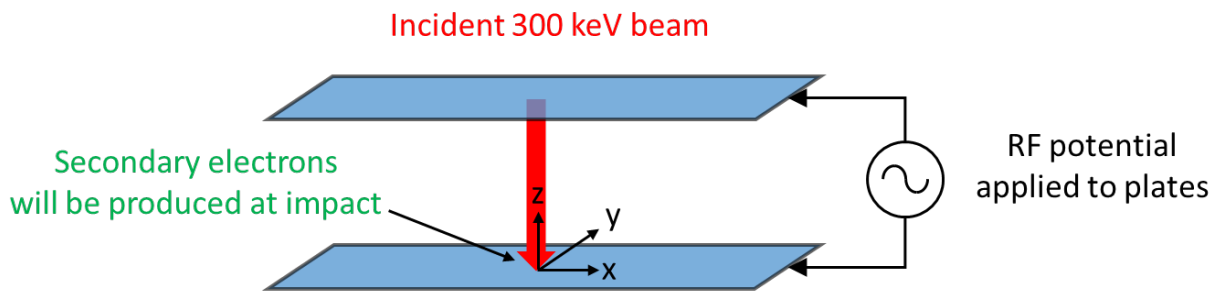


Figure 42: Parallel-Plate Multipactor Scenario.

The SEY for both parallel plates was defined to use the classical ICEPIC SEY curve (Vaughan SEY) with a peak occurring at an incident energy of 637.2 eV which corresponds to the theoretical impact energy for multipacting electrons starting from rest, augmented with an additive high incident energy response with a peak occurring at an incident energy of 300 keV (ie. $E_c = 300$ keV in model definition) and model parameters $n=2$ and $k(\theta=0^\circ)=1$ in the model definition given by Equation (7) of section 4.1. See Figure 43 for a notional example of such a composite SEY curve, with the Vaughan normal-incidence SEY peak δ_{max0} being set to 1.2 and the additive correction normal-incidence SEY peak $A(0)$ being set to 0.4. Unless otherwise noted, the emission energy distribution of the secondary electrons consists of 90% true secondaries modelled by a Maxwell-Boltzmann distribution with a temperature of 3 eV, and 10% scattered secondaries modelled by a uniform energy distribution between 0 and the incident energy.

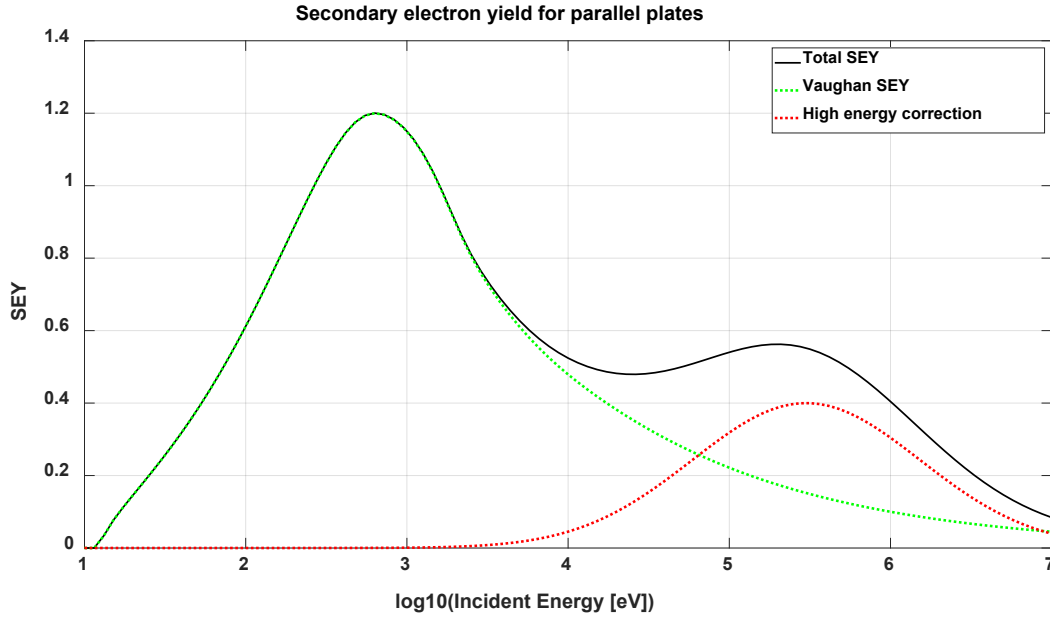


Figure 43: Notional Secondary Electron Yield Composed of Both a Vaughan SEY Component with a Peak Value δ_{max0} of 1.2 and a High Energy Correction Component with a Peak Value $A(0)$ of 0.4.

Swept-parameter trials were run in which the peak of the Vaughan SEY curve and the peak of the additive high-energy correction SEY curve were allowed to independently vary. The Vaughan normal-incidence SEY peak δ_{max0} was varied from 1.0 to 1.4 in steps of 0.01, and the high-energy correction normal-incidence SEY peak $A(0)$ was varied from 0.0 to 0.8 in steps of 0.1. Figure 44 shows the results of such trials.

A few noteworthy behaviors are observed in the results. We first note that even for the high energy SEY set to zero, multipactor is still initiated due to the nonzero SEY from the Vaughan component with a tail extending to high energies as shown in Figure 43. We also note that for a peak Vaughan SEY component of 1.2 (as shown above in Figure 43), the Vaughan SEY has a value of approximately 0.15 at an incident energy of 300 keV, and thus a sweep of 0.0 to 0.8 in the high energy SEY peak (which occurs at 300 keV) corresponds to approximately 0x to 5.3x of the Vaughan SEY contribution. In the trials used to generate Figure 44, for a peak Vaughan SEY of 1.2, we observe 3.54E3 multipacting particles when the high energy SEY peak is 0.0, and 1.90E4 multipacting particles when the high energy SEY peak is 0.8; this corresponds to an increase by a factor of approximately 5.4, very close to the above-noted factor of 5.3. Thus, before space-charge limits the multipactor current, we see a linear relationship between the high energy (300 keV) SEY and the resulting low-energy multipactor current.

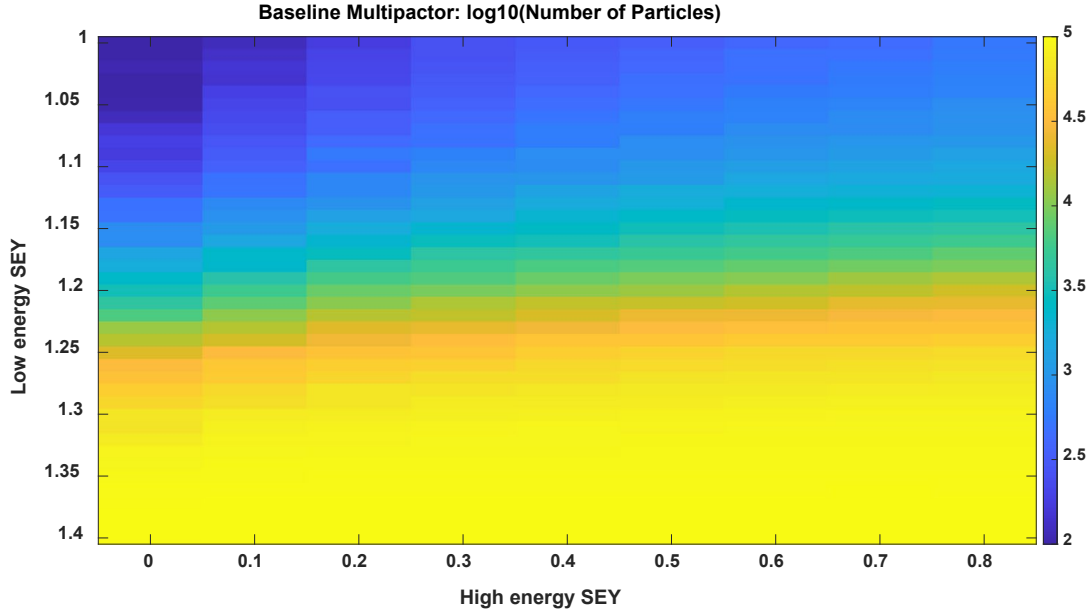


Figure 44: Average Number of Multipacting Particles in Final RF Period of Simulation, as a Function of the Peak SEY of the Low Energy (Vaughan) SEY Component and the High Energy SEY Component.

4.2.3 Parallel-plate multipactor with E_{override}

With these baseline results examined, we next examine the effect of the optional secondary energy override threshold E_{override} described in Section 4.1.6; incident electrons greater than E_{override} produce secondaries with energy spectra uniformly distributed between 0 and the incident energy. We set E_{override} (sec_e_over parameter in the ICEPIC input file) to be 30 keV, and otherwise run the same trials as described above. The results are shown in Figure 45. We observe that the number of multipacting particles is reduced as compared to the previous results, due to high-energy incident electrons tending to produce more high-energy secondary electrons, instead of primarily low-energy true secondary electrons which can directly phase-lock with the multipactor resonance.

In the trials used to generate Figure 45, for a peak Vaughan SEY of 1.2, we observe 200.6 average multipacting particles when the high energy SEY peak is 0.0, and 4.13E3 multipacting particles when the high energy SEY peak is 0.8; this corresponds to a nonlinear increase by a factor of 20.6, significantly greater than the previous linear increase by a factor of 5.36. An examination of the number of secondary particles vs. time is shown in Figure 46, for both high energy SEY peaks $A=0.0$ and $A=0.8$, with and without using E_{override} ; a peak Vaughan SEY of 1.2 was used in all cases. The plots show that all curves are tending towards the same asymptotic slope as time progresses, representing the same exponential growth factor of multipactor current, as expected. However, we see that multipactor initiation is delayed when the optional E_{override}

parameter is used, as compared to the baseline results without E_{override} . The exact mechanism for this multipactor initiation delay is not well understood, but presumably is related to the actual number of secondary electrons in the proper phase space to be susceptible to multipactor resonance, and not just their relative number in relation to the total population of secondary electrons.

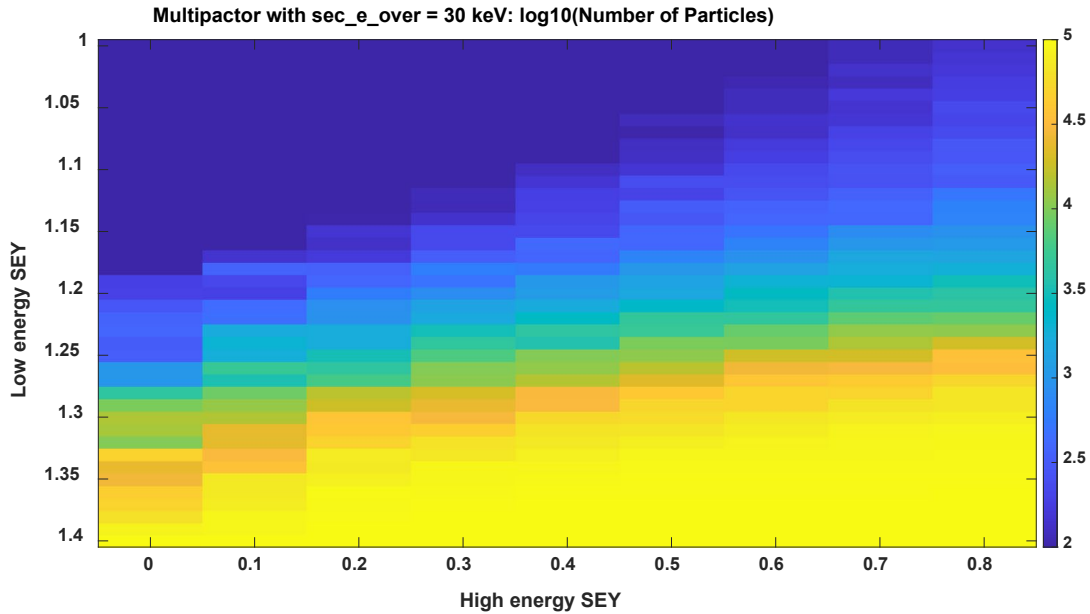


Figure 45: Average Number of Multipacting Particles in Final RF Period of Simulation, as a Function of the Peak SEY of the Low Energy (Vaughan) SEY Component and the High Energy SEY Component, with the Optional E_{override} Parameter set to 30 keV.

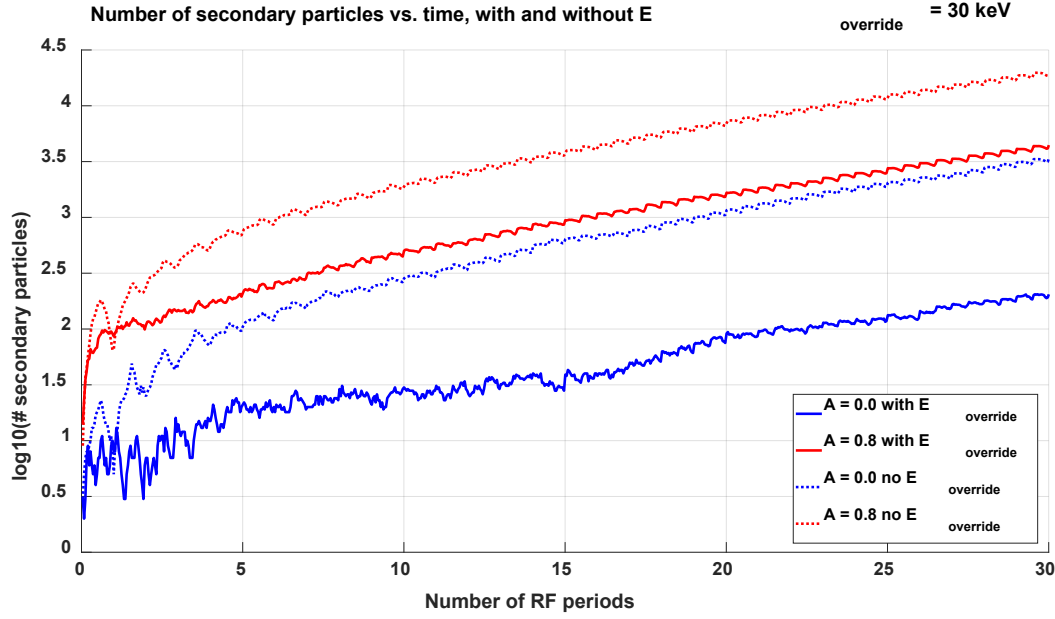


Figure 46: Number of Secondary Particles vs. Time, With and Without Setting $E_{\text{override}} = 30$ keV; A Vaughan SEY peak of 1.2 was Used, and Two Different High Energy SEY Peaks of $A=0$ and $A=0.8$ were Used: The Presence of E_{override} Delays Simulated Multipactor Initiation.

4.2.4 Parallel-plate multipactor with magnetic containment

We next consider the effect of non-normal incidence angles on the resulting multipactor currents. To do this, continue with E_{override} set to 30 keV, and introduce a z-directed magnetic field (normal to the plate faces) as shown in Figure 47. This will result in secondary electrons orbiting the magnetic flux lines, with a consequence that more electrons will impact the plates at steeper incidence angles, because these steeply-inclined incidence trajectories would otherwise have been lost to the sides of the simulation volume. We can then adjust the incidence angle sensitivity factors k_{se} , k_{sd} , k_{se2} , and k_{sd2} in equations (4), (5), (8), (9), and (10) of section 4.1 and observe the change in the multipacting current.

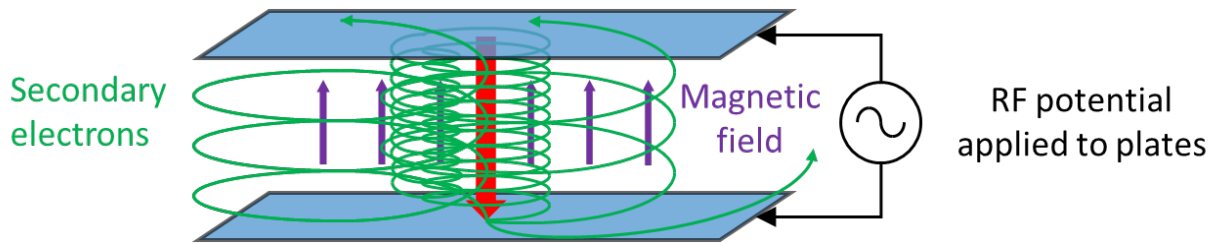


Figure 47: Parallel-Plate Multipactor Scenario in the Presence of a z-Directed Magnetic Field: Secondary Electron Trajectories Will Orbit the Magnetic Flux Lines and Undergo Less Loss to the Sides of the Simulation Volume.

Figure 48 shows the number of multipacting particles in the presence of a z-directed magnetic field of strength 0.1 T. When compared with the previous results of Figure 45 without a magnetic field, we see a reduction in multipacting particles. Figure 49 shows the number of secondary particles vs. time for comparison cases with and without the presence of the magnetic field. As seen in the plotted curves, the early-time number of secondary particles in the simulation tends to increase due to the presence of the magnetic containment, as expected. However, the containment also results in multipactor trajectories concentrated near the center of the plates, which appears to hasten space-charge limitation of multipactor growth, as can be seen by the late-time number of secondary particles having a reduced slope as compared to the previous case without the magnetic field. The net result is a diminishing of the overall number of secondary particles as seen in Figure 48, especially in the lower right quadrant where low and high energy SEY is large.

We next sequentially adjust the angle sensitivity factors k_{se} , k_{sd} , k_{se2} , and k_{sd2} to values of 1, 2, 4, and 8 while holding all other parameters the same; these four parameters were varied identically, and a single parameter k_s is used to denote all of them, ie. $k_{se} = k_{sd} = k_{se2} = k_{sd2} = k_s$. The results are shown respectively in Figure 50, Figure 51, Figure 52, and Figure 53. We tend to see a modest increase in the total number of secondary particles observed as k_s is increased, as would be expected due to the SEY increasing for off-normal incident electrons.

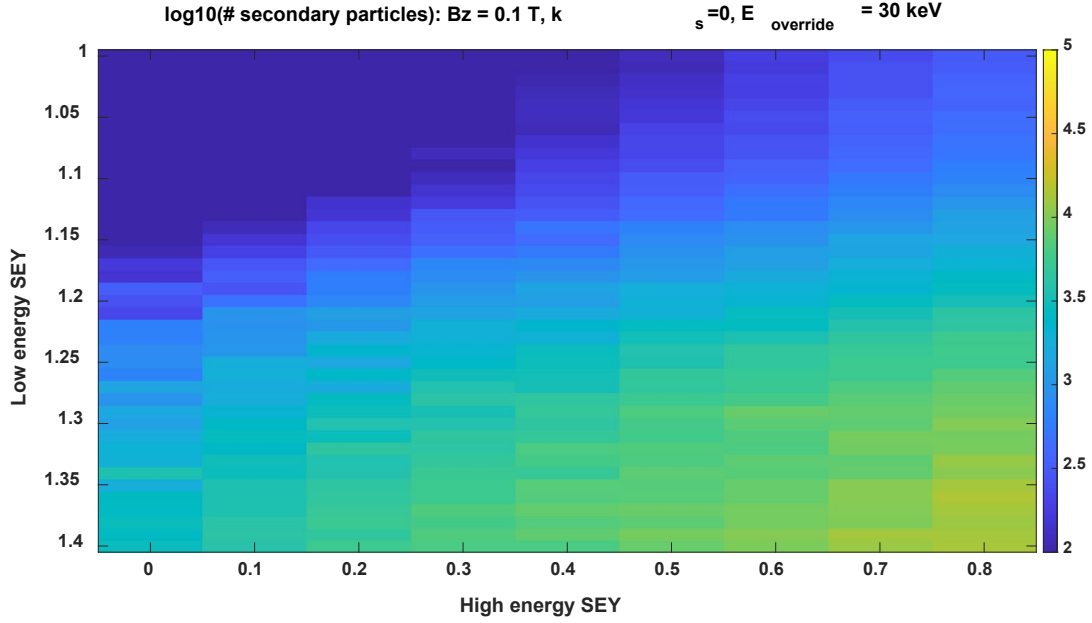


Figure 48: Average Number of Multipacting Particles in Final RF Period of Simulation, as a Function of the Peak SEY of the Low Energy (Vaughan) SEY Component and the High Energy SEY Component. Angle-Dependent Factor $k_s = 0$ with a Z-Directed Magnetic Field of 0.1 T.

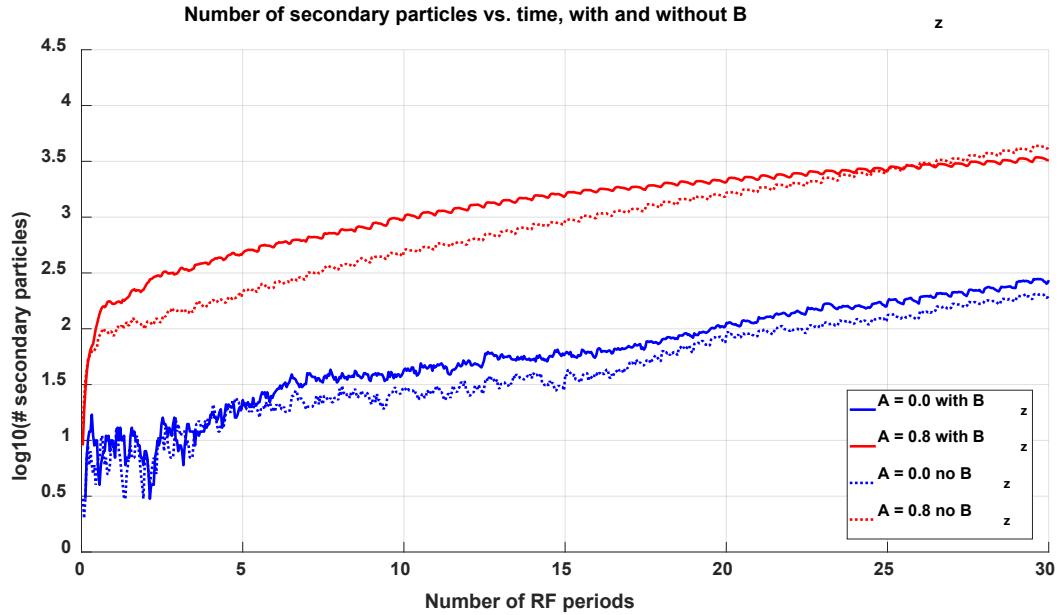


Figure 49: Number of Secondary Particles vs. Time, With and Without the Presence of B_z . A Vaughan SEY Peak of 1.2 Was Used, and Two Different High Energy SEY Peaks of $A=0$ and $A=0.8$ Were Used; $E_{\text{override}} = 30$ keV for All Cases.

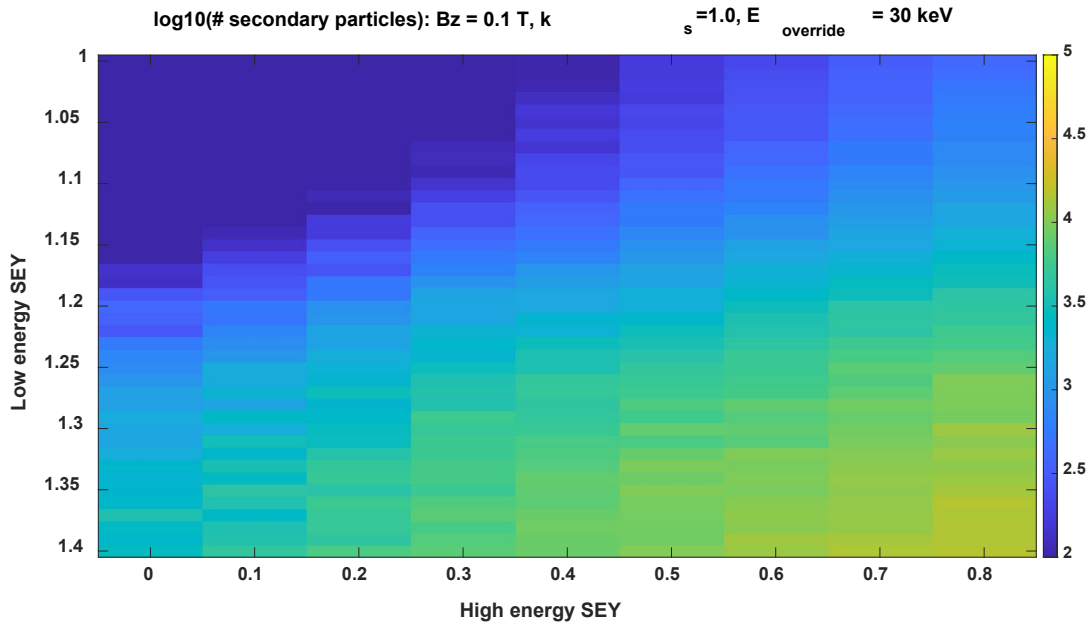


Figure 50: Average Number of Multipacting Particles in Final RF Period of Simulation, as a Function of the Peak SEY of the Low Energy (Vaughan) SEY Component and the High Energy SEY Component; Angle-Dependent Factor $k_s = 1$ With a Z-Directed Magnetic Field of 0.1 T.

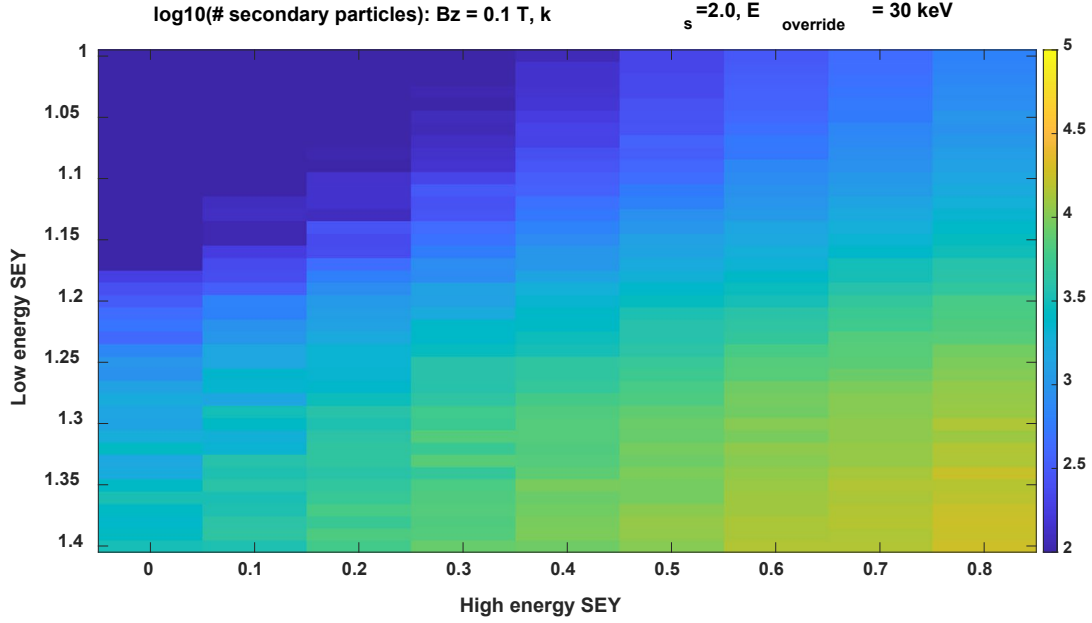


Figure 51: Average Number of Multipacting Particles in Final RF Period of Simulation, as a Function of the Peak SEY of the Low Energy (Vaughan) SEY Component and the High Energy SEY Component. Angle-Dependent Factor $k_s = 2$ with a Z-Directed Magnetic Field of 0.1 T.

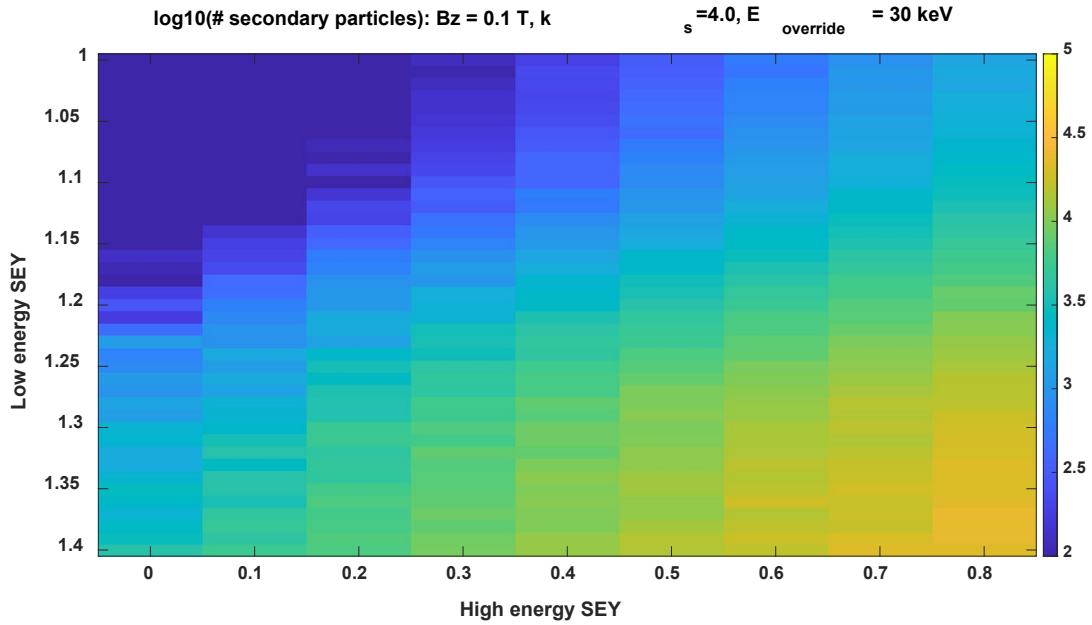


Figure 52: Average Number of Multipacting Particles in Final RF Period of Simulation, as a Function of the Peak SEY of the Low Energy (Vaughan) SEY Component and the High Energy SEY Component; Angle-Dependent Factor $k_s = 4$ with a Z-Directed Magnetic Field of 0.1 T.

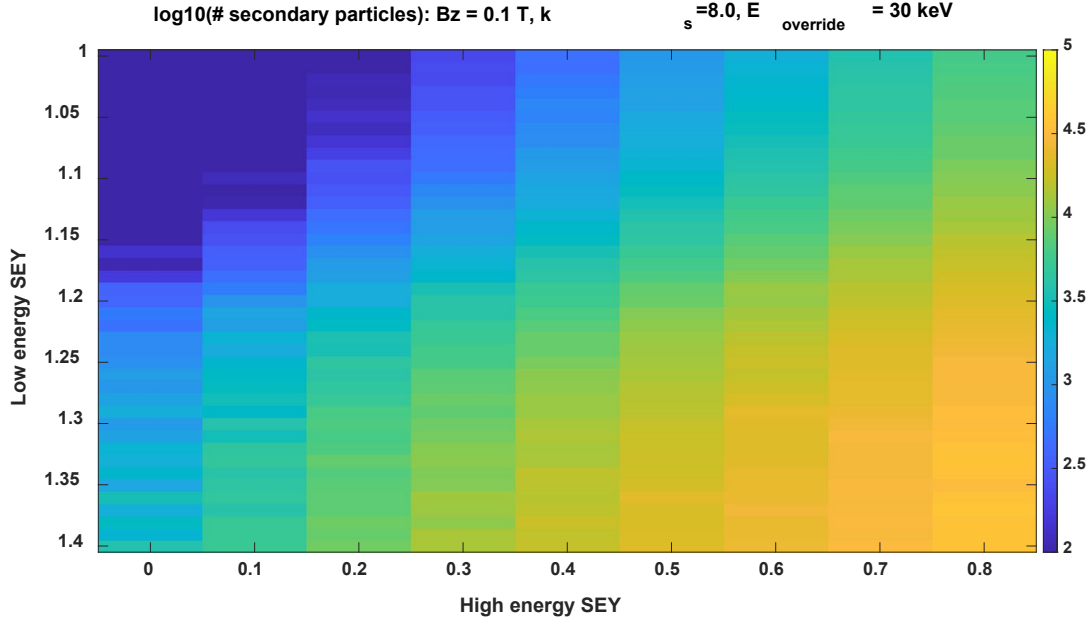


Figure 53: Average Number of Multipacting Particles in Final RF Period of Simulation, as a Function of the Peak SEY of the Low Energy (Vaughan) SEY Component and the High Energy SEY Component; Angle-Dependent Factor $k_s = 8$ with a Z-Directed Magnetic Field of 0.1 T.

4.2.5 Conclusion

In section 4.2 we have provided an evaluation of the updated ICEPIC high-energy SEE model by simulating parallel-plate multipactor, which is seeded from secondary electrons generated by a relatively high energy electron beam incident upon one of the plates. We examined how the predicted multipactor current growth changed as the SEE model parameters were changed. The observed results can be explained to a large part by first-principles multipactor analysis and the assumption of eventual space-charge saturation which limits further multipactor growth. However, adjustment of the SEE energy spectra (section 4.2.3) was shown to unexpectedly affect the simulation time before multipactor current growth was observed, presumably by changing the absolute number of electrons within an appropriate portion of the phase space to phase-lock with the RF excitation.

5.0 CONCLUSIONS

This report has detailed work performed to improve the ICEPIC high-energy SEE model. A literature search revealed that despite being a problem of interest for a century, there are significant inconsistencies in experimental data due to the high SEY sensitivity to material preparation and purity; there is also relatively little data for incident energies above a few tens of keV. One key takeaway for anyone seeking to model SEE is that there may not be a precisely known SEY curve for a given material in real-world situations, but rather a range of possible SEY values depending on such factors as material purity, surface contamination, roughness, temperature, and even prior dosing of incident particles. It is hard to precisely quantify such effects, but if simulated results for a given device are expected to be sensitive to SEE, then regardless of the SEE model employed, it may be prudent to assess device behavior with the secondary electron yield modified by perhaps $\pm 50\%$ from the expected value.

Due to insufficiency of the available measured data, we next turned our attention to the simulation code GEANT4, which is perhaps the most recognized and validated code presently available for high-energy particle-material interaction simulations. The best available GEANT4 physics models are presently unable to generate secondary electrons at energies of less than 10 eV, resulting in the omission of a significant portion of the secondary electron population and a likely under-estimation in SEY. However, the authors do believe that taken together, the GEANT4 results for seven materials do qualitatively represent a sufficient breadth of SEE behavior, allowing for the definition of a more general parametric SEE model, which was described in section 4.1 and implemented in ICEPIC. This more general parametric SEE model can be tuned to fit future available SEE data as it becomes available.

The updated high energy SEE model was evaluated using a well-understood parallel-plate multipactor scenario, and sensitivity to various model parameters were examined. The observed results behaved mostly as anticipated, except for an unforeseen multipactor initiation delay when the EES was adjusted to include more energetic secondary electrons. The authors attribute this unanticipated initiation delay to the nonlinearities inherent in multipactor formation and phase-locking of random particle trajectories, and not suggestive of any problems in the high energy SEE model.

6.0 RECOMMENDATIONS

The main limitations in the present work relate to the lack of robust SEE data for high incident energy electrons. The available high energy experimental data does not cover a wide range of materials, and the data which is available tends to be for normal incidence at relatively few incident energies. Similarly, the available GEANT4 simulated data suffers from deficiencies in the predicted number of secondary electrons with low emission energies, and recent successive GEANT4 releases do not always yield consistent results, both of which suggest caution when assessing GEANT4 validity for accurate material characterization.

Based on the above realities, it is the recommendation of the author that further high energy secondary electron model development be halted until better validated data is available, against which the existing high energy model can be tuned and/or modified as needed. In the meantime, when secondary electrons are important to device physics being simulated in ICEPIC, it is recommended that the user assess device sensitivity with the secondary electron yield modified by perhaps $\pm 50\%$ from the expected value.

Reliable high energy experimental data would require numerous measurements with varying samples, preparation, and measurement conditions in order to assess repeatability. Such data would be very valuable, but would also be quite costly to obtain and validate. The authors do not believe it reasonable to anticipate a well-developed library of such data in the public domain any time within the foreseeable future. It may be feasible for well-resourced groups to characterize the high energy SEE for a limited number of specific materials present in devices they wish to simulate, with the materials subject to the particular preparations and environments anticipated with the eventual real-world devices.

The limitations presented with GEANT4 results are more easily overcome than the lack of experimental data, and the authors would recommend focusing any available resources towards obtaining improved high energy secondary electron data from GEANT4. This could be accomplished by modification of the GEANT4 Livermore physics models, or the implementation of new models, in order to reduce the minimum energy threshold from the present 10 eV. In order to capture the majority of low-energy secondary electrons which tend to follow a Maxwell-Boltzmann distribution with a temperature of a few eV, a low energy threshold of 1 eV or lower is recommended. Such work would require considerable technical sophistication, with a level of effort estimated by the authors to be three person-years for PhD-trained physicists, assuming that validated experimental data of the relevant atomic physical processes is available in the 1-10 eV range for the engineering materials of interest.

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APPENDIX A: EES for Copper and Stainless Steel

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A.1 Overview

This appendix provides an exhaustive list of the GEANT4 EES plots for copper and stainless steel, generated using the three GEANT4 electromagnetic models discussed in Section 3.2.6. Each plot shows the emission energy spectra (EES) for a particular incident energy and has distributions for the incident angles between 0 and 60 degrees. The 80 degree EES were not included because all electrons were perfectly reflected, with emission energy equal to the incident energy. All EES x-axis ranges are normalized so that a value of 1 corresponds to the incident energy. In order to best observe the spectra over a wide range of incident energies, the EES y-axes are scaled such that each curve has an integrated area of unity, and the total yield for that incident energy is listed in the legend; note that when yield curves are displayed in isolation in the literature, a common convention is for the integral of the yield curve not to equal unity, but rather to equal the total yield.

A.2 Copper

A.2.1 Default Models

The EES for the GEANT4 default model with the GEANT4 built-in copper material definition are as shown in Figure A-1 through Figure A-5.

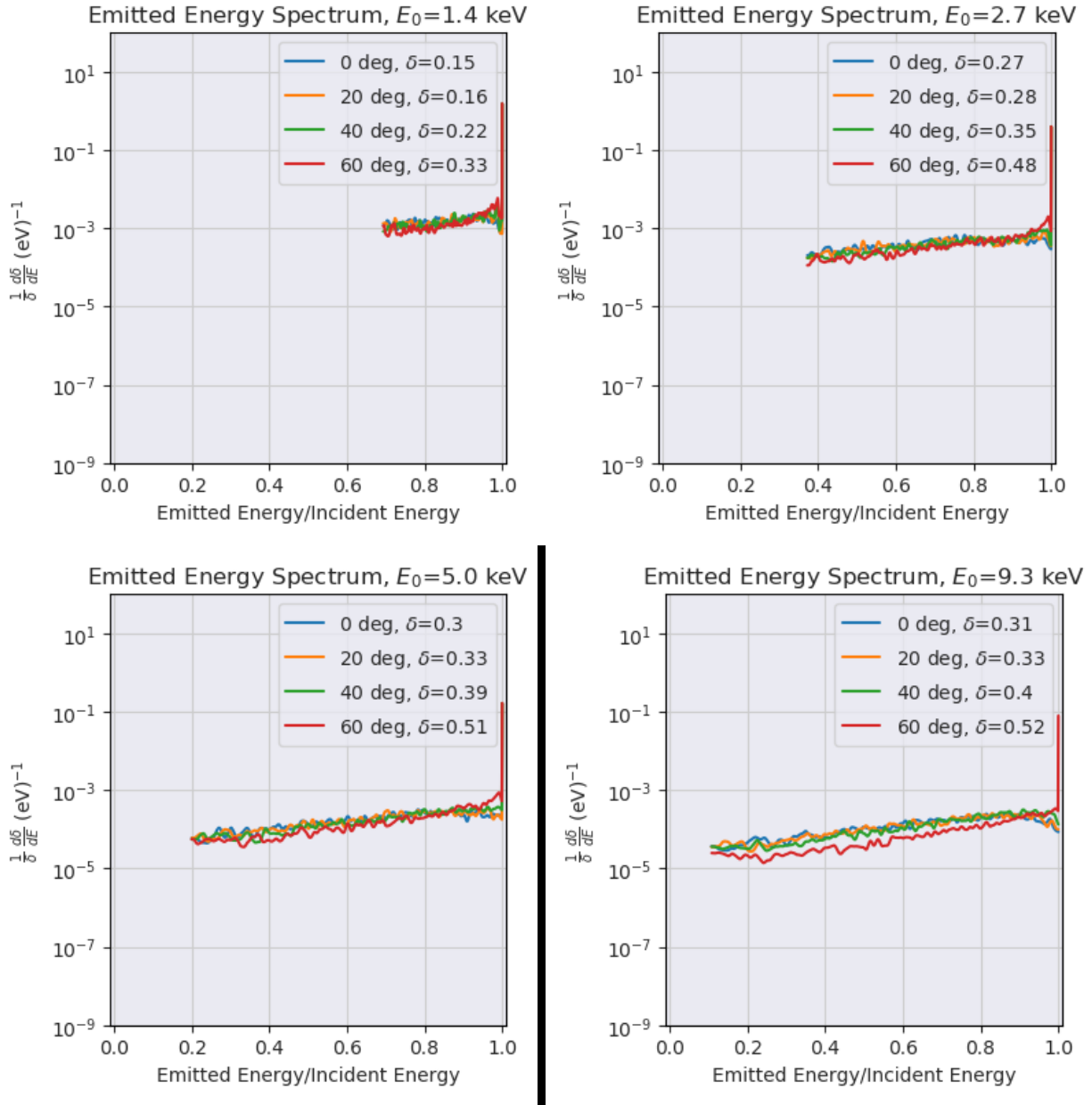


Figure A- 1: EES from GEANT4's Default Models for Electrons Incident on Copper with Energies E_0 of 1.4 to 9.3 keV.

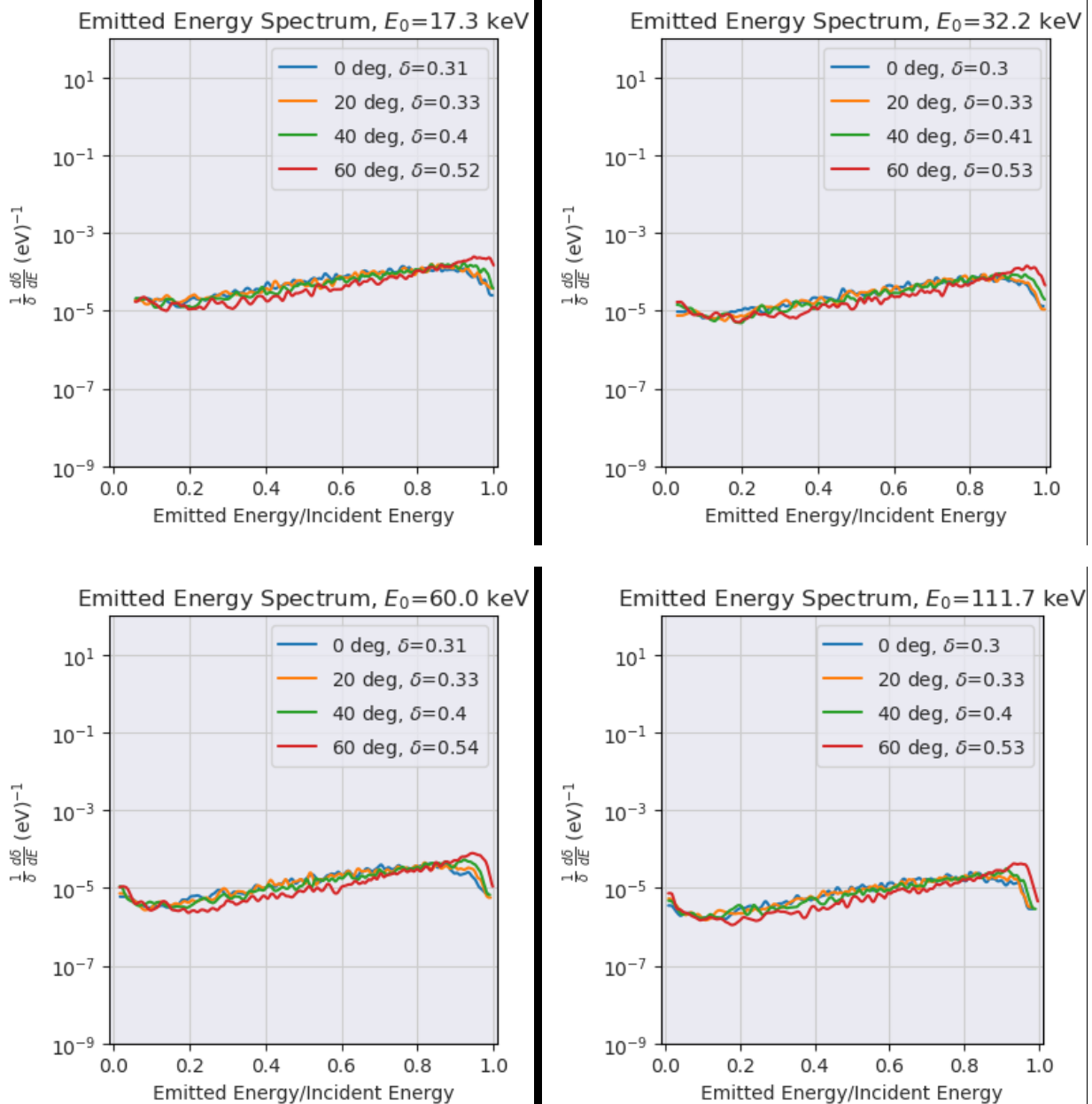


Figure A- 2: EES from GEANT4's Default Models for Electrons Incident on Copper with Energies E_0 of 17.3 to 111.7 keV.

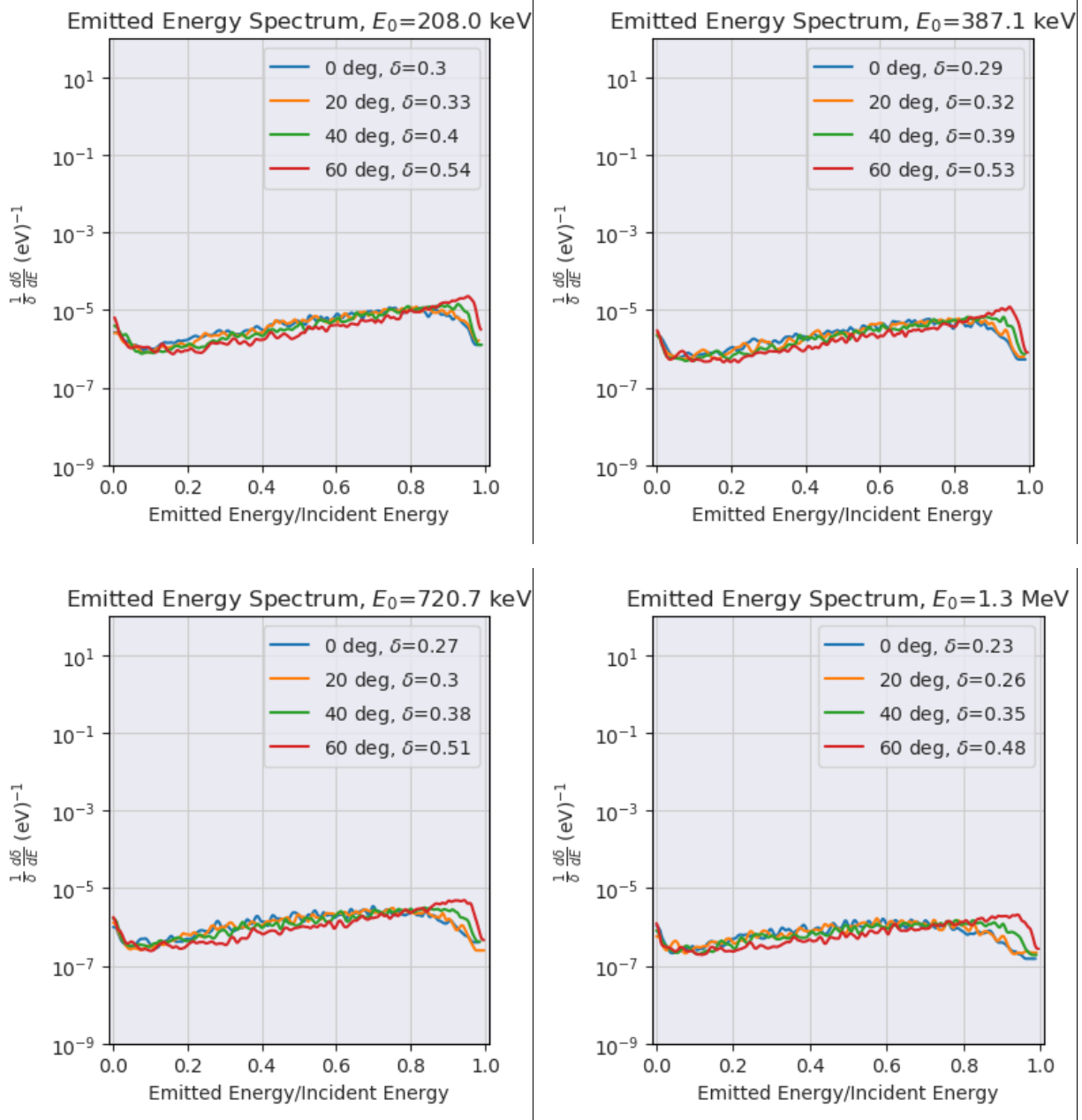


Figure A- 3: EES from GEANT4's Default Models for Electrons Incident on Copper with Energies E_0 of 208 keV to 1.3 MeV.

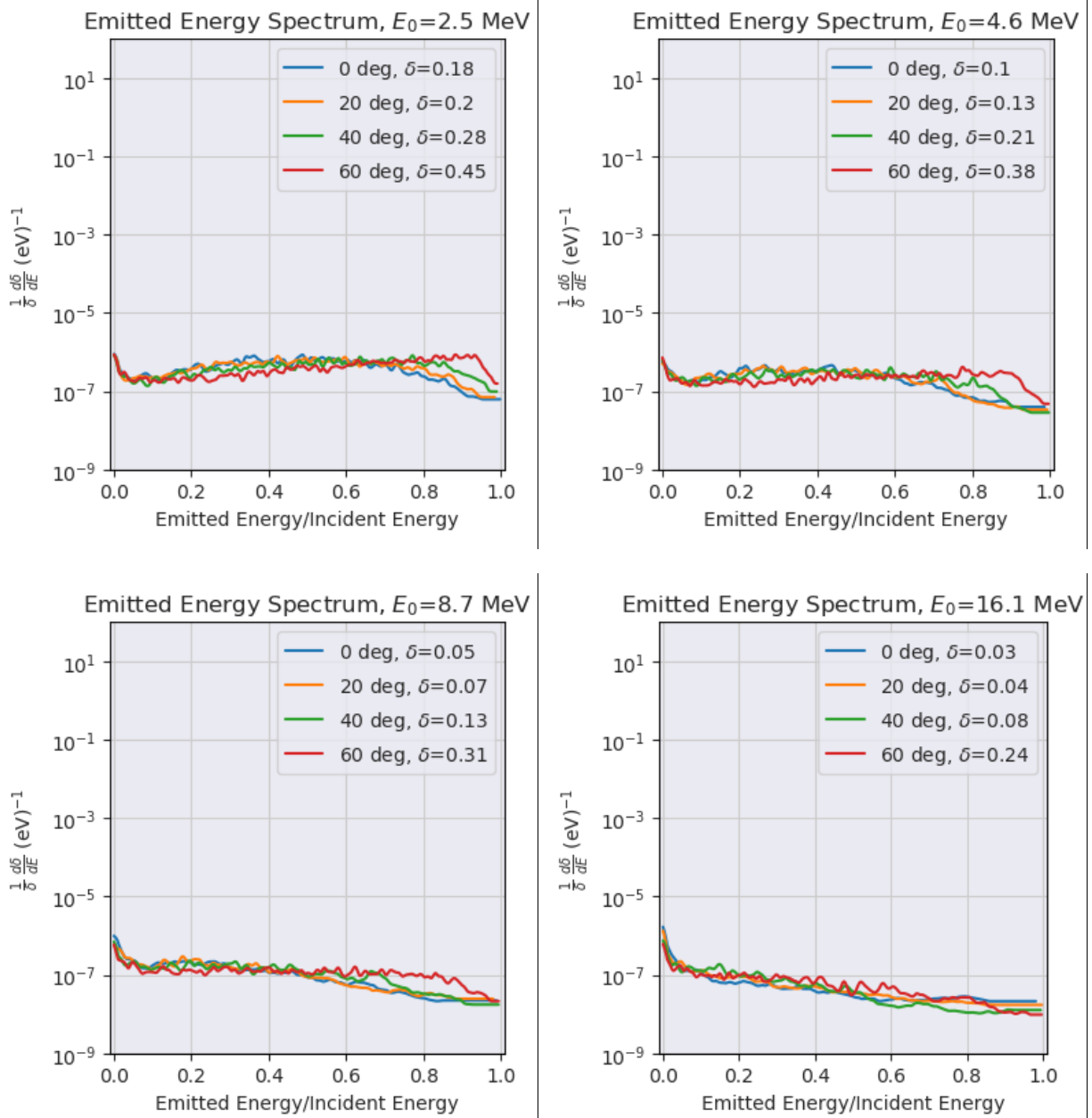


Figure A- 4: EES from GEANT4's Default Models for Electrons Incident on Copper with Energies E_0 of 2.5 to 16.1 MeV.

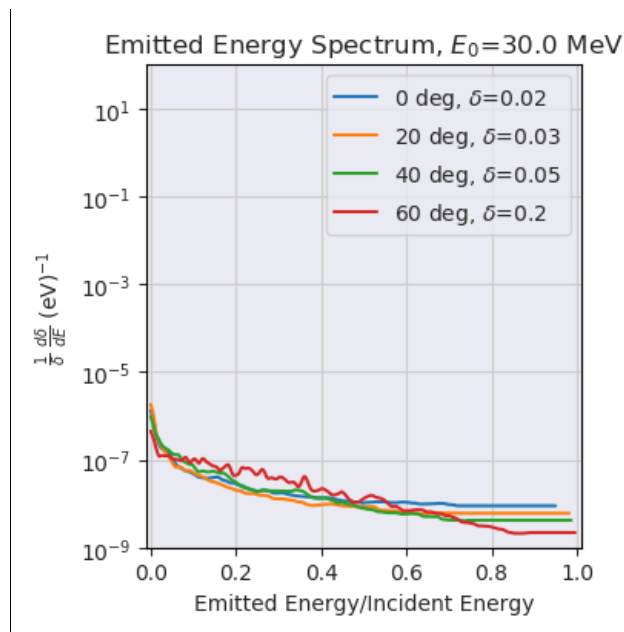


Figure A- 5: EES from GEANT4's Default Models for Electrons Incident on Copper with Energy E_0 of 30.0 MeV.

A.2.2 Penelope Models

The EES for the GEANT4 Penelope model with the GEANT4 built-in copper material definition are as shown in Figure A-6 through Figure A-11.

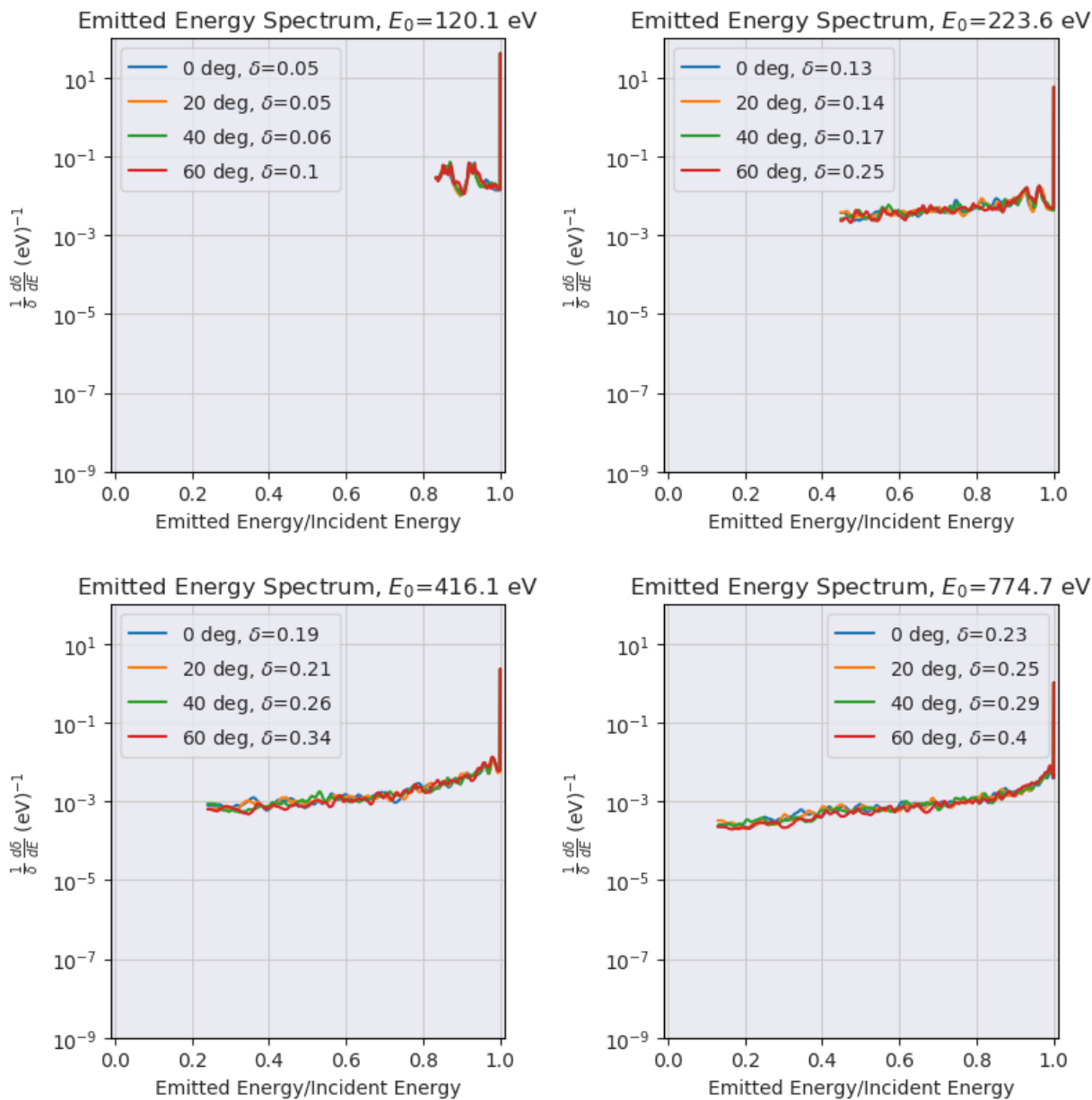


Figure A- 6: EES from GEANT4's Penelope Models for Electrons Incident on Copper with Energies E_0 of 120.1 to 774.7 eV.

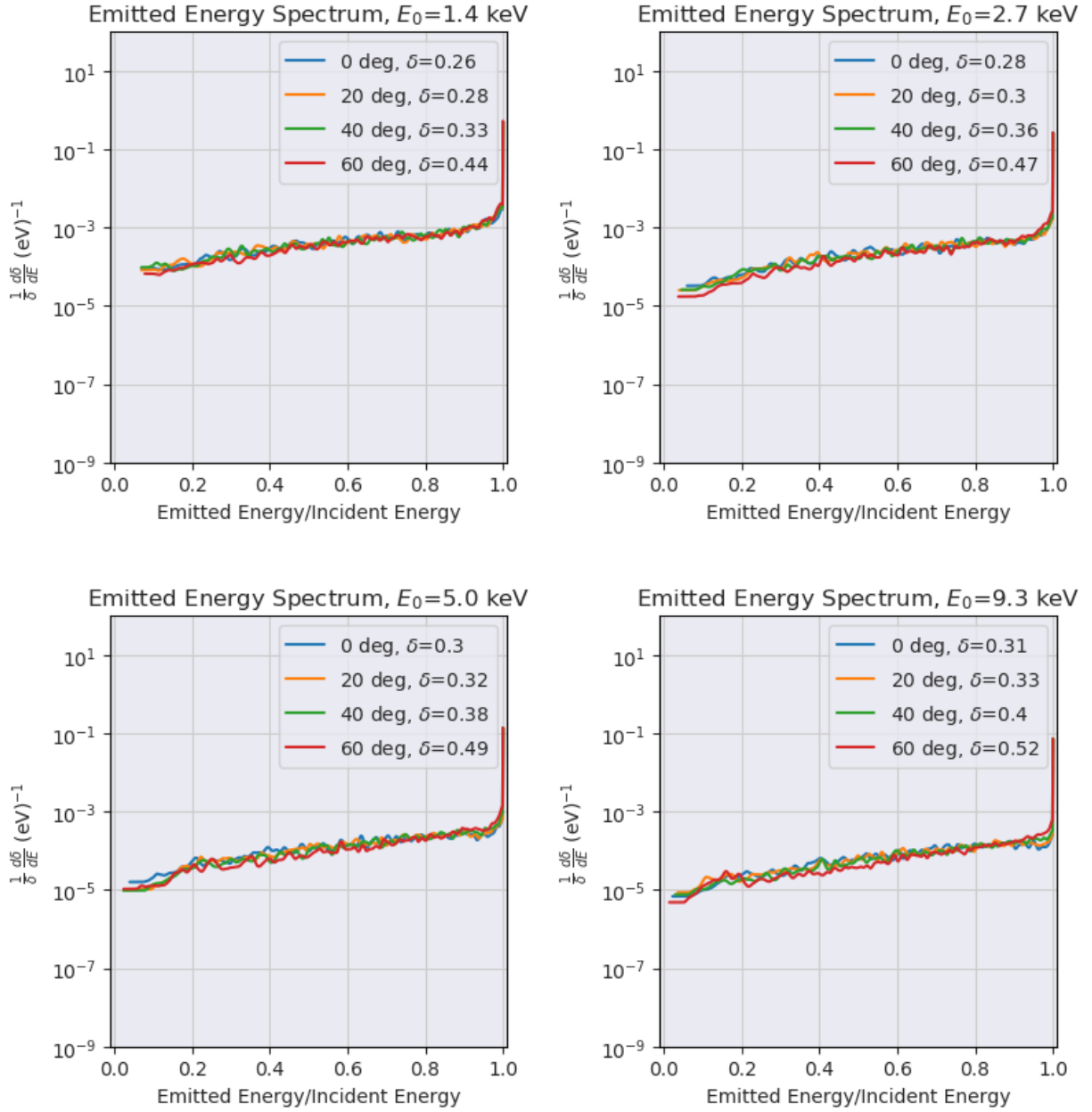


Figure A- 7: EES from GEANT4's Penelope Models for Electrons Incident on Copper with Energies E_0 of 1.4 to 9.3 keV.

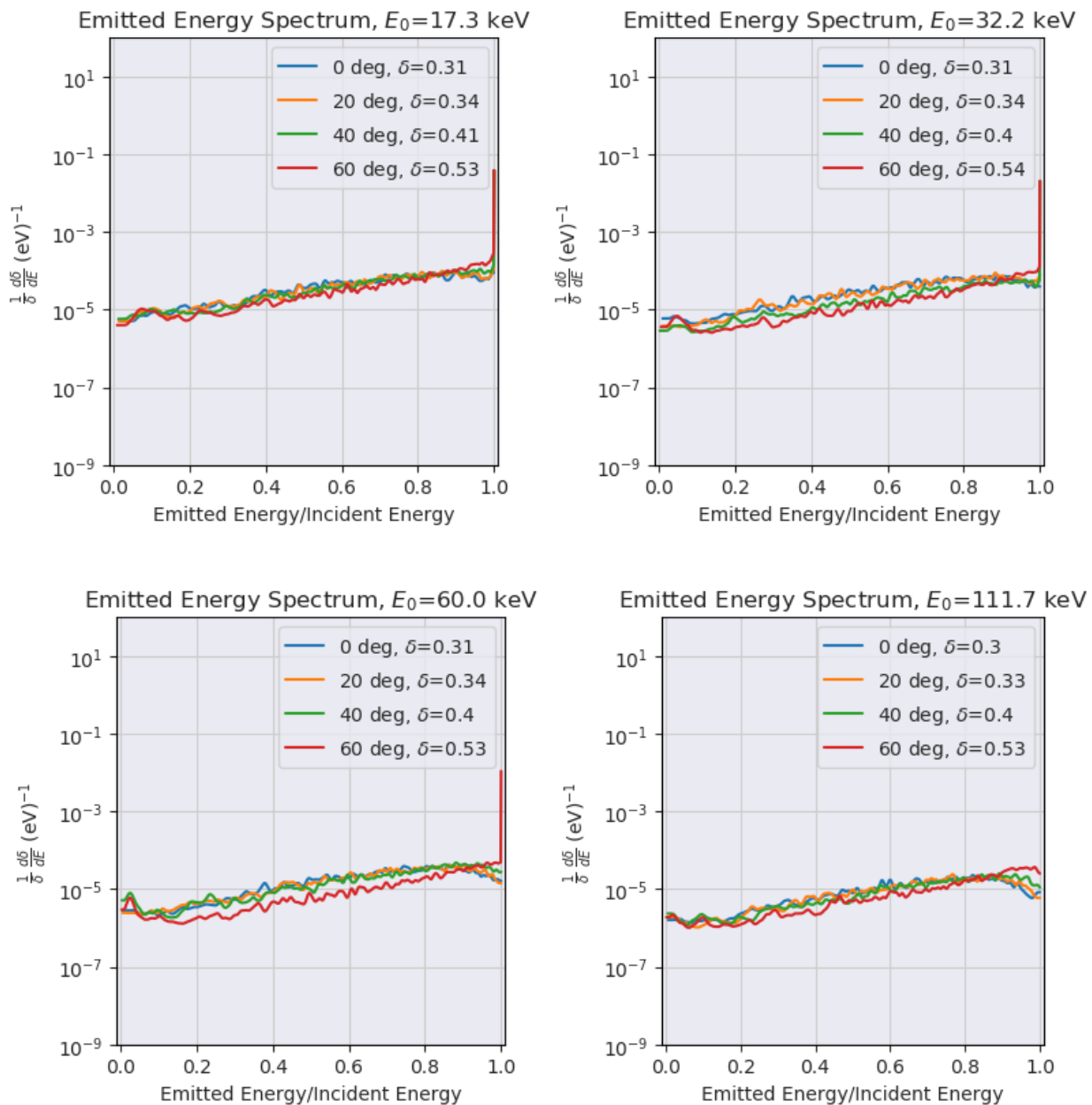


Figure A- 8: EES from GEANT4's Penelope Models for Electrons Incident on Copper with Energies E_0 of 17.3 to 111.7 keV.

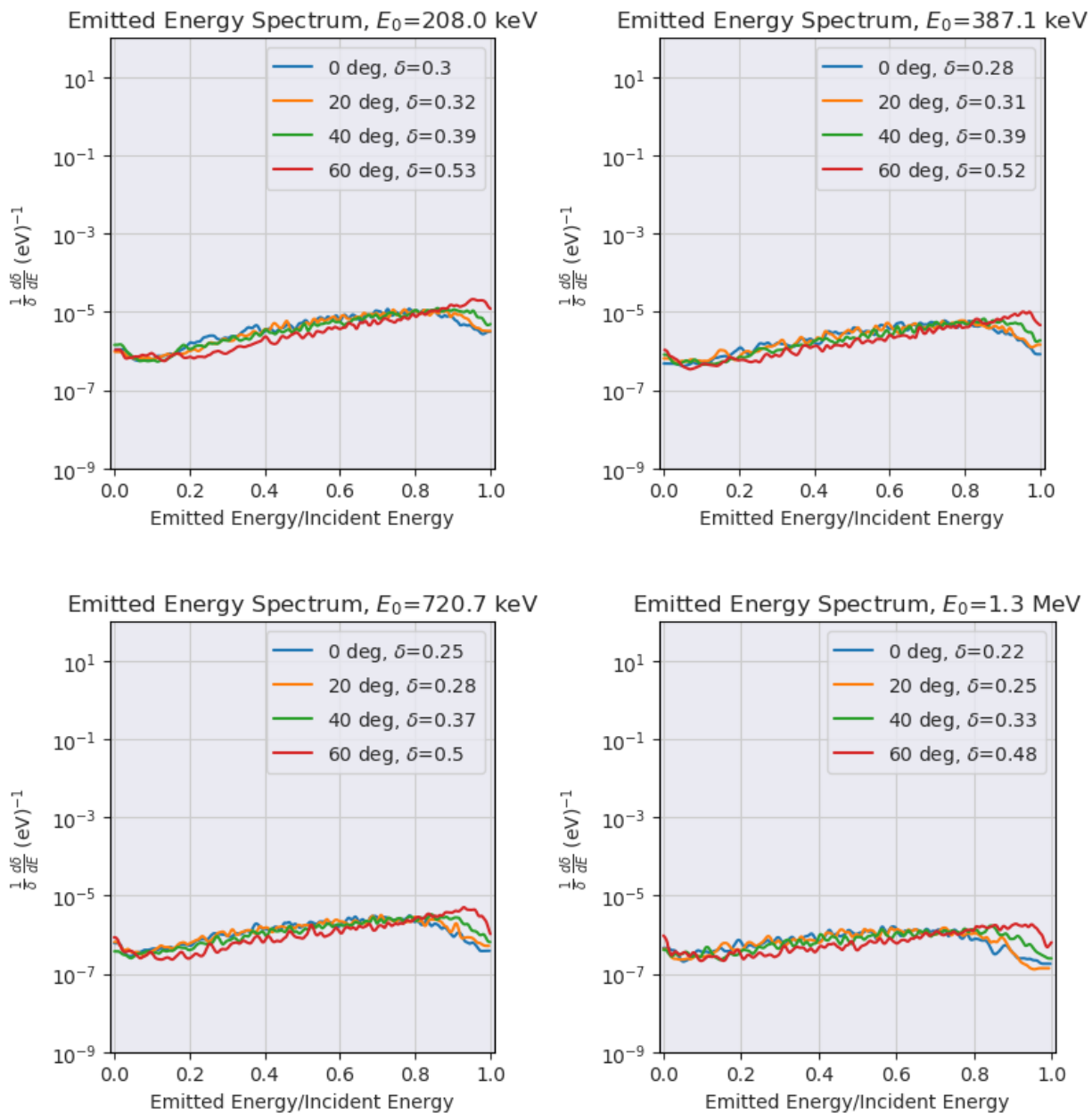


Figure A- 9: EES from GEANT4's Penelope Models for Electrons Incident on Copper with Energies E_0 of 208 keV to 1.3 MeV.

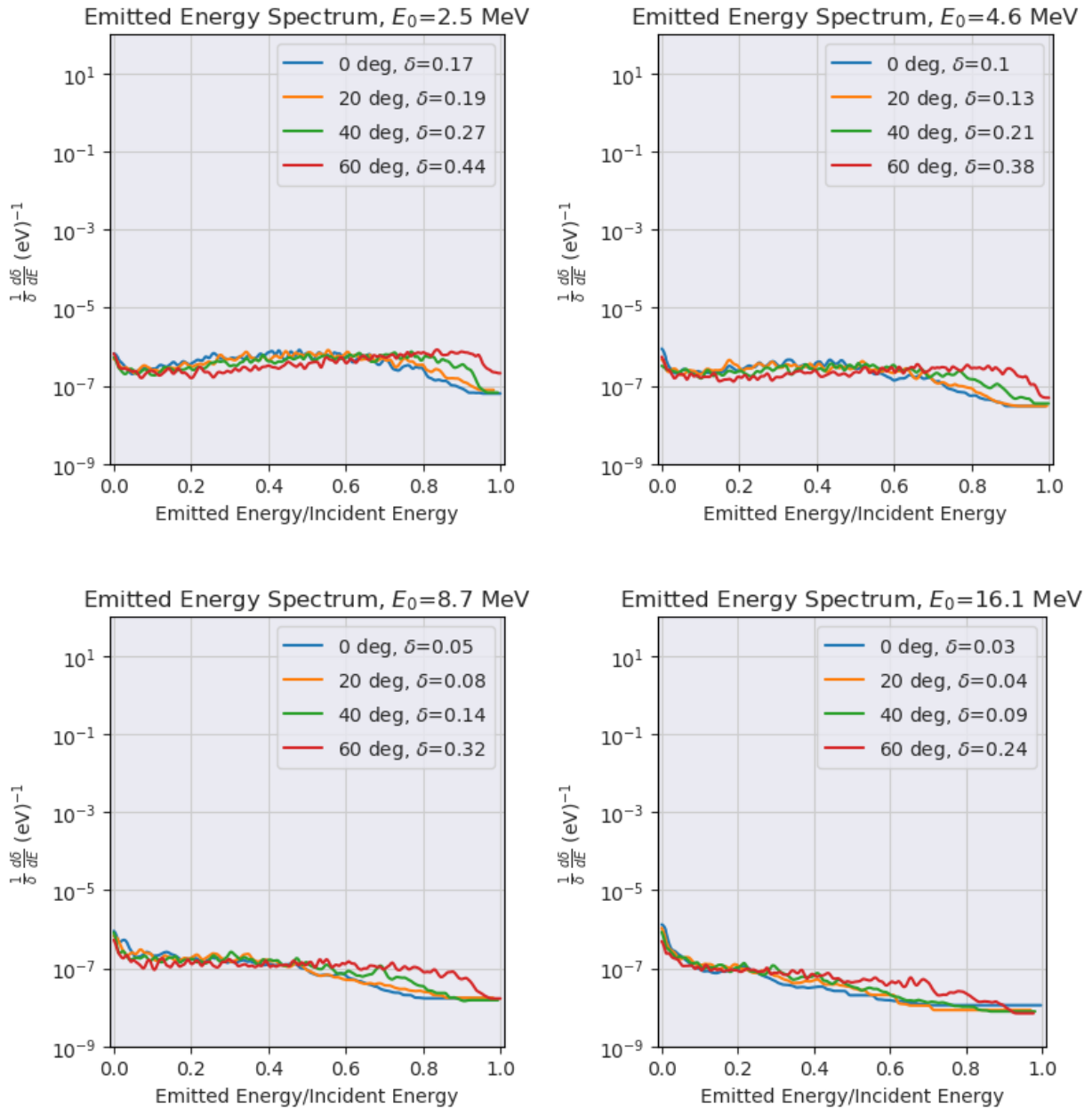


Figure A- 10: EES from GEANT4's Penelope Models for Electrons Incident on Copper with Energies E_0 of 2.5 to 16.1 MeV.

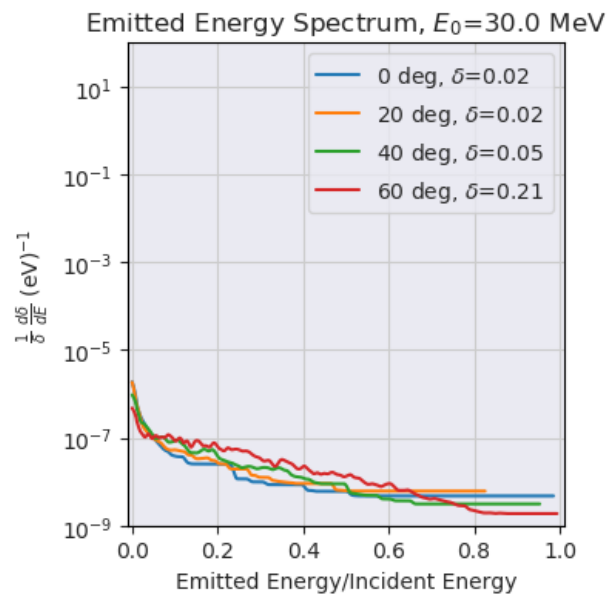


Figure A- 11: EES from GEANT4's Penelope Models for Electrons Incident on Copper with Energy E_0 of 30.0 MeV.

A.2.3 Livermore Models

The EES for the GEANT4 Livermore model with GEANT4 built-in copper material definition are provided in Figure A-12 through Figure A-24. In addition to the EES plotted over the full range of secondary energies, these plots also show the EES zoomed into the range 10-20 eV. This is because the Livermore SEY curves have an emission peak in this range that is not observed in the default and Penelope EES. This peak is likely the reason that the GEANT4 Livermore SEY curves agree with the Furman and Vaughan SEY curves better than the results from the GEANT4 default and Penelope models. Note that despite this low energy emission peak being present, the GEANT4 Livermore model still significantly underestimates the SEY for energies below a few tens of keV as compared to the Furman and Vaughan models.

It should be noted that due to the different sample widths used for plotting the EES distributions on the normal and zoomed x-axes, the displayed probability densities will appear somewhat different, although the areas under the curves (probability) for the corresponding distributions is the same over the zoomed 10-20 eV intervals. Note also that in Figure A-14 and some subsequent results in this report, some narrow spikes are seen in the GEANT4 emission energy spectra. We suspect that these are due to GEANT4 trying to model discrete energies corresponding to quantum mechanical energy transitions, but we do not understand why they only appear in some emission spectra.

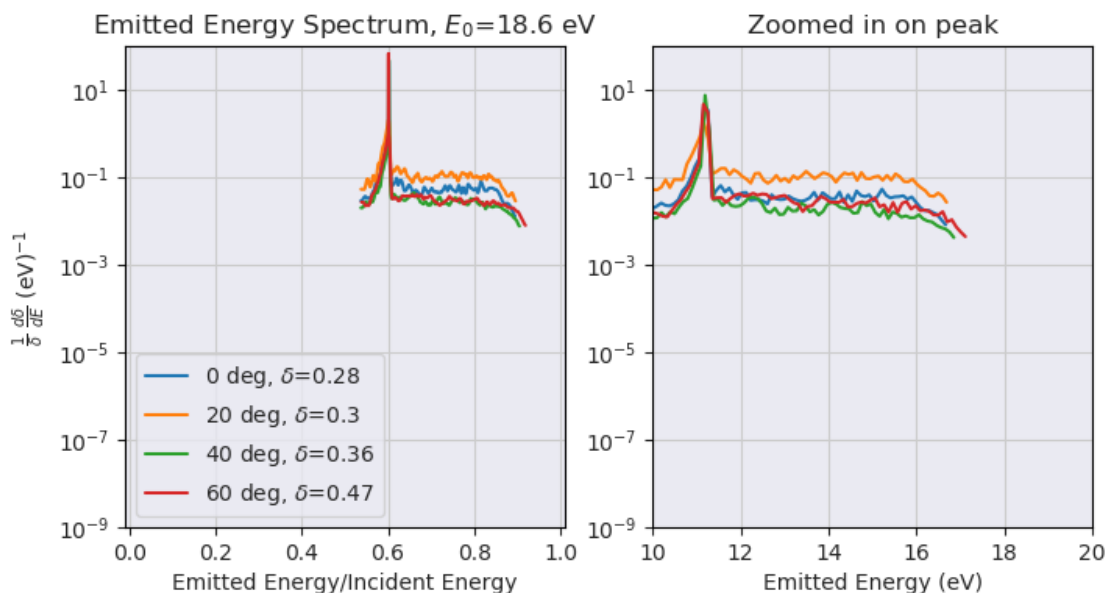


Figure A- 12: EES from GEANT4's Livermore Models for Electrons Incident on Copper with Energy E_0 of 18.6 eV.

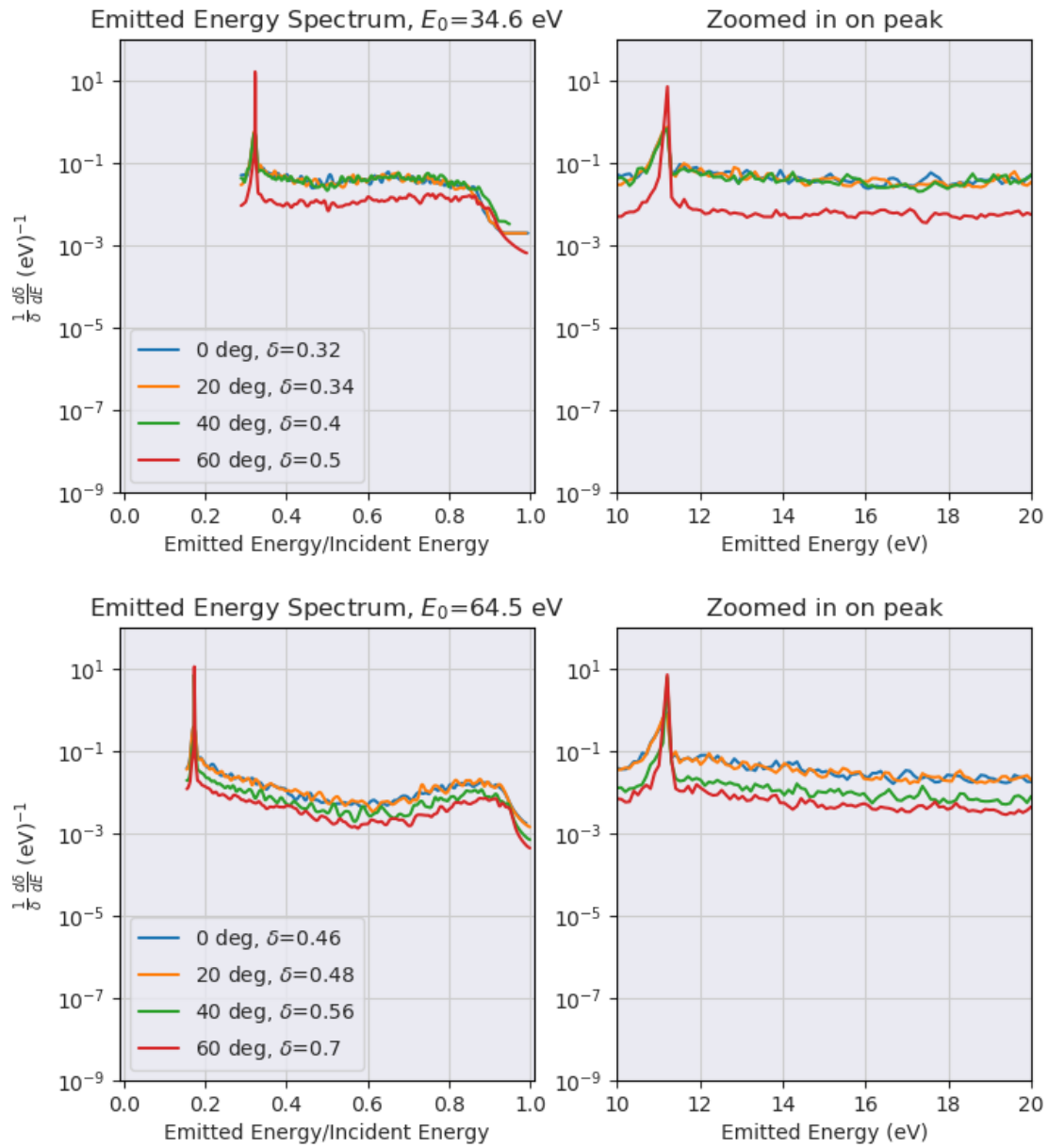


Figure A- 13: EES from GEANT4's Livermore Models for Electrons Incident on Copper with Energies E_0 of 34.6 and 64.5 eV.

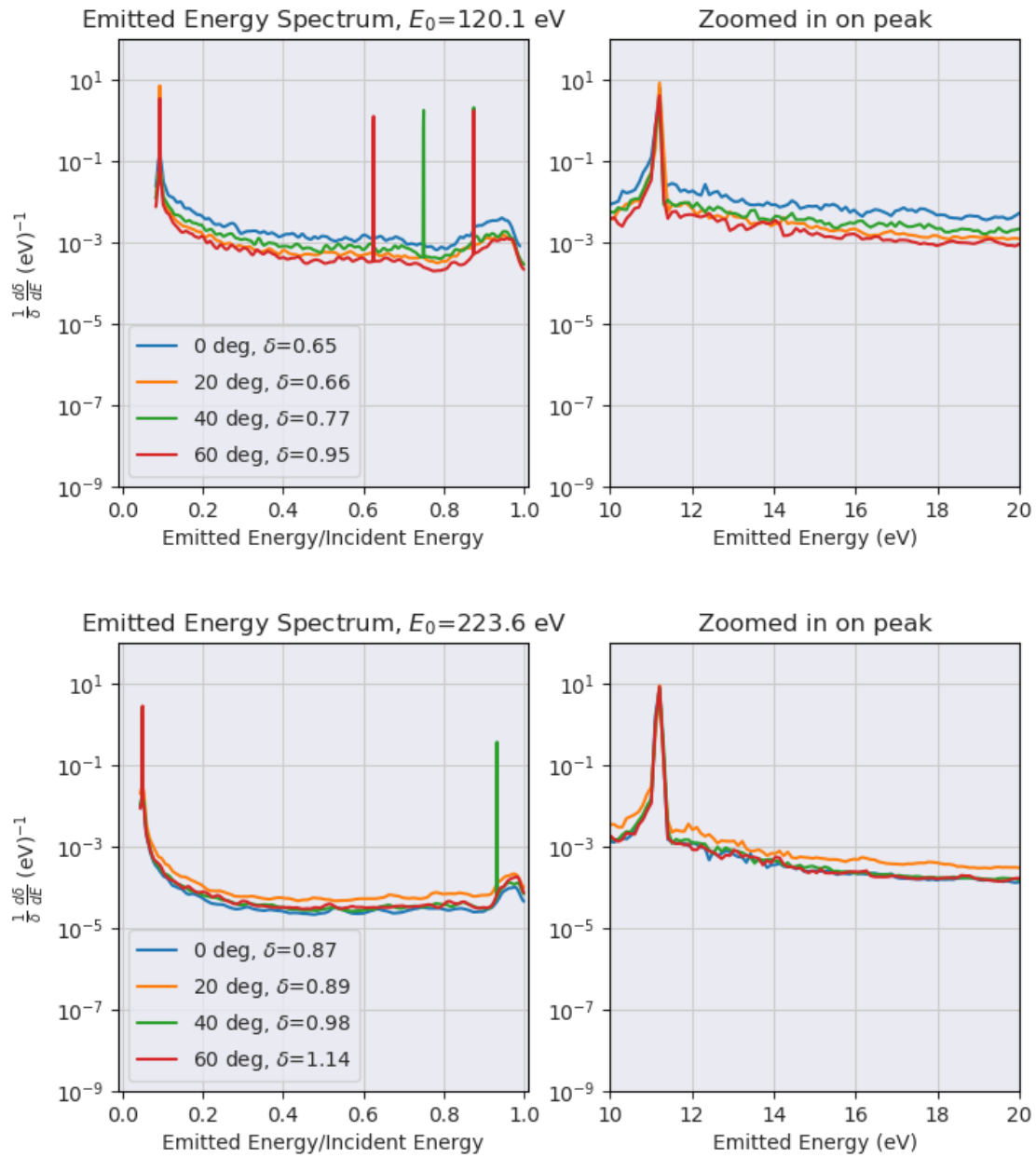


Figure A- 14: EES from GEANT4's Livermore Models for Electrons Incident on Copper with Energies E_0 of 120.1 and 223.6 eV.

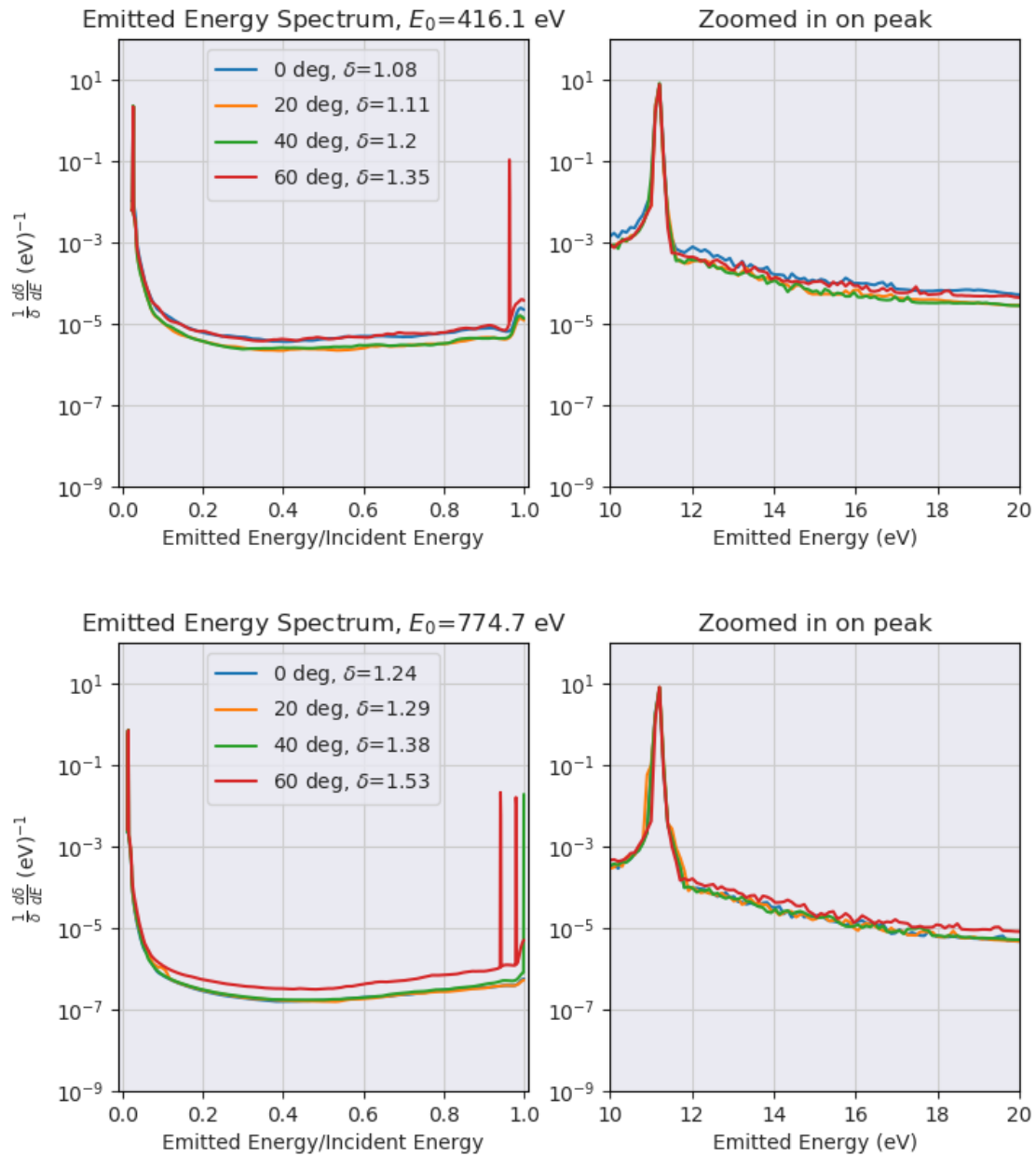


Figure A- 15: EES from GEANT4's Livermore Models for Electrons Incident on Copper with Energies E_0 of 416.1 and 774.7 eV.

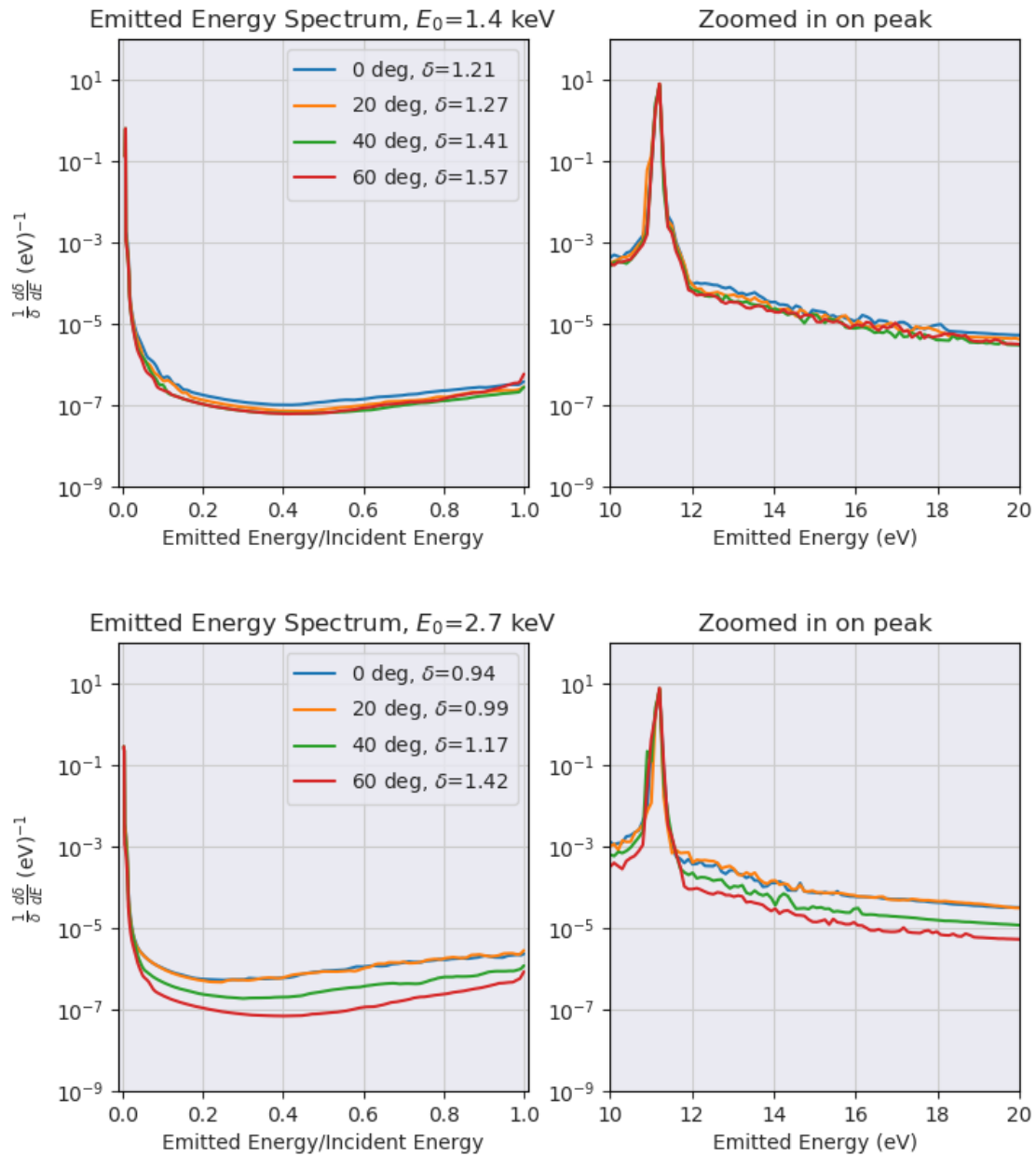


Figure A- 16: EES from GEANT4's Livermore Models for Electrons Incident on Copper with Energies E_0 of 1.4 and 2.7 keV.

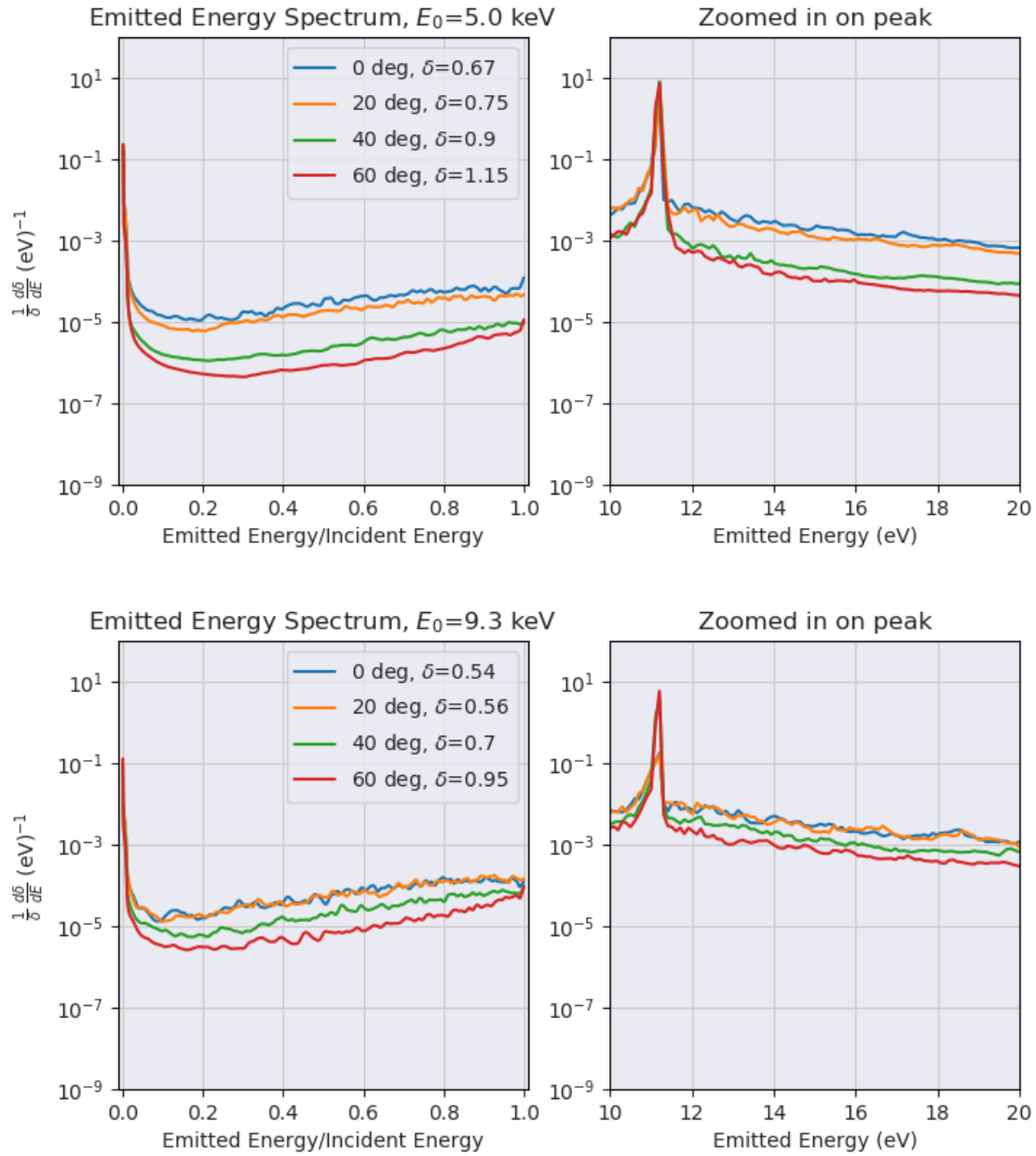


Figure A- 17: EES from GEANT4's Livermore Models for Electrons Incident on Copper with Energies E_0 of 5.0 and 9.3 eV.

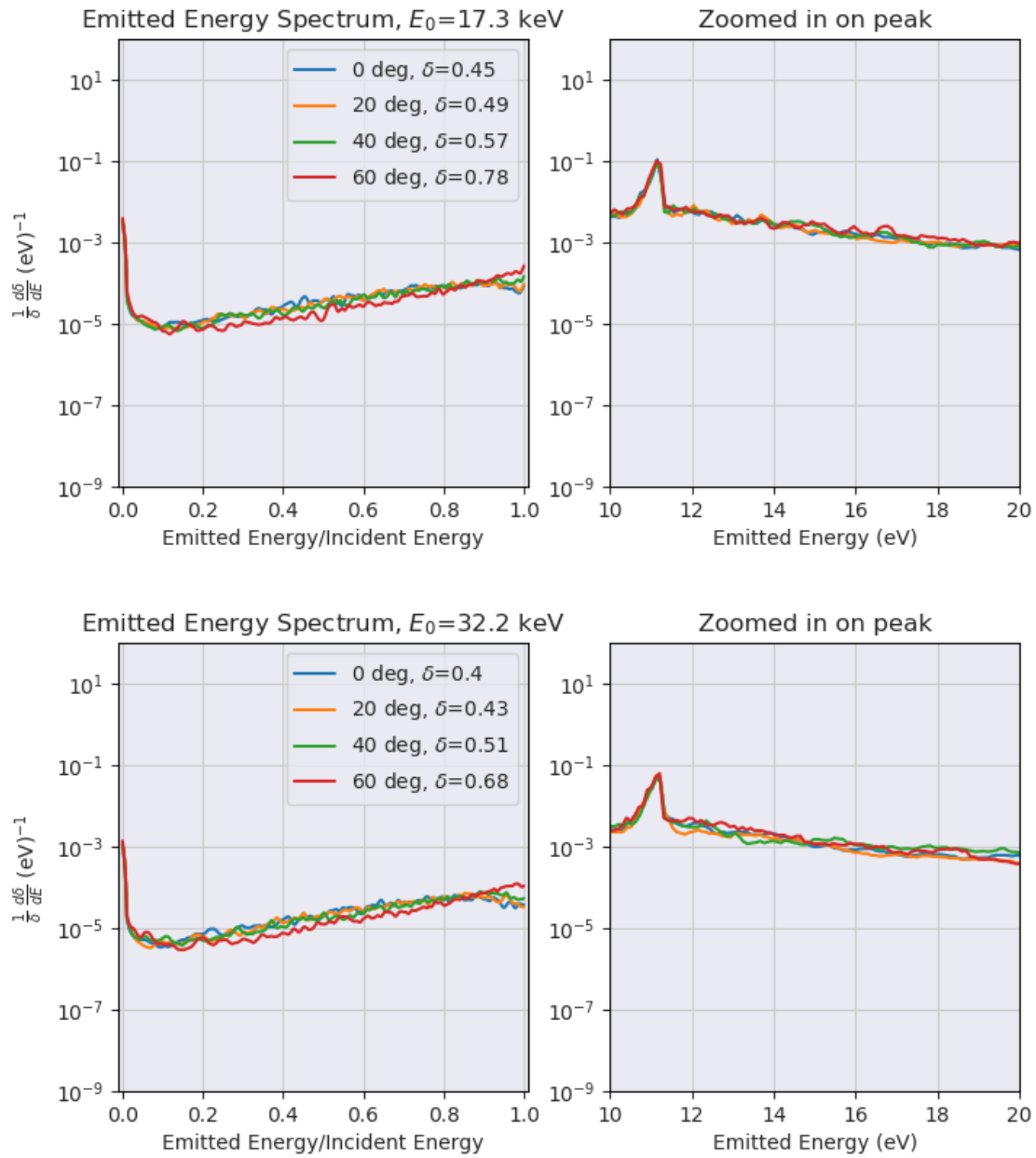


Figure A- 18: EES from GEANT4's Livermore Models for Electrons Incident on Copper with Energies E_0 of 17.3 and 32.2 keV.

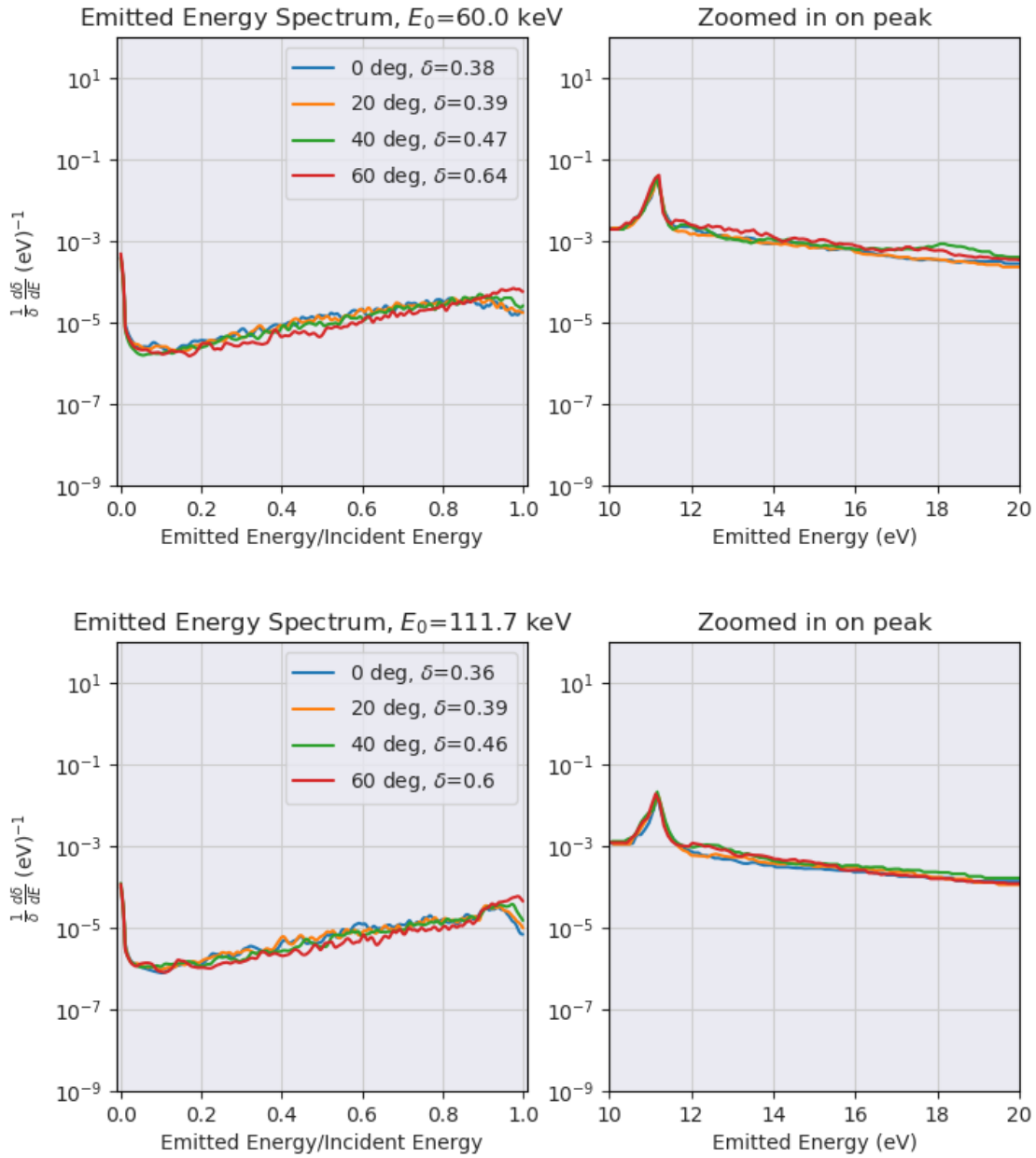


Figure A- 19: EES from GEANT4's Livermore Models for Electrons Incident on Copper with Energies E_0 of 60.0 and 111.7 keV.

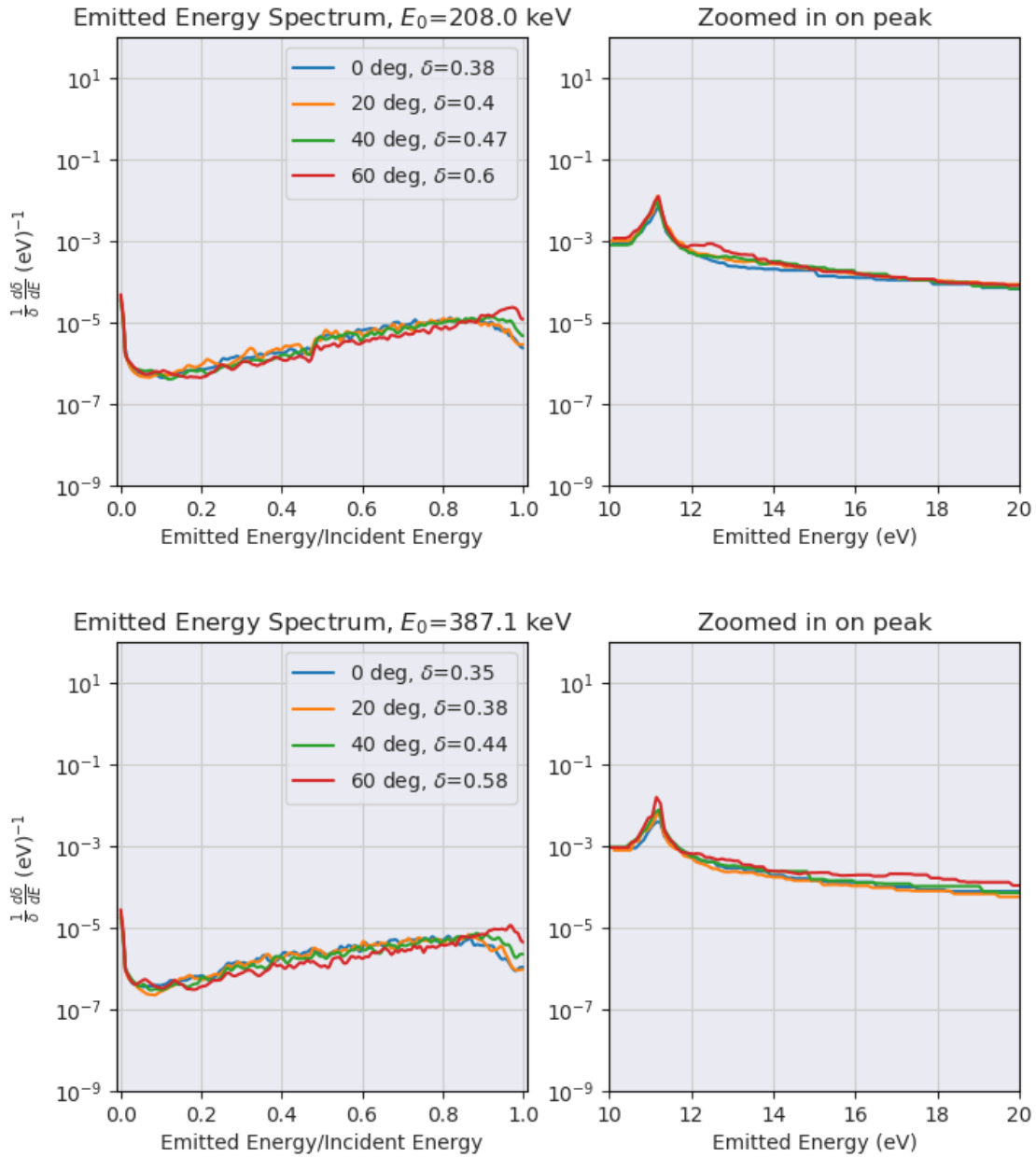


Figure A- 20: EES from GEANT4's Livermore Models for Electrons Incident on Copper with Energies E_0 of 208.0 and 387.1 keV.

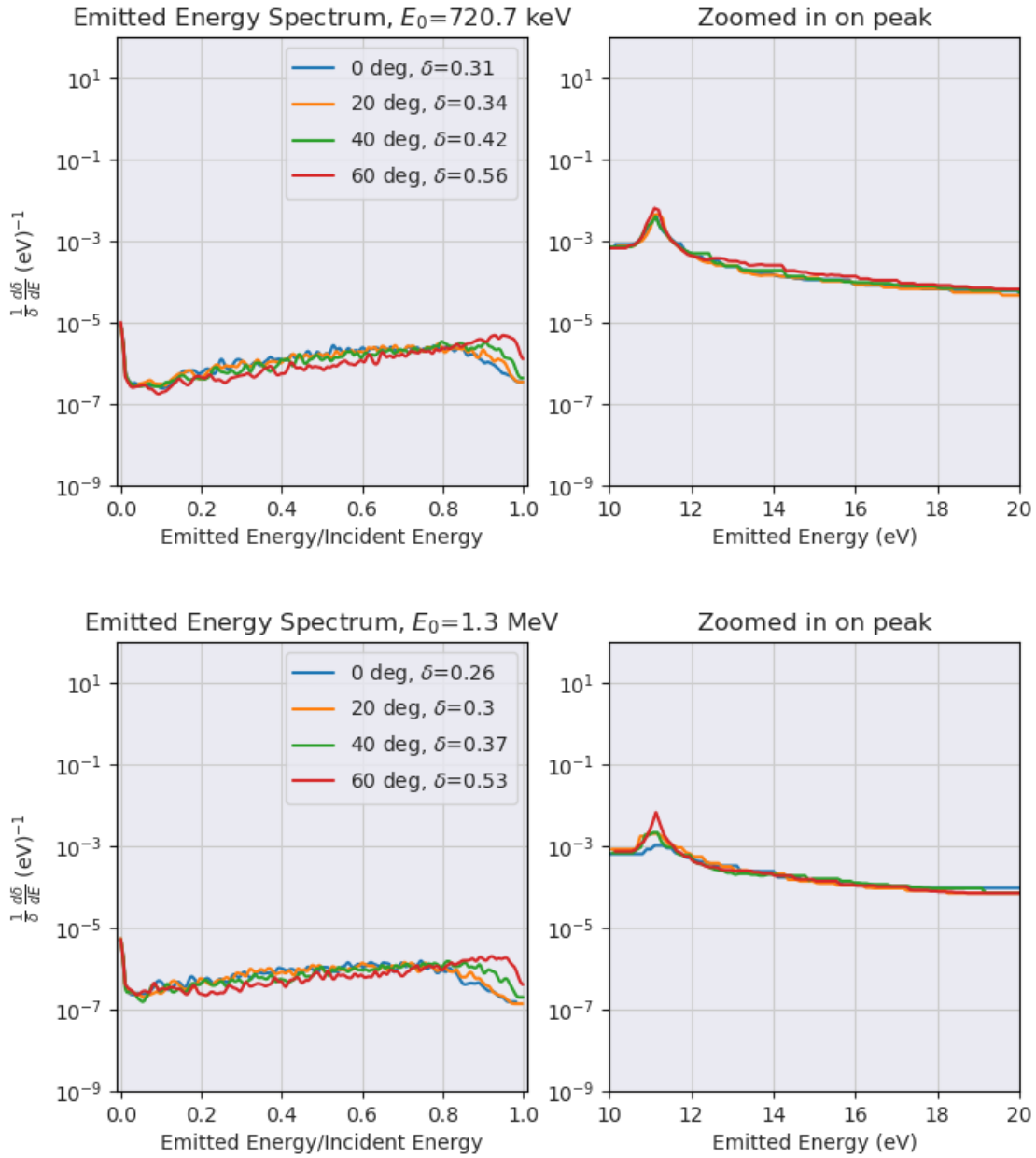


Figure A- 21: EES from GEANT4's Livermore Models for Electrons Incident on Copper with Energies E_0 of 720.7 keV and 1.3 MeV.

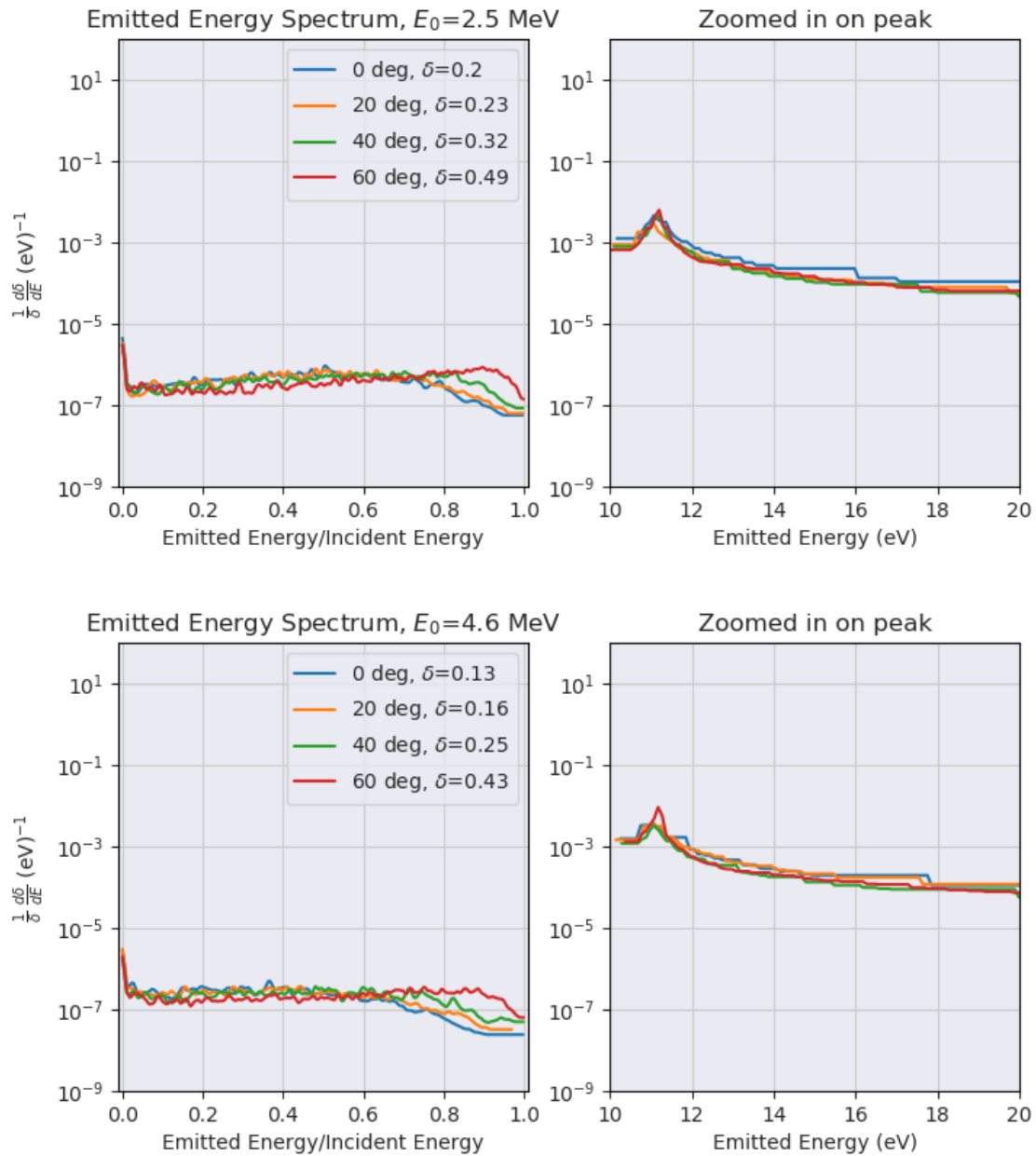


Figure A- 22: EES from GEANT4's Livermore Models for Electrons Incident on Copper with Energies E_0 of 2.5 and 4.6 MeV.

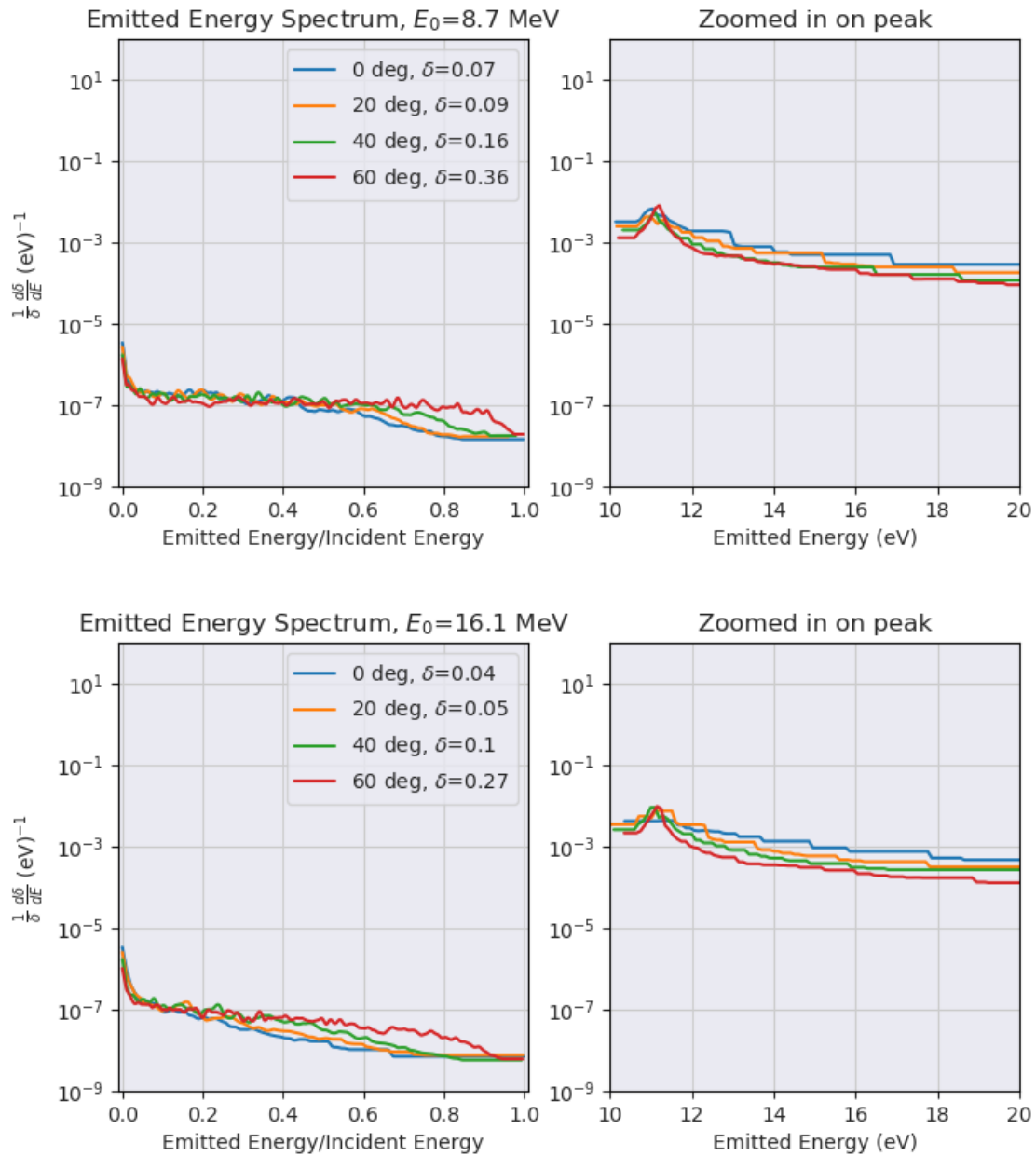


Figure A- 23: EES from GEANT4's Livermore Models for Electrons Incident on Copper with Energies E_0 of 8.7 and 16.1 MeV.

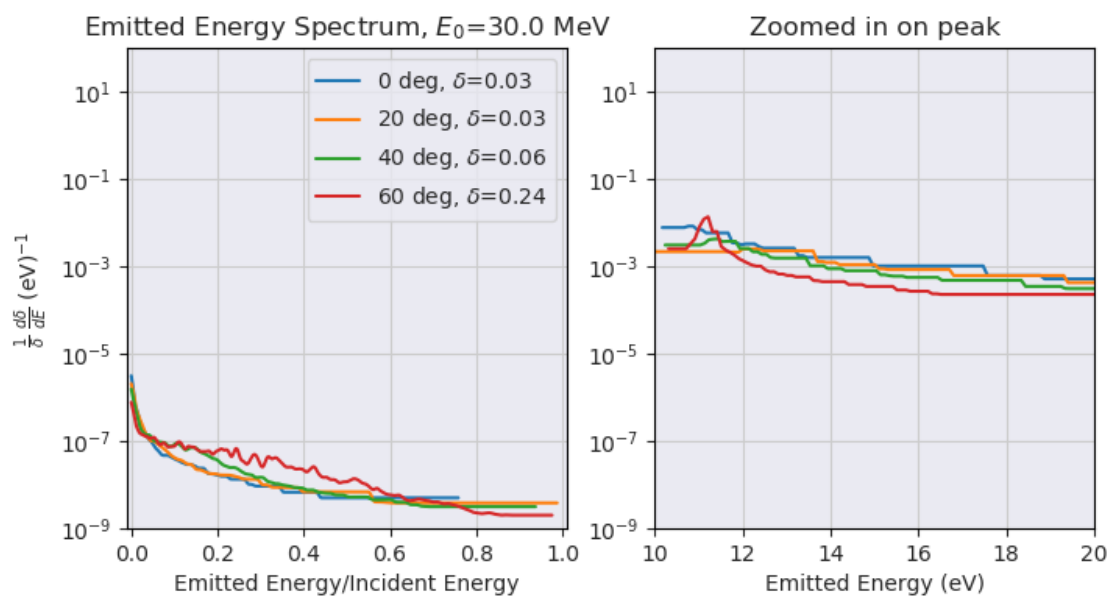


Figure A- 24: EES from GEANT4's Livermore Models for Electrons Incident on Copper with Energy E_0 of 30.0 MeV.

A.3 Stainless Steel

A.3.1 Default Models

The EES for the GEANT4 default model with the GEANT4 built-in stainless steel material definition are as shown in Figure A-25 through A-29

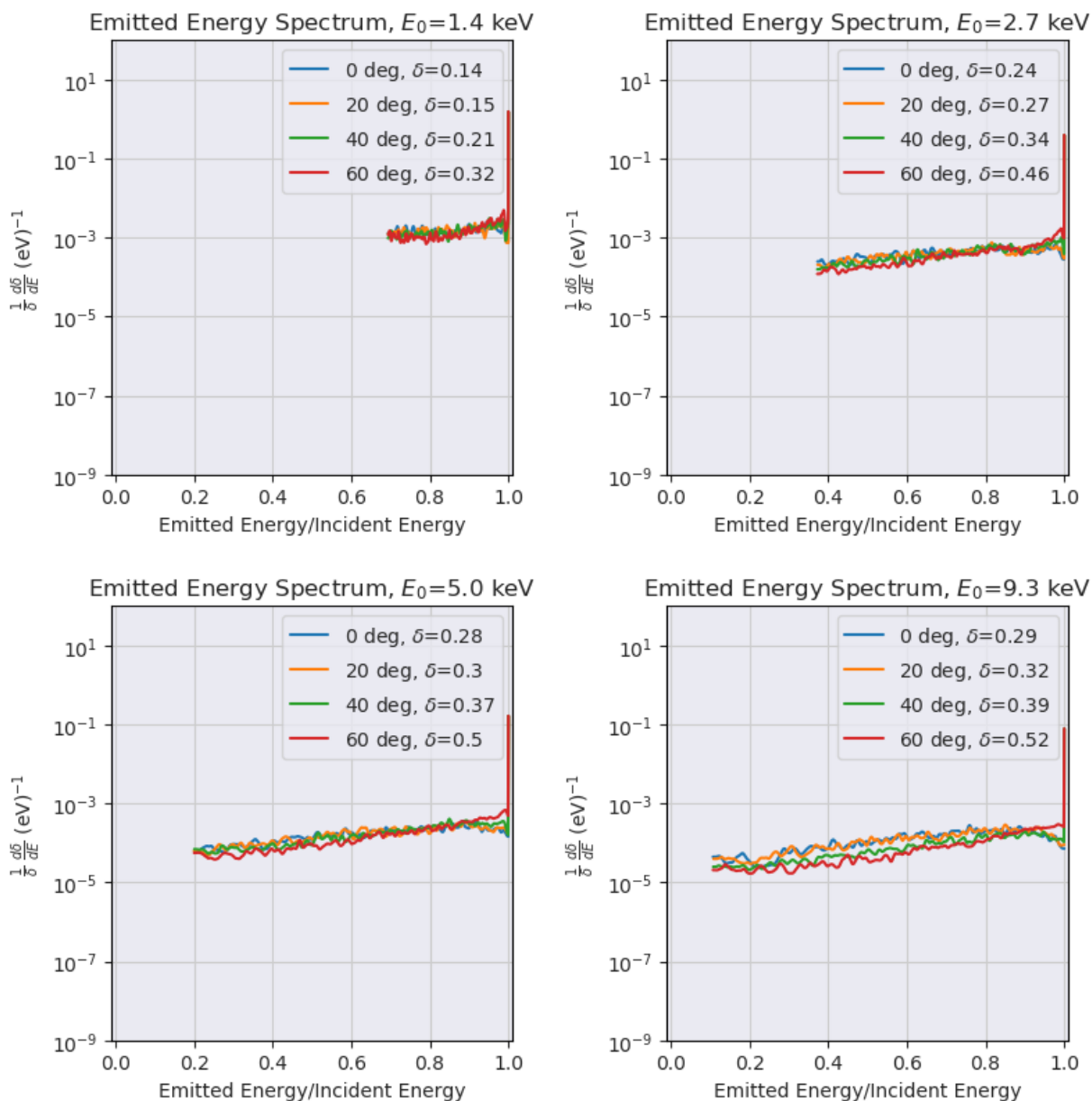


Figure A- 25: EES from GEANT4's Default Models for Electrons Incident on Stainless Steel with Energies E_0 of 1.4 to 9.3 keV.

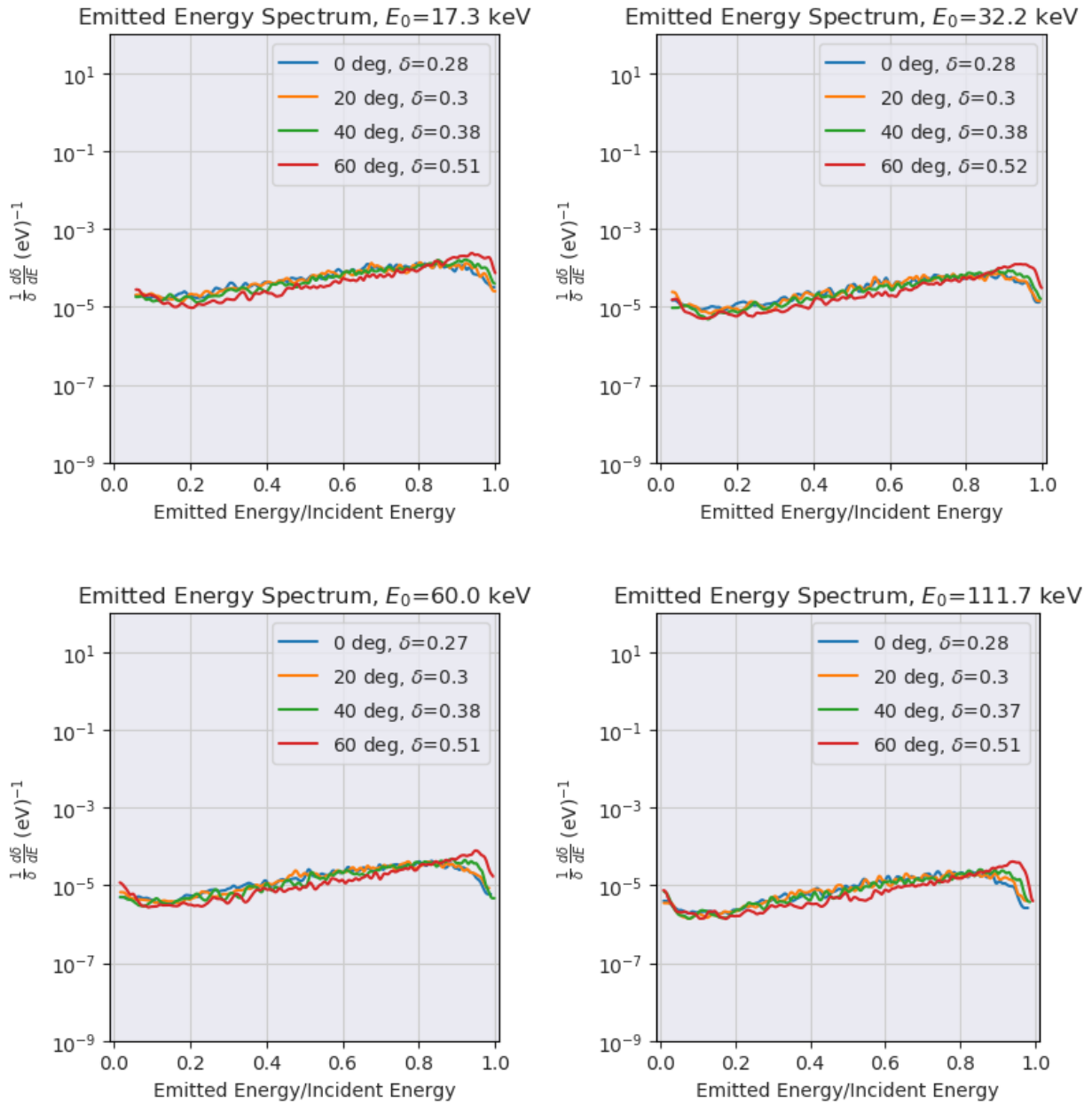


Figure A- 26: EES from GEANT4's Default Models for Electrons Incident on Stainless Steel with Energies E_0 of 17.3 to 111.7 keV.

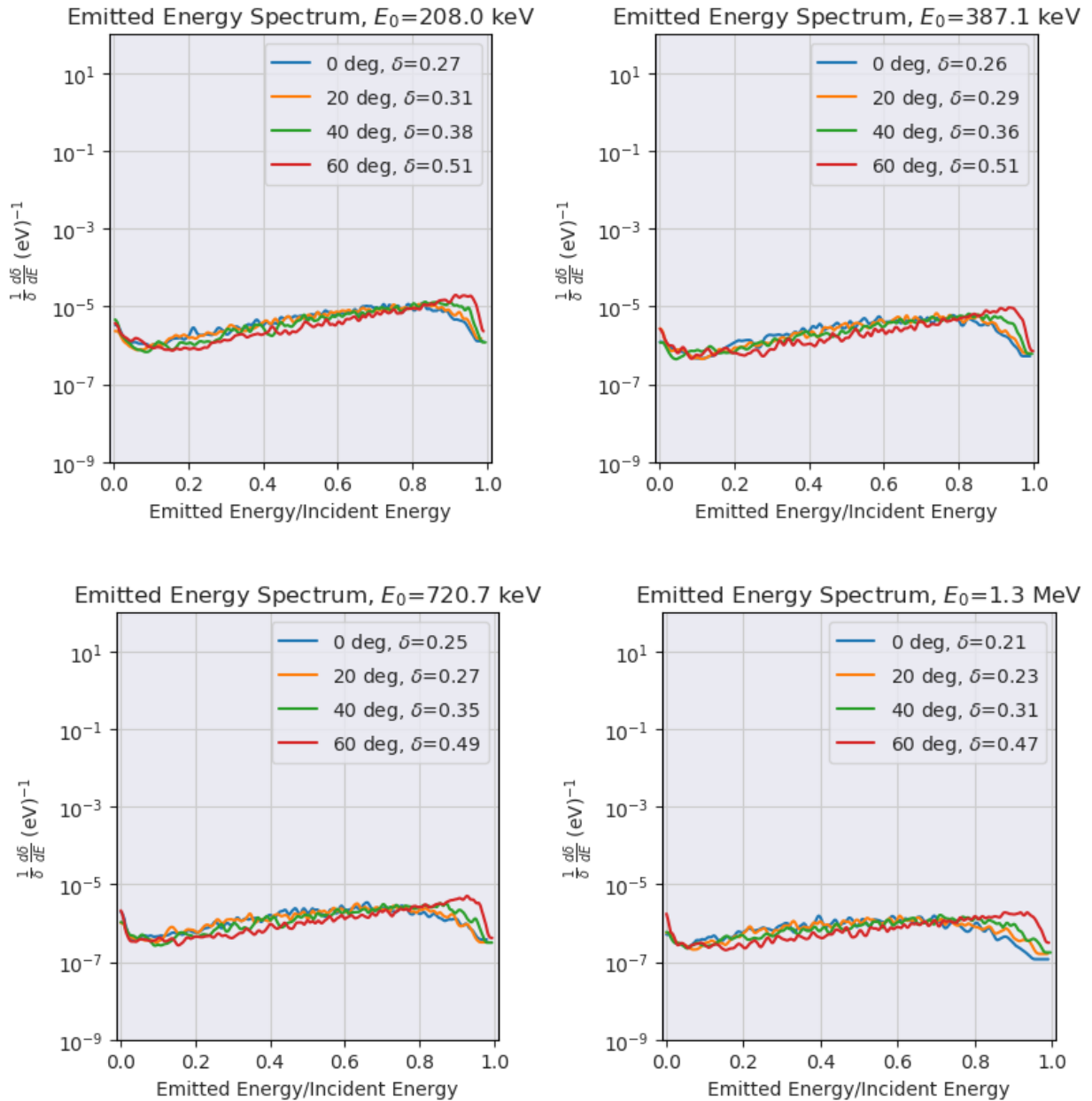


Figure A- 27: EES from GEANT4's Default Models for Electrons Incident on Stainless Steel with Energies E_0 of 208 keV to 1.3 MeV.

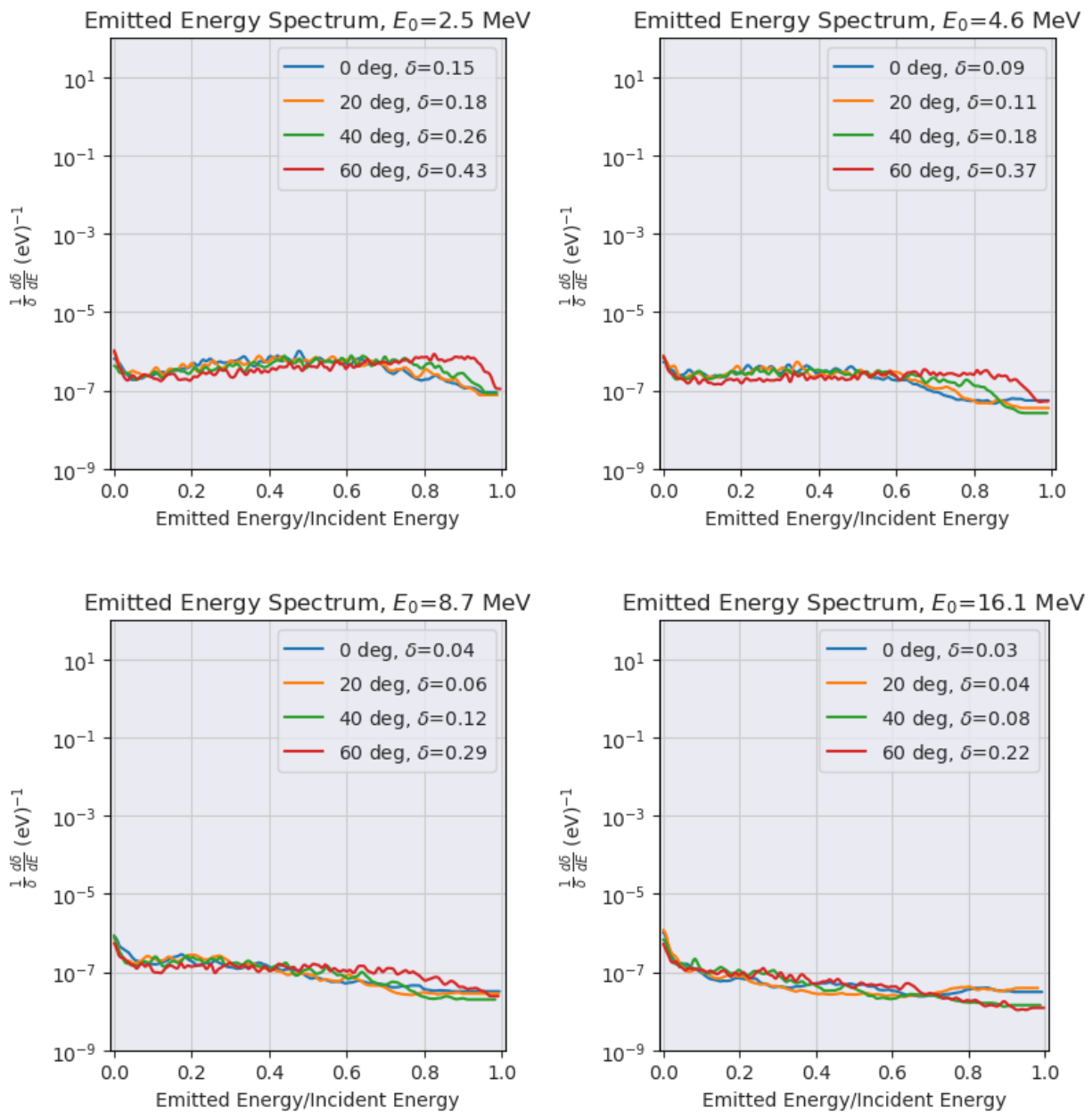


Figure A- 28: EES from GEANT4's Default Models for Electrons Incident on Stainless Steel with Energies E_0 of 2.5 to 16.1 MeV.

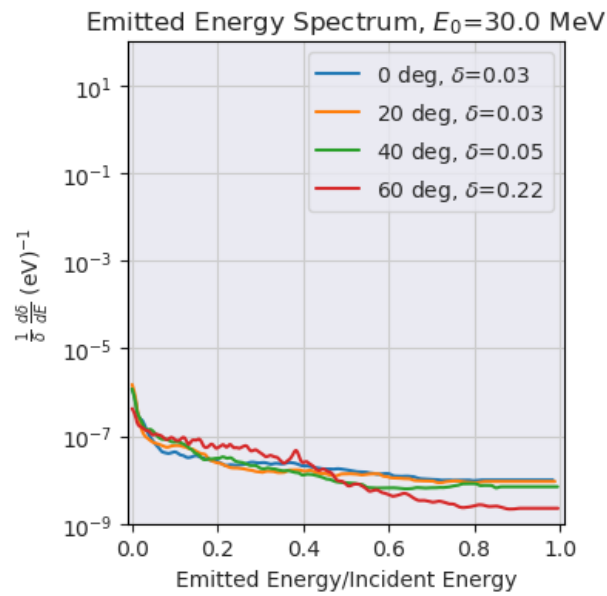


Figure A- 29: EES from GEANT4's Default Models for Electrons Incident on Stainless Steel with Energy E_0 of 30.0 MeV.

A.3.2 Penelope Models

The EES for the GEANT4 Penelope model with the GEANT4 built-in stainless steel material definition are as shown in Figure A-30 through A-35.

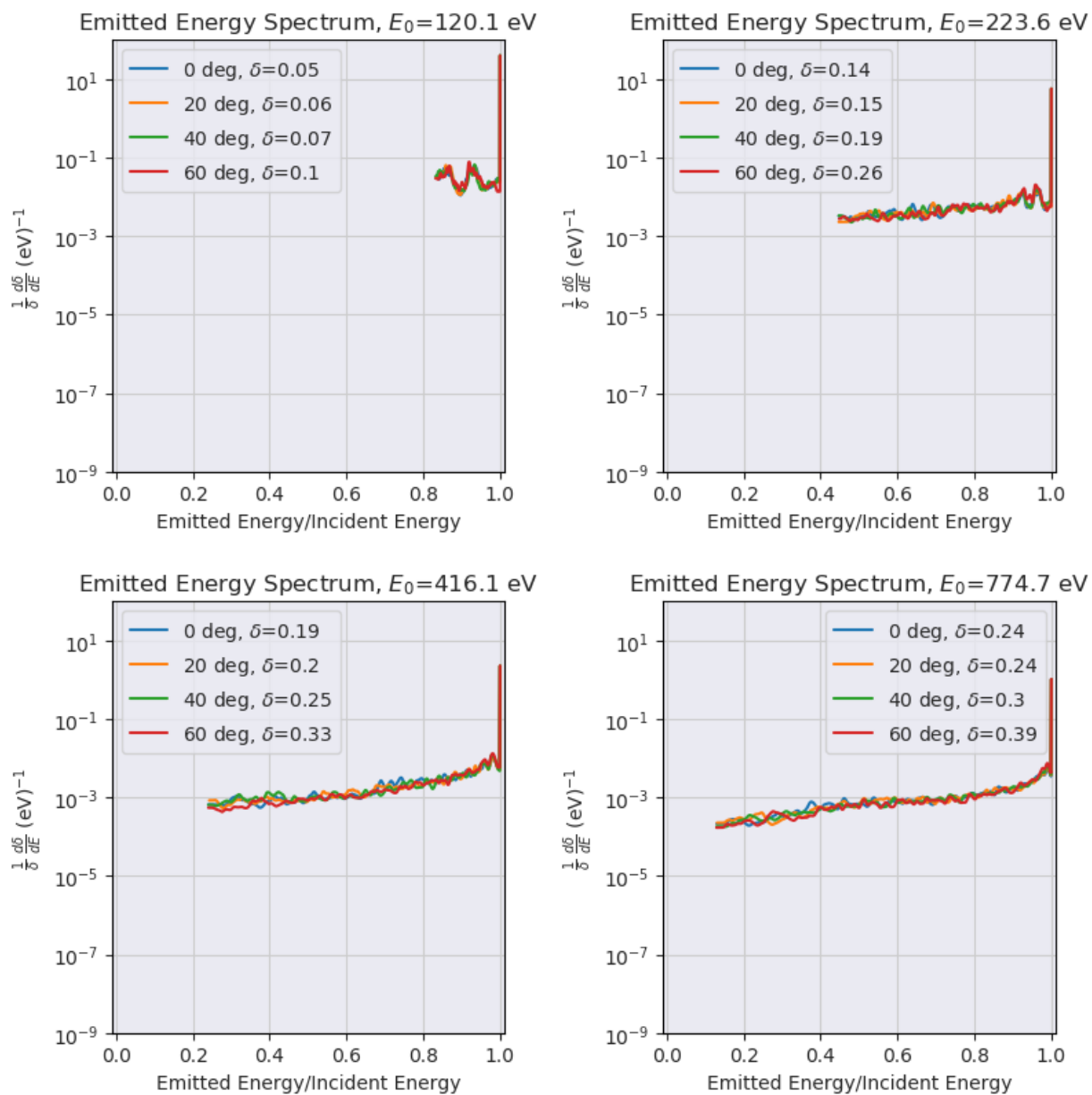


Figure A- 30: EES from GEANT4's Penelope Models for Electrons Incident on Stainless Steel with Energies E_0 of 120.1 to 774.7 eV.

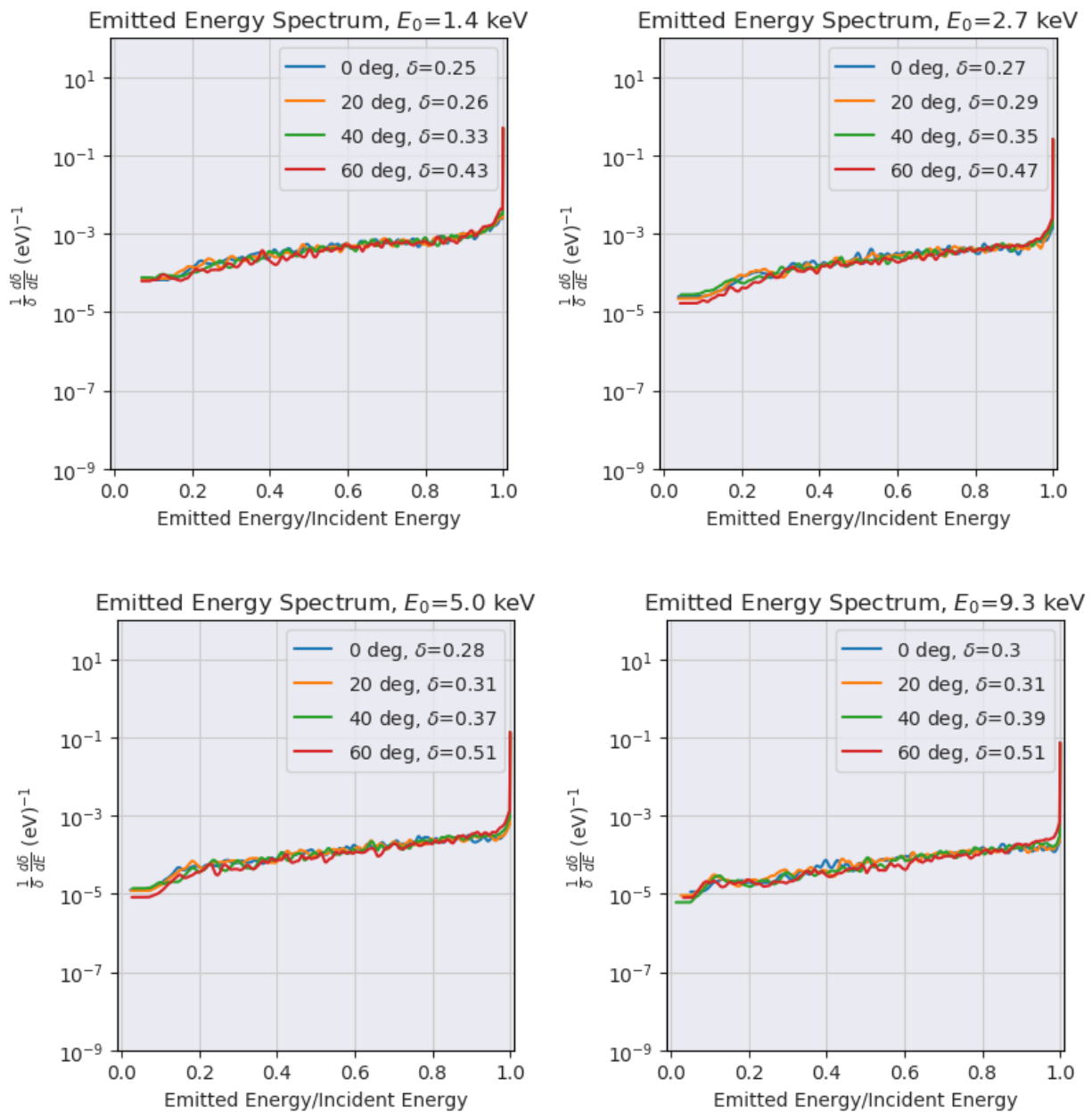


Figure A- 31: EES from GEANT4’s Penelope Models for Electrons Incident on Stainless Steel with Energies E_0 of 1.4 to 9.3 keV.

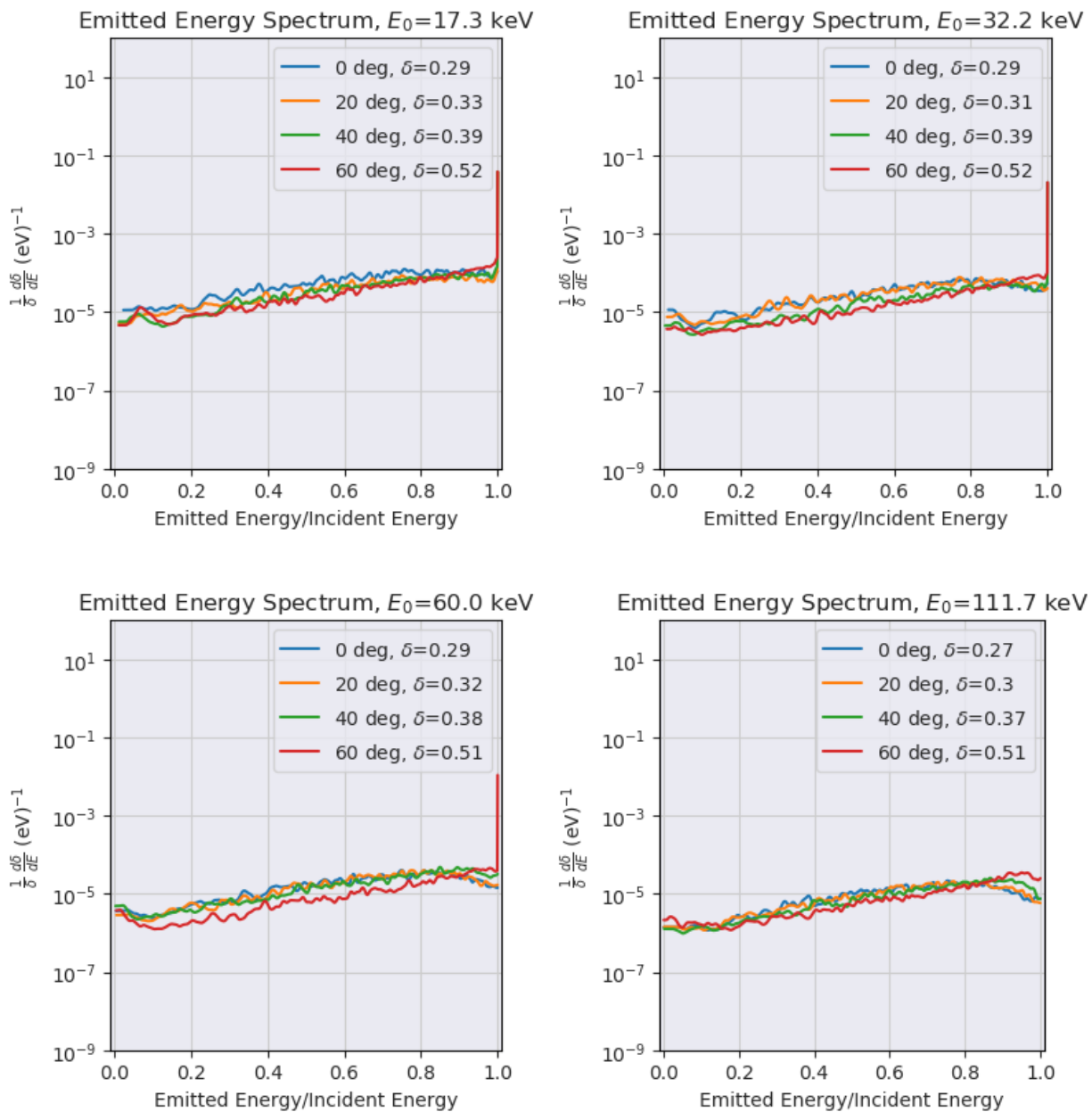


Figure A- 32: EES from GEANT4’s Penelope Models for Electrons Incident on Stainless Steel with Energies E_0 of 17.3 to 111.7 keV.

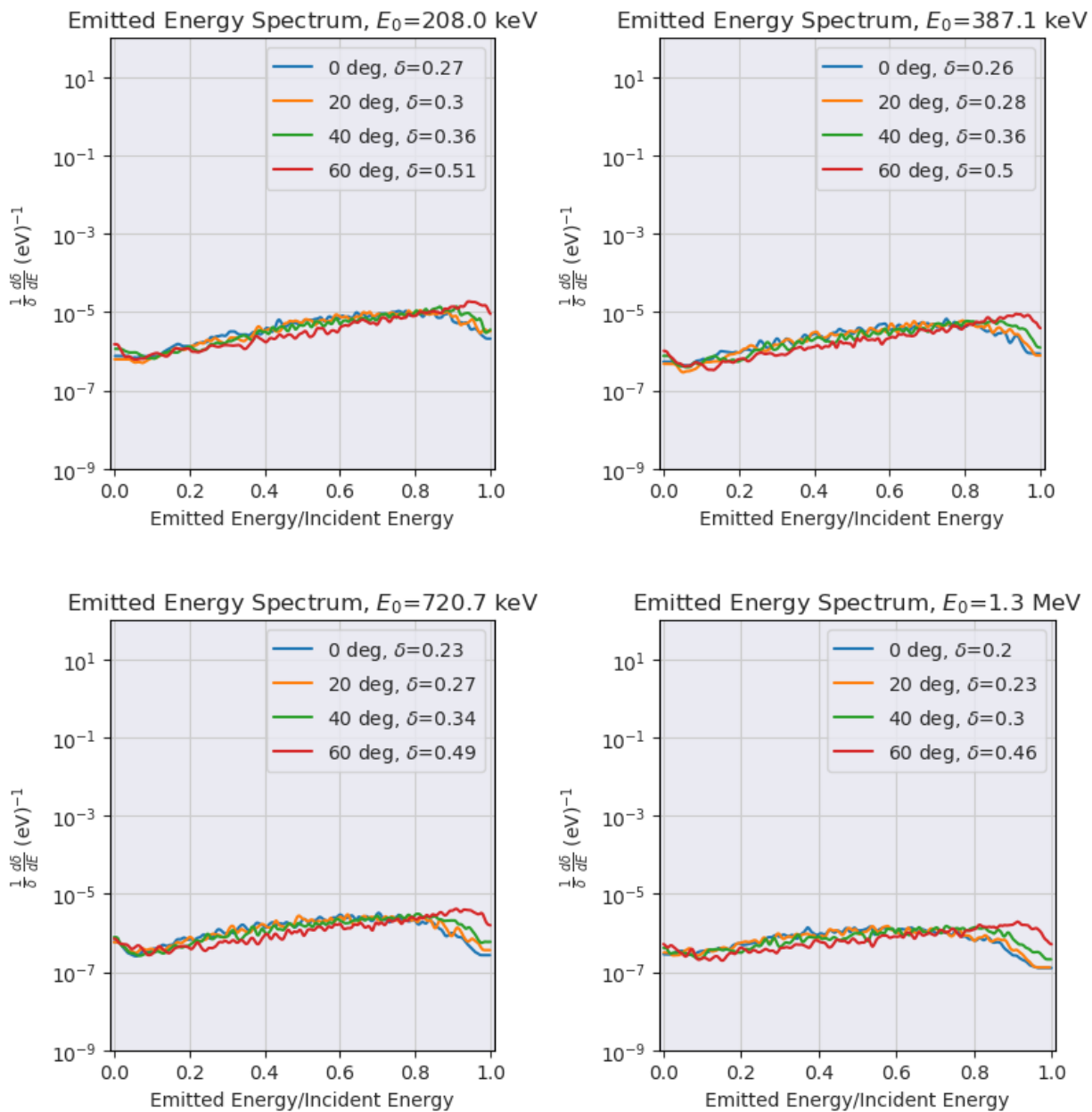


Figure A- 33 : EES from GEANT4's Penelope Models for Electrons Incident on Stainless Steel with Energies E_0 of 208 keV to 1.3 MeV.

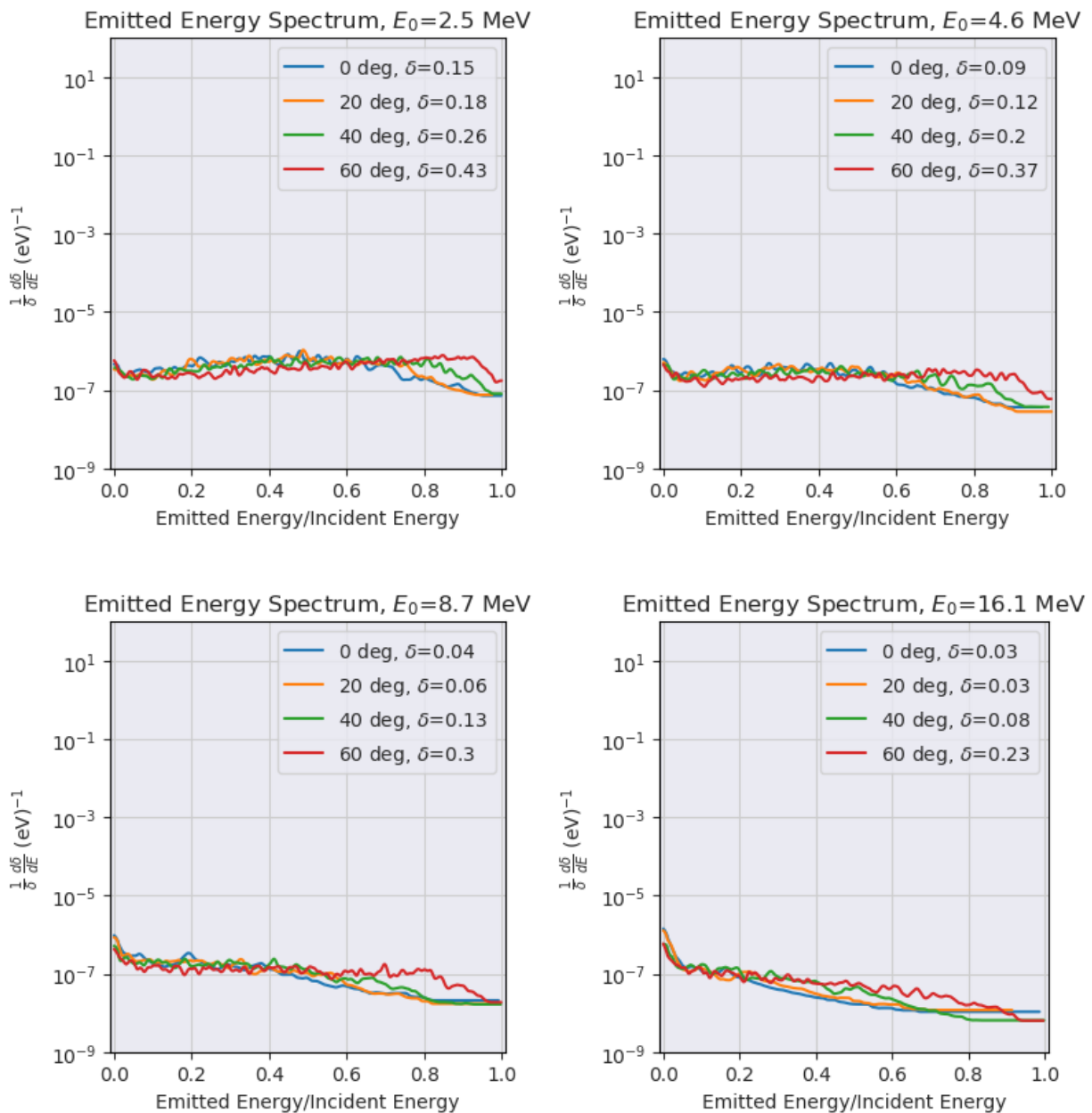


Figure A- 34: EES from GEANT4's Penelope Models for Electrons Incident on Stainless Steel with Energies E_0 of 2.5 to 16.1 MeV.

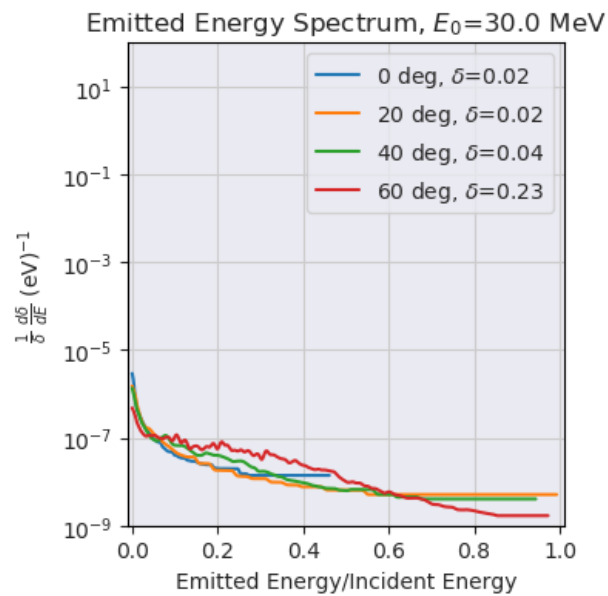


Figure A- 35: EES from GEANT4's Penelope Models for Electrons Incident on Stainless Steel with Energy E_0 of 30.0 MeV.

A.3.3 Livermore Models

The EES for the GEANT4 Livermore model with the GEANT4 built-in stainless steel material definition are as shown in Figure A-36 through A-48; both the full energy range and a view zoomed from 10-20 eV are shown. Unlike the EES distributions produced from GEANT4 using copper, the EES from stainless steel do not exhibit an emission peak around 10-12 eV. Between incident energies of 64 and 1,400 eV, several periodic delta functions can be seen. It is not yet known what physics processes are causing the delta functions. It is possible this effect could be caused by a quantum mechanical phenomenon similar to the photoelectric effect (which produces electrons with very specific energies) occurring near the surface of the material (so that they do not interact with the material before exiting).

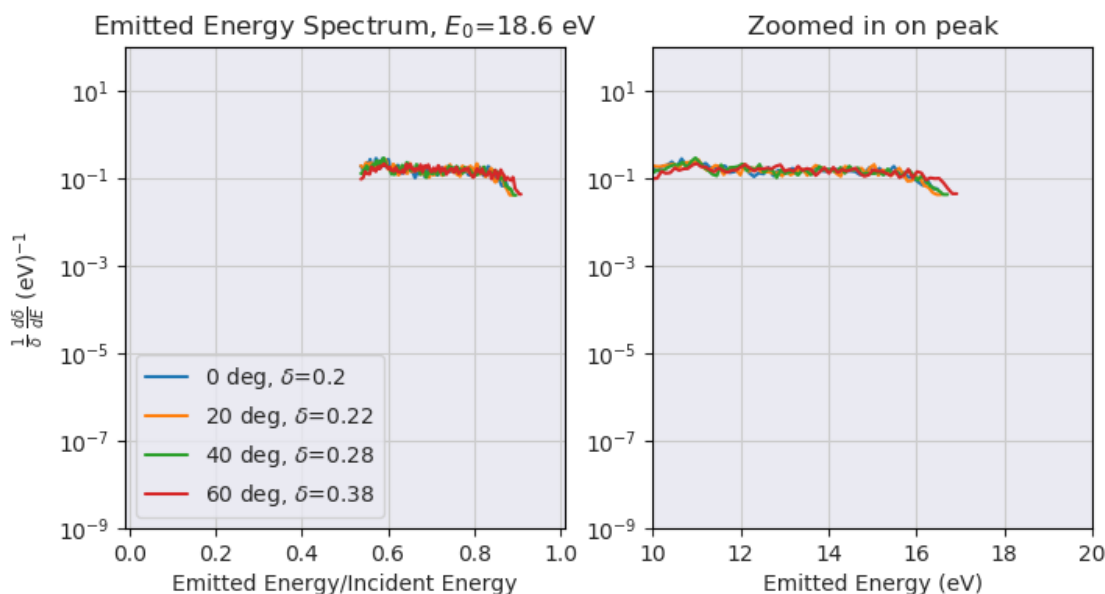


Figure A- 36: EES from GEANT4's Livermore Models for Electrons Incident on Stainless Steel with Energy E_0 of 18.6 eV (left), and over the Emitted Energy Range 10-20 eV (right).

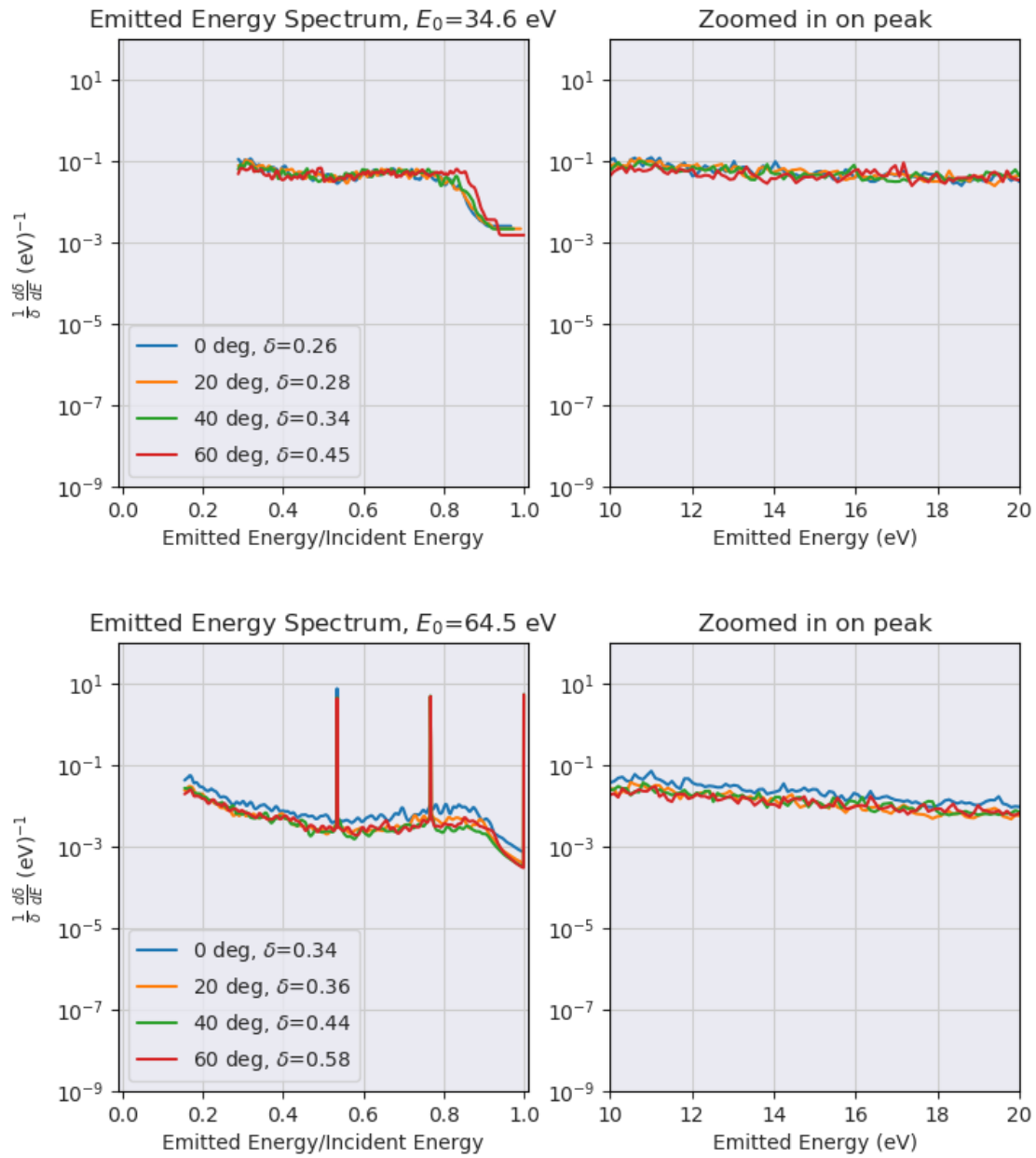


Figure A- 37: EES from GEANT4's Livermore Models for Electrons Incident on Stainless Steel with Energies E_0 of 34.6 eV and 64.5 eV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

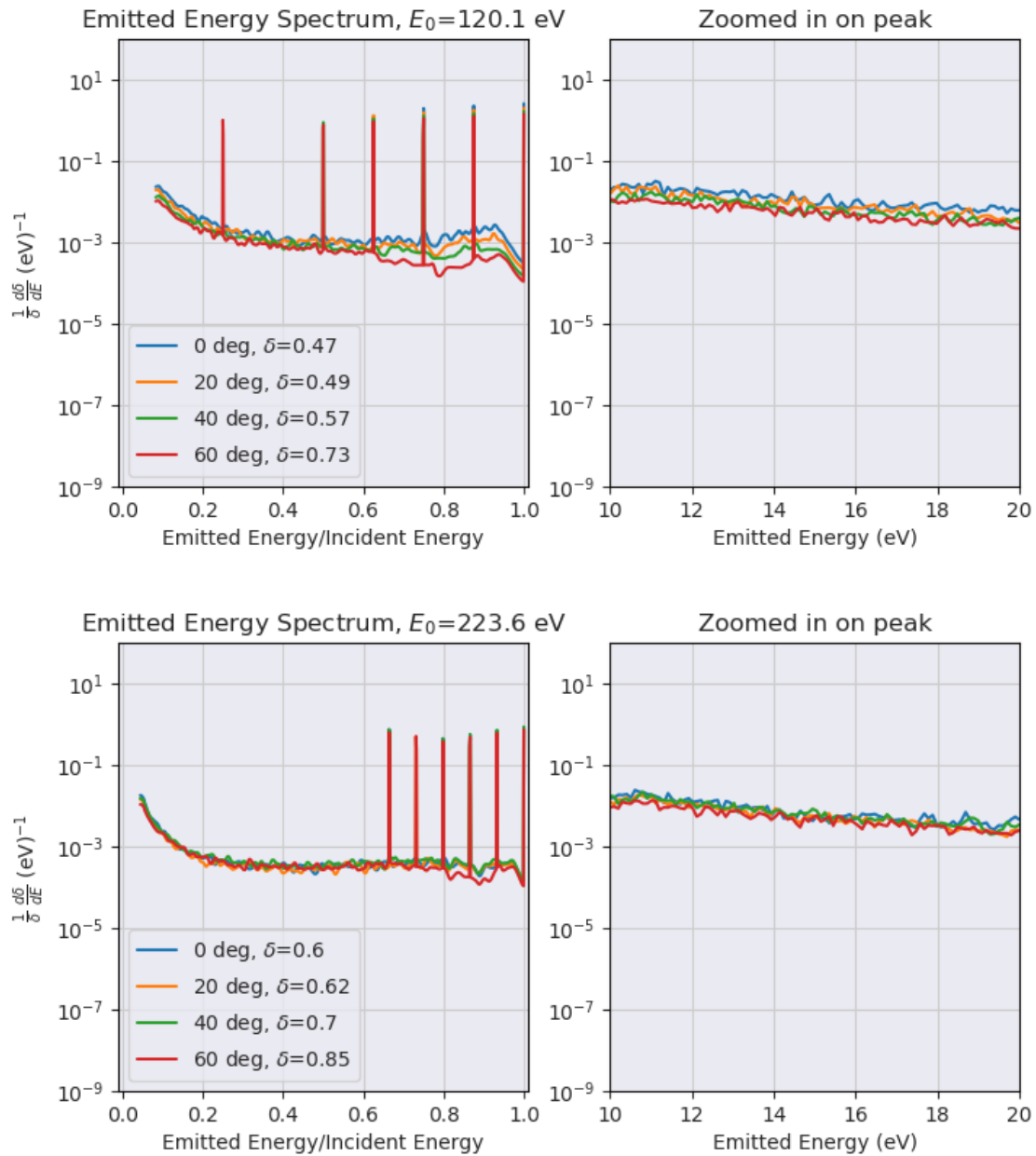


Figure A- 38: EES from GEANT4's Livermore Models for Electrons Incident on Stainless Steel with Energies E_0 of 120.1 eV and 223.6 eV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

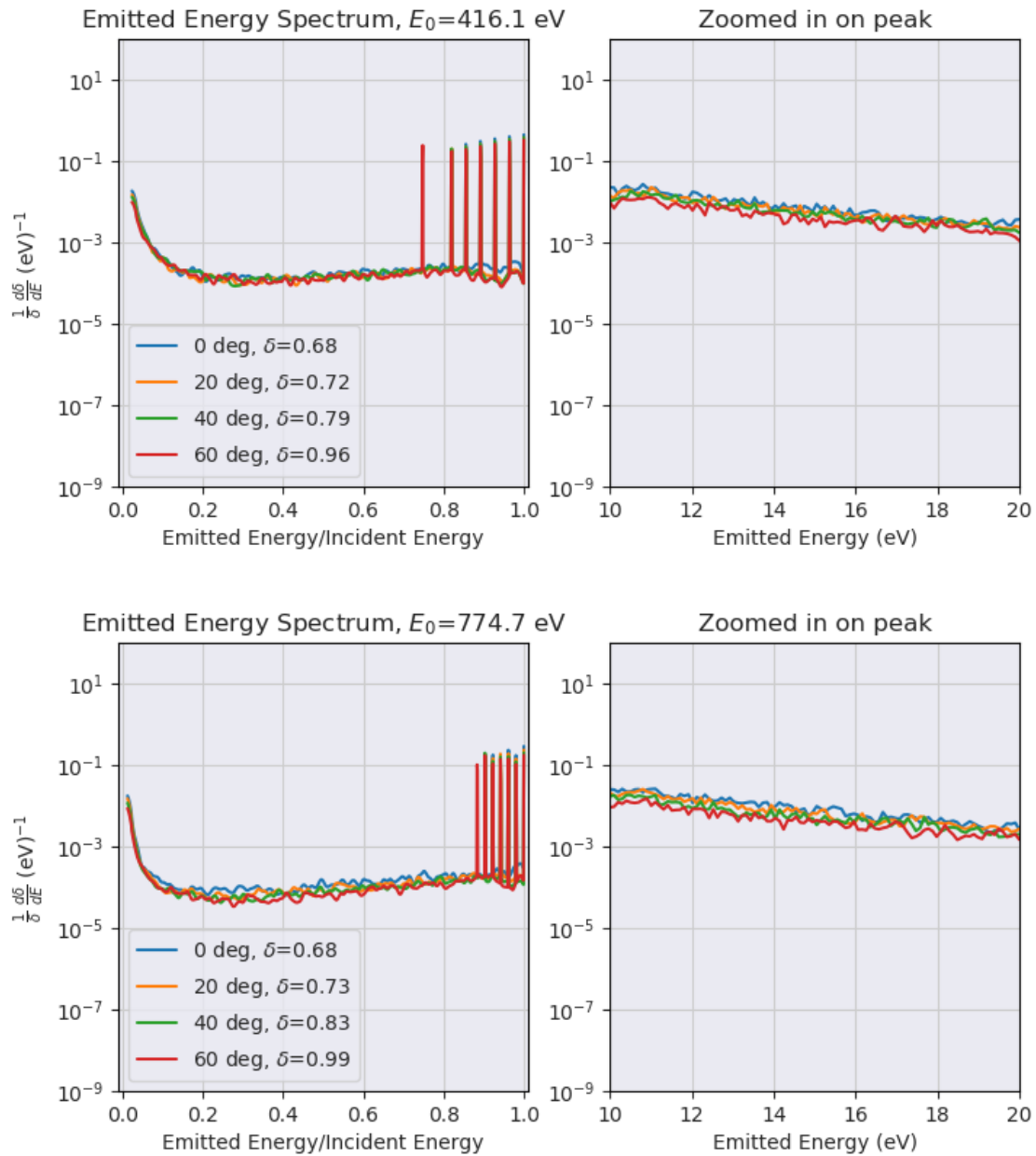


Figure A- 39: EES from GEANT4’s Livermore Models for Electrons Incident on Stainless Steel with Energies E_0 of 416.1 eV and 774.7 eV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

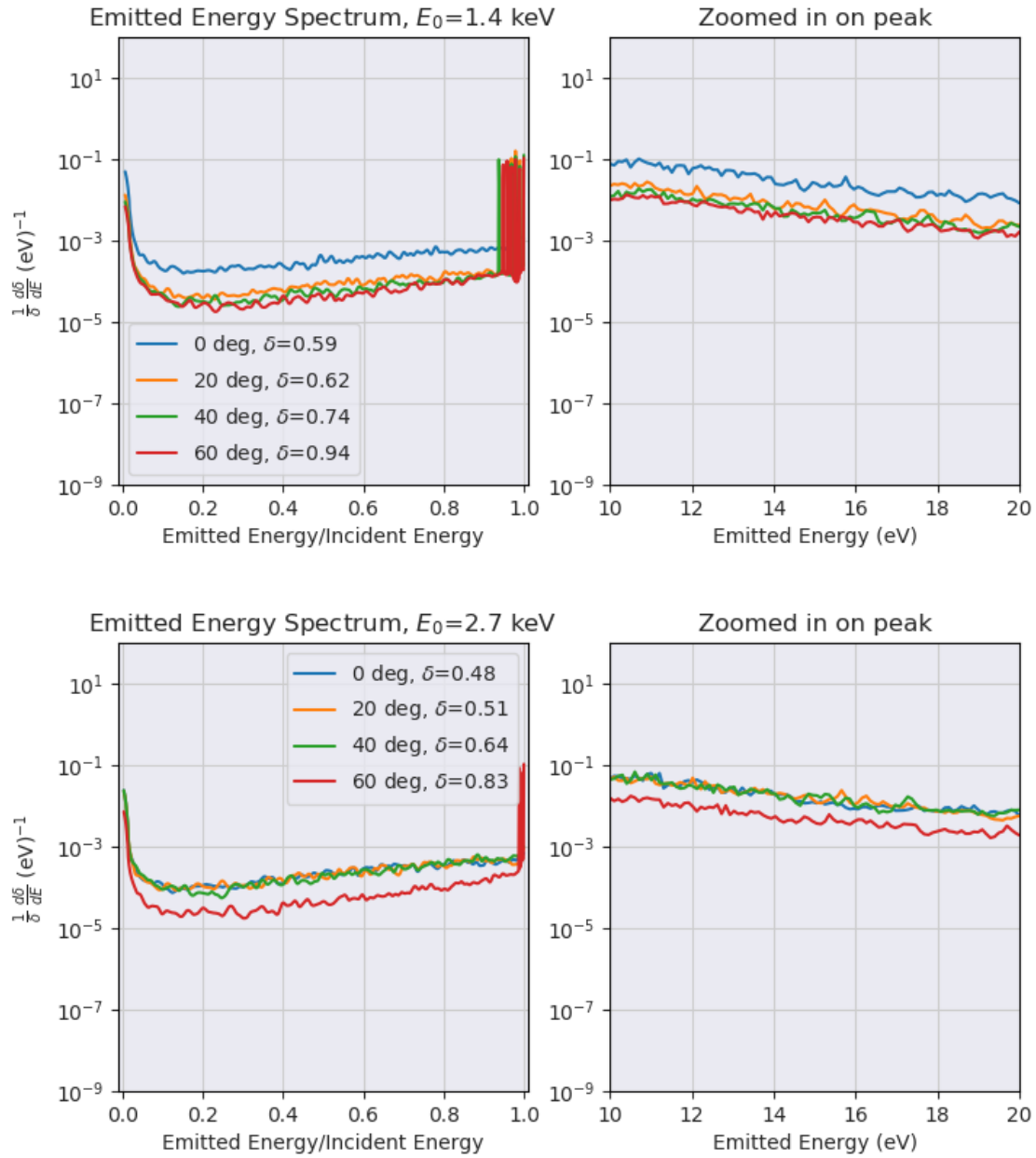


Figure A- 40: EES from GEANT4’s Livermore Models for Electrons Incident on Stainless Steel with Energies E_0 of 1.4 keV and 2.7 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

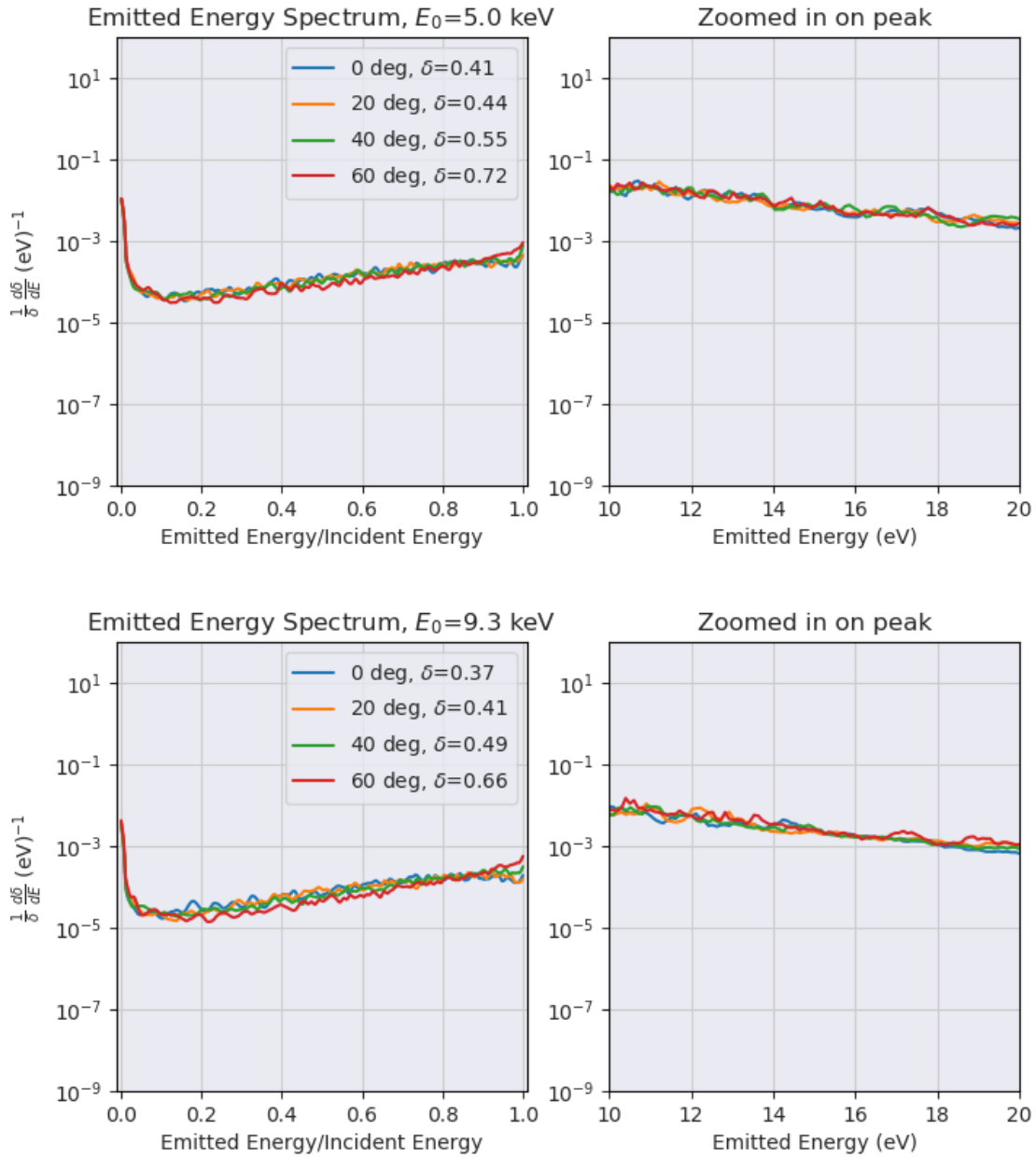


Figure A- 41: EES from GEANT4's Livermore Models for Electrons Incident on Stainless Steel with Energies E_0 of 5.0 keV and 9.3 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

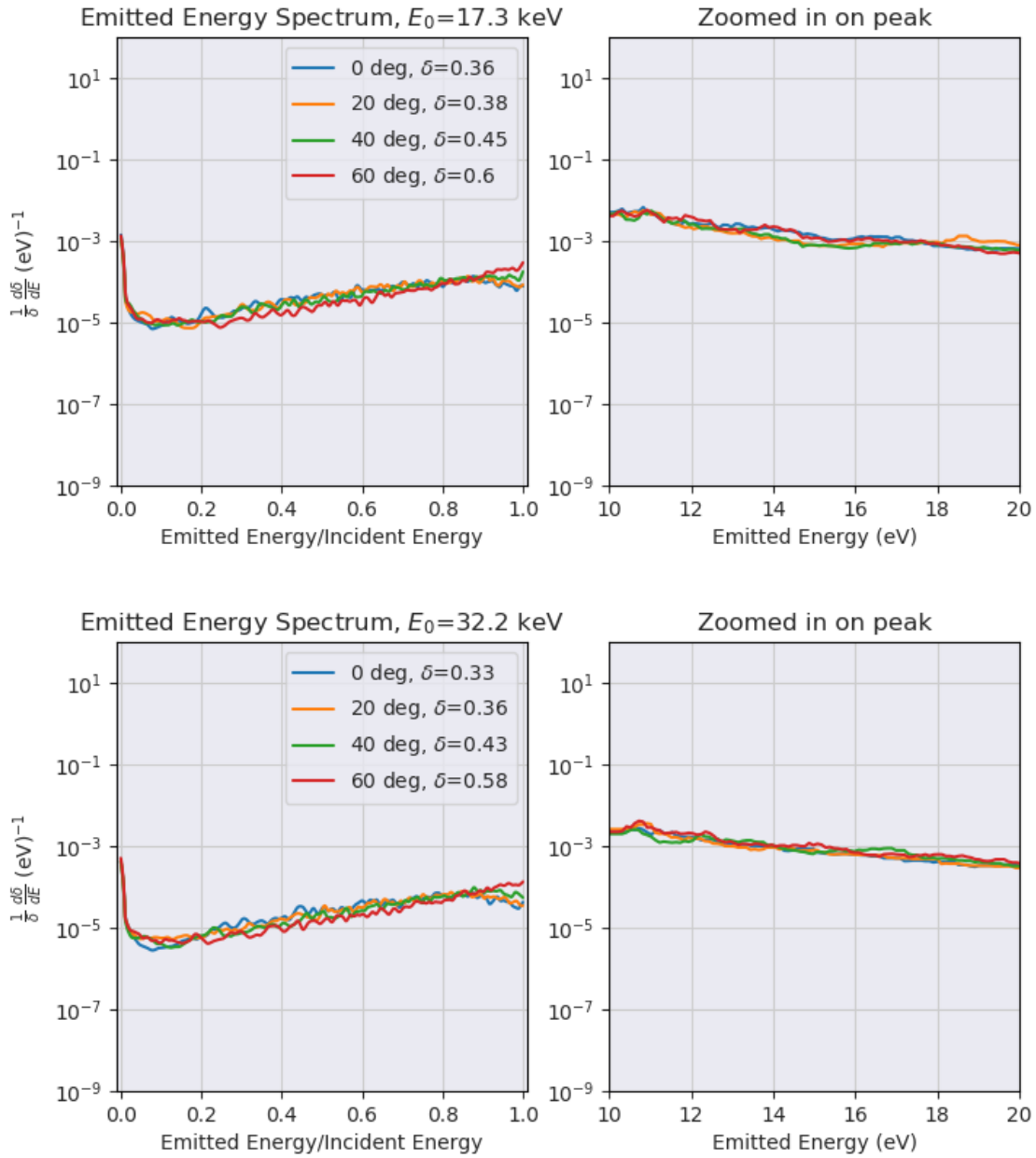


Figure A- 42: EES from GEANT4's Livermore Models for Electrons Incident on Stainless Steel with Energies E_0 of 17.3 keV and 32.2 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

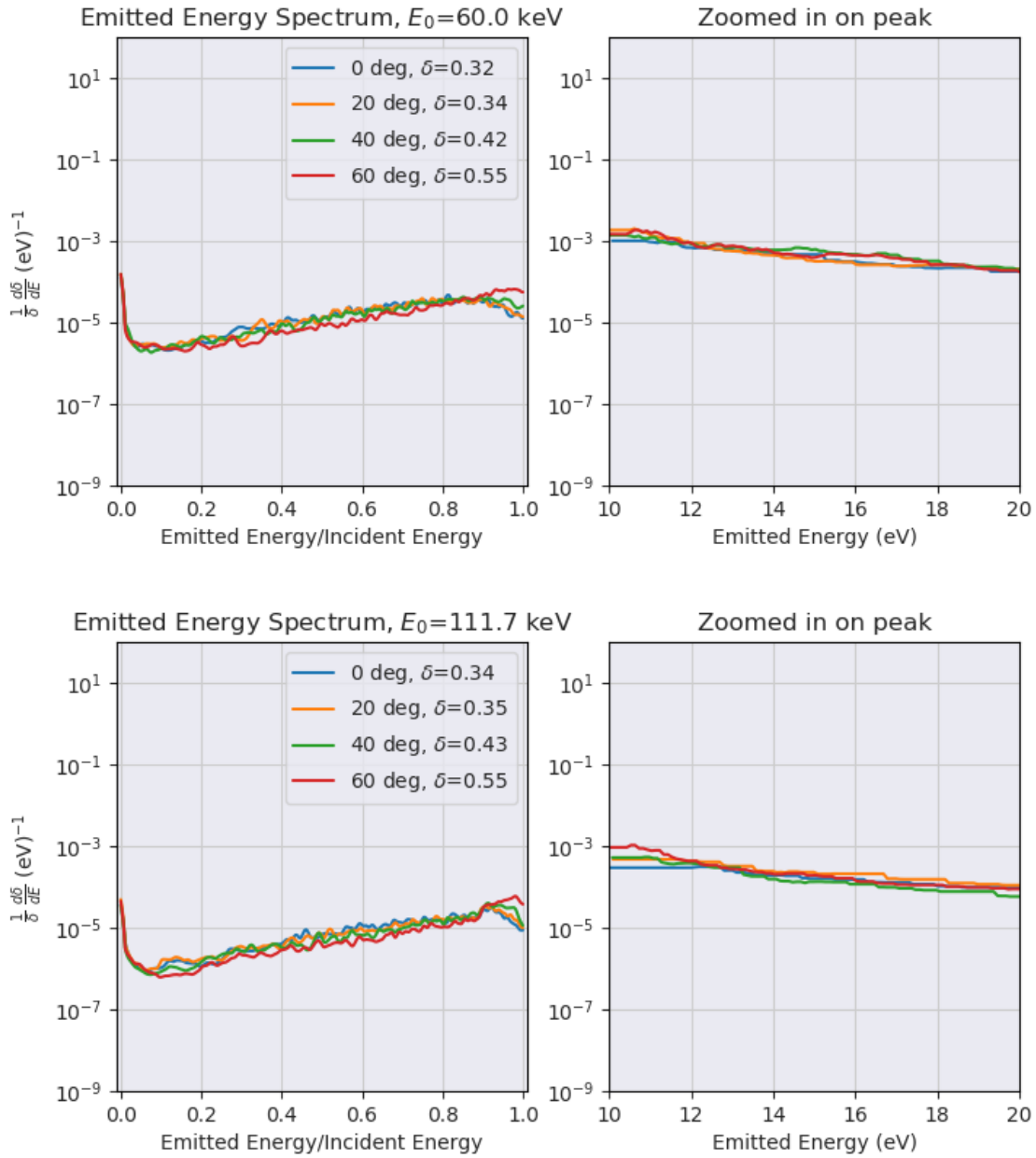


Figure A- 43: EES from GEANT4's Livermore Models for Electrons Incident on Stainless Steel with Energies E_0 of 60.0 keV and 111.7 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

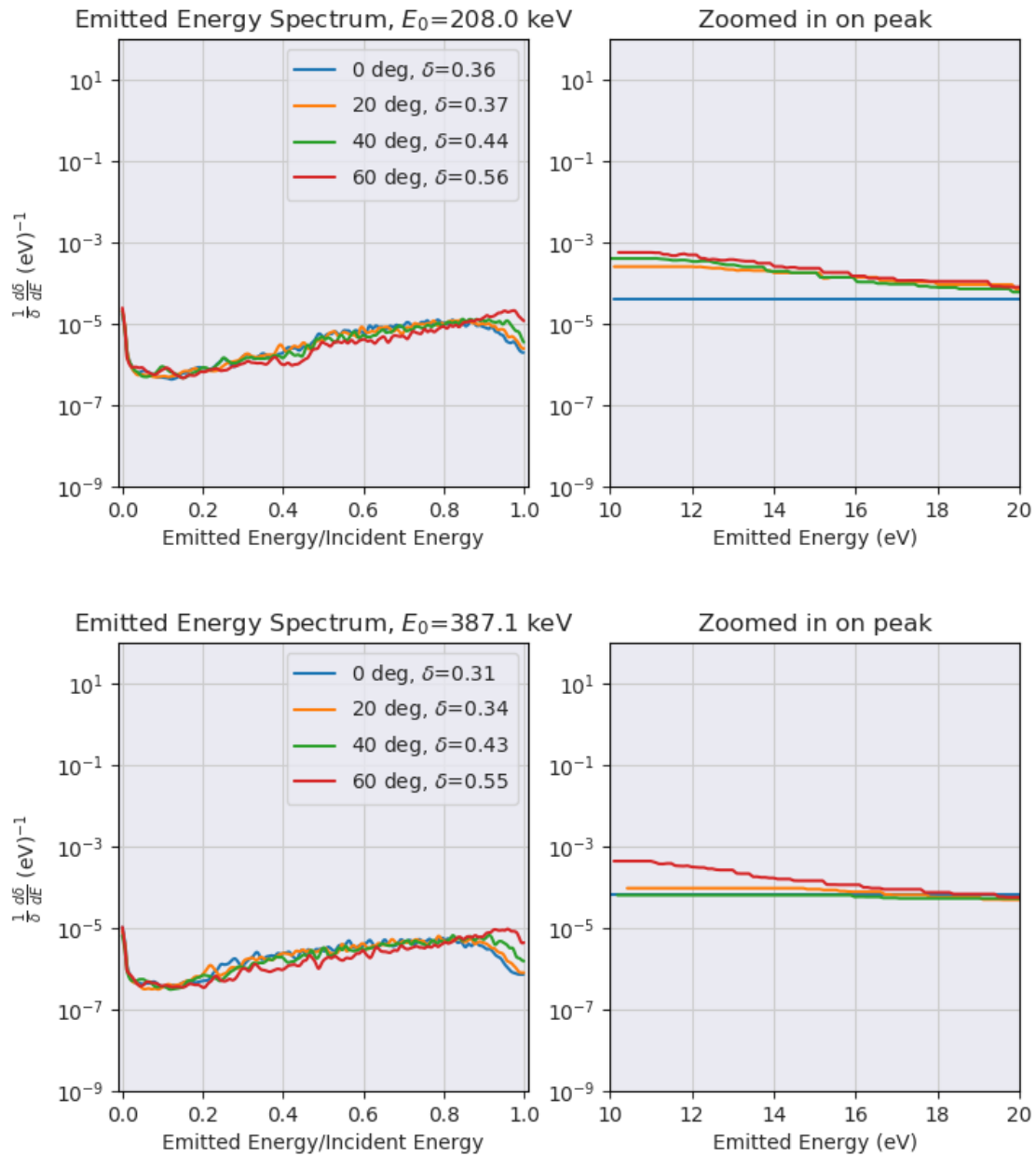


Figure A- 44: EES from GEANT4's Livermore Models for Electrons Incident on Stainless Steel with Energies E_0 of 208.0 keV and 387.1 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

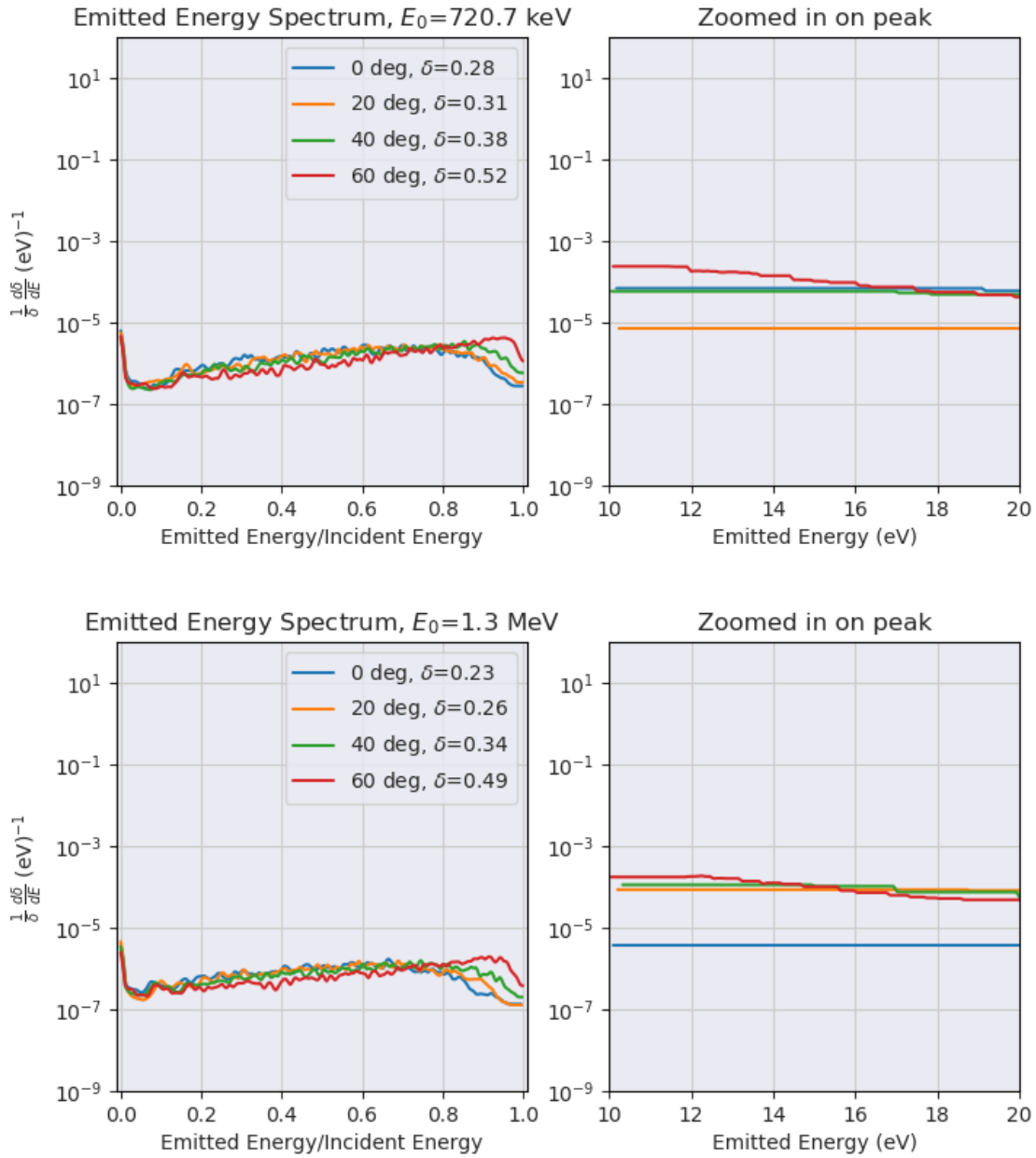


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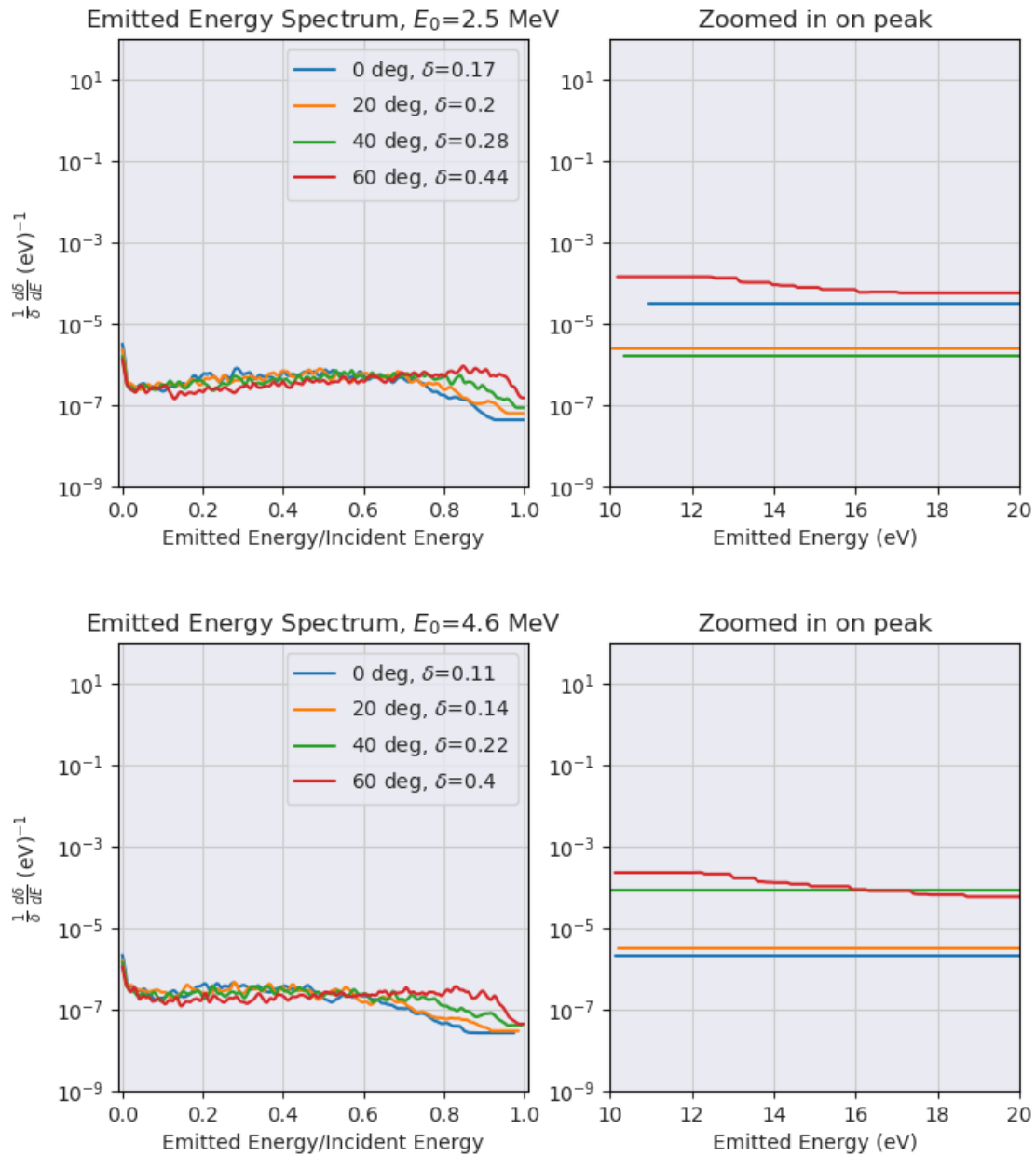


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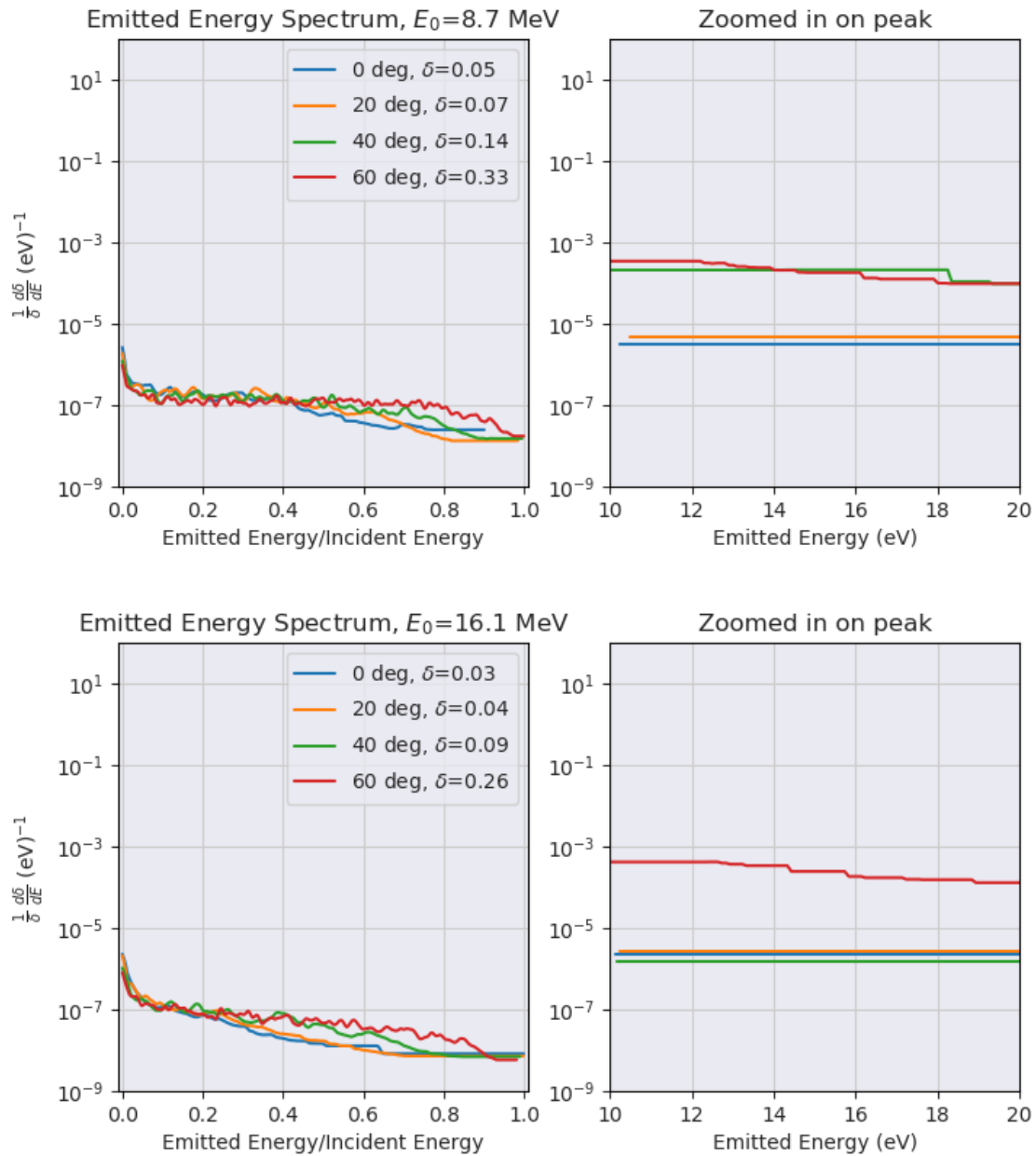


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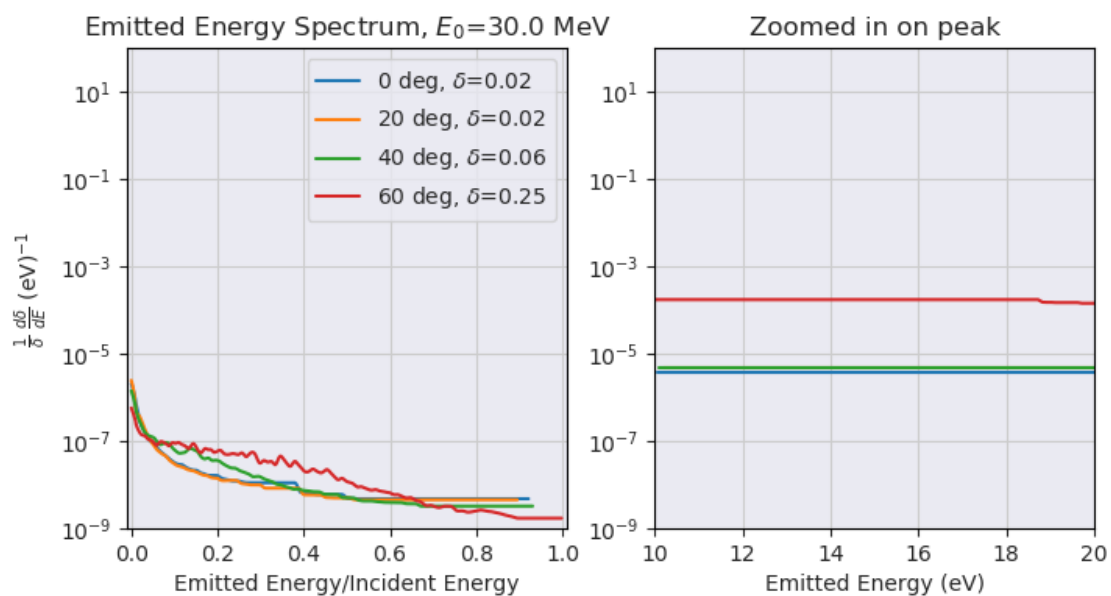


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B.1 Overview

This appendix provides an exhaustive list of the GEANT4 EES plots for aluminum, niobium, graphite, aluminum oxide (alumina), and beryllium oxide using the Livermore physics models. All plots were generated similarly to those in Appendix A: The 80 degree EES were not included because all electrons were perfectly reflected, with emission energy equal to the incident energy. All EES x-axis ranges are normalized so that a value of 1 corresponds to the incident energy. In order to best observe the spectra over a wide range of incident energies, the EES y-axes are scaled such that each curve has an integrated area of unity, and the total yield for that incident energy is listed in the legend; note that when yield curves are displayed in isolation in the literature, a common convention is for the integral of the yield curve not to equal unity, but rather to equal the total yield.

B.2 Aluminum

In this section we provide the EES of aluminum, as simulated using the built-in GEANT4 aluminum material definition. The results are as shown in Figure B-1 through Figure B-13. As

with stainless steel, the aluminum EES lack an emission peak between 10-12 eV. In addition, they are often much flatter than the stainless steel distributions. Delta functions like those seen in stainless steel occur here as well. Similarly, they are not yet understood, but could correspond to a phenomenon similar to the photoelectric effect.

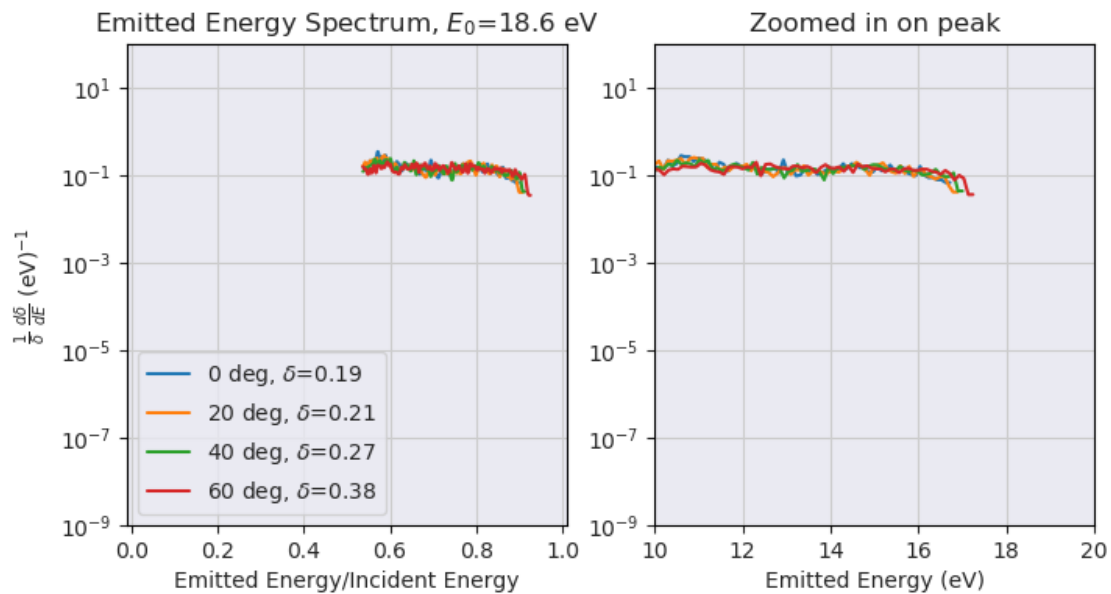


Figure B- 1: EES from GEANT4's Livermore Models for Electrons Incident on Aluminum with Energy E_0 of 18.6 eV (left), and over the Emitted Energy Range 10-20 eV (right).

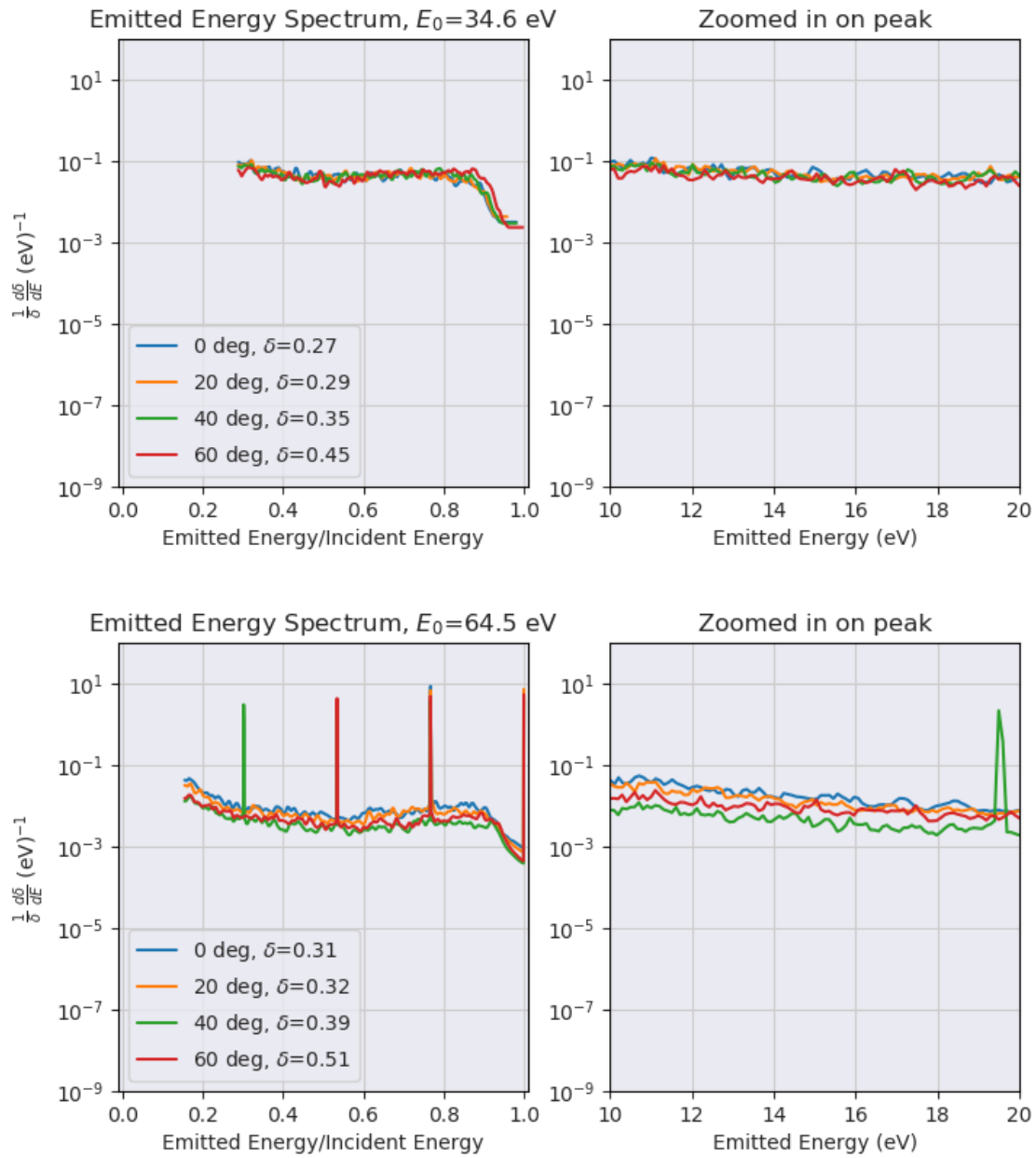


Figure B- 2: EES from GEANT4's Livermore Models for Electrons Incident on Aluminum with Energies E_0 of 34.6 eV and 64.5 eV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

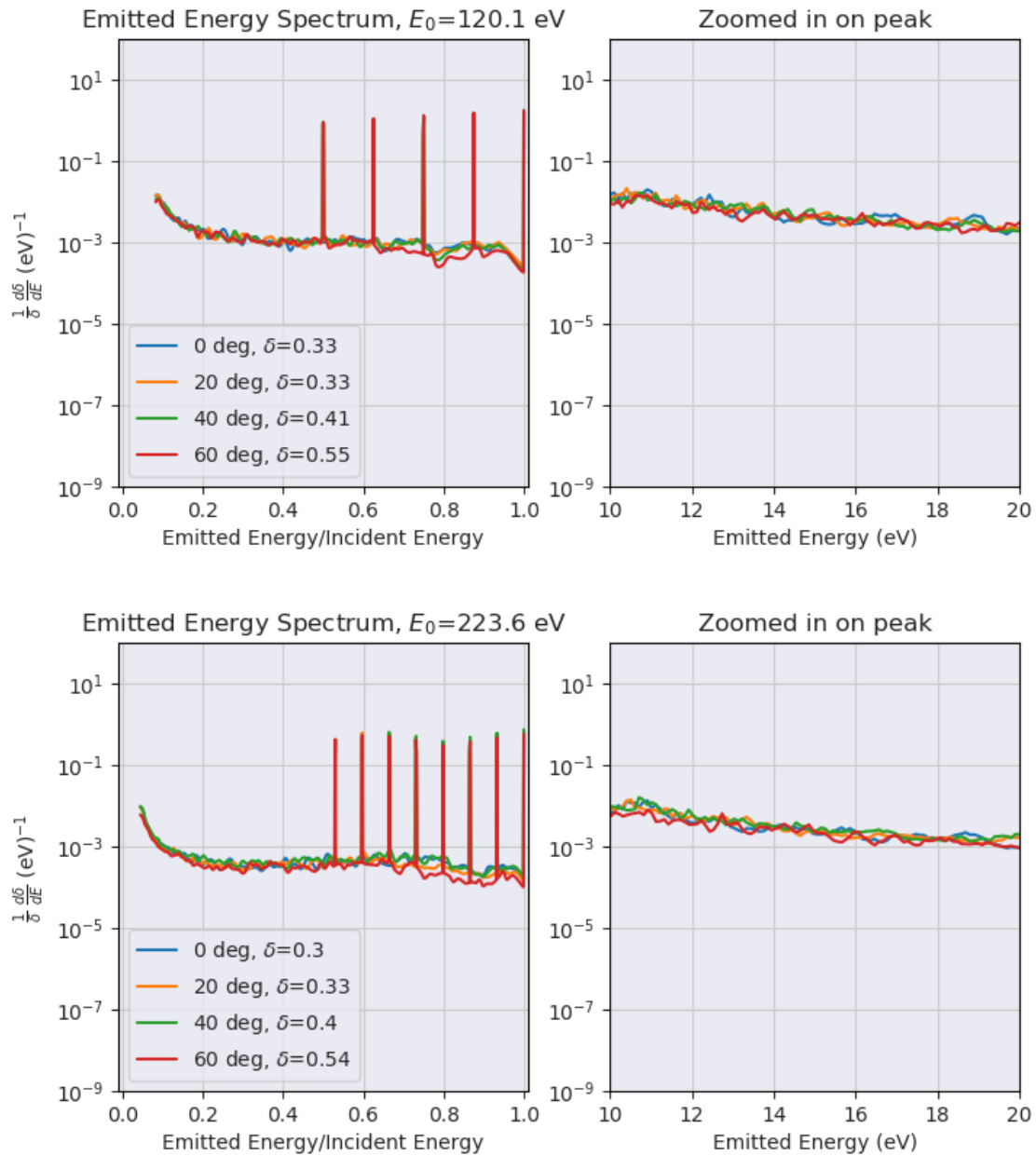


Figure B- 3: EES from GEANT4's Livermore Models for Electrons Incident on Aluminum with Energies E_0 of 120.1 eV and 223.6 eV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

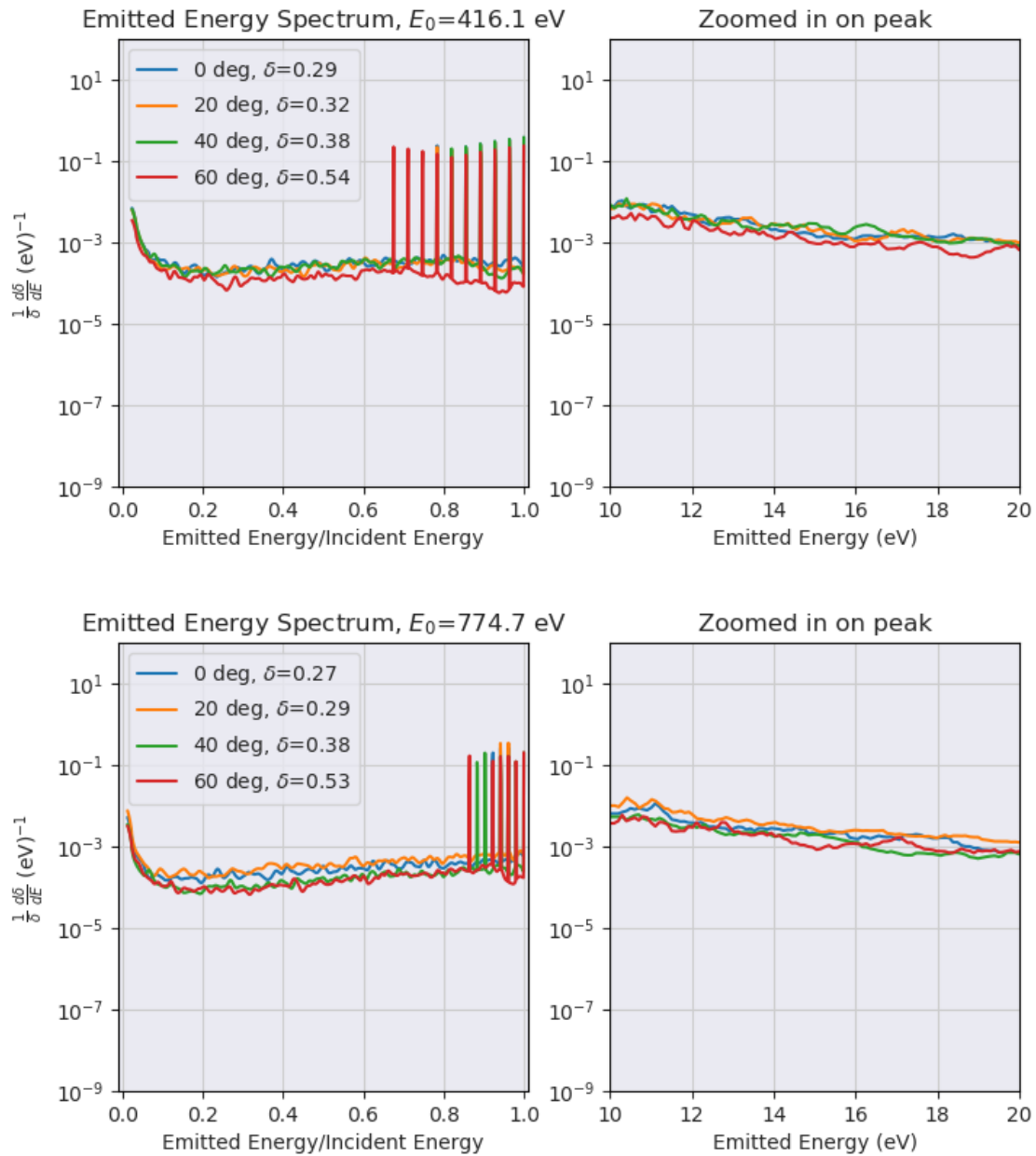


Figure B- 4: EES from GEANT4's Livermore Models for Electrons Incident on Aluminum with Energies E_0 of 416.1 eV and 774.7 eV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

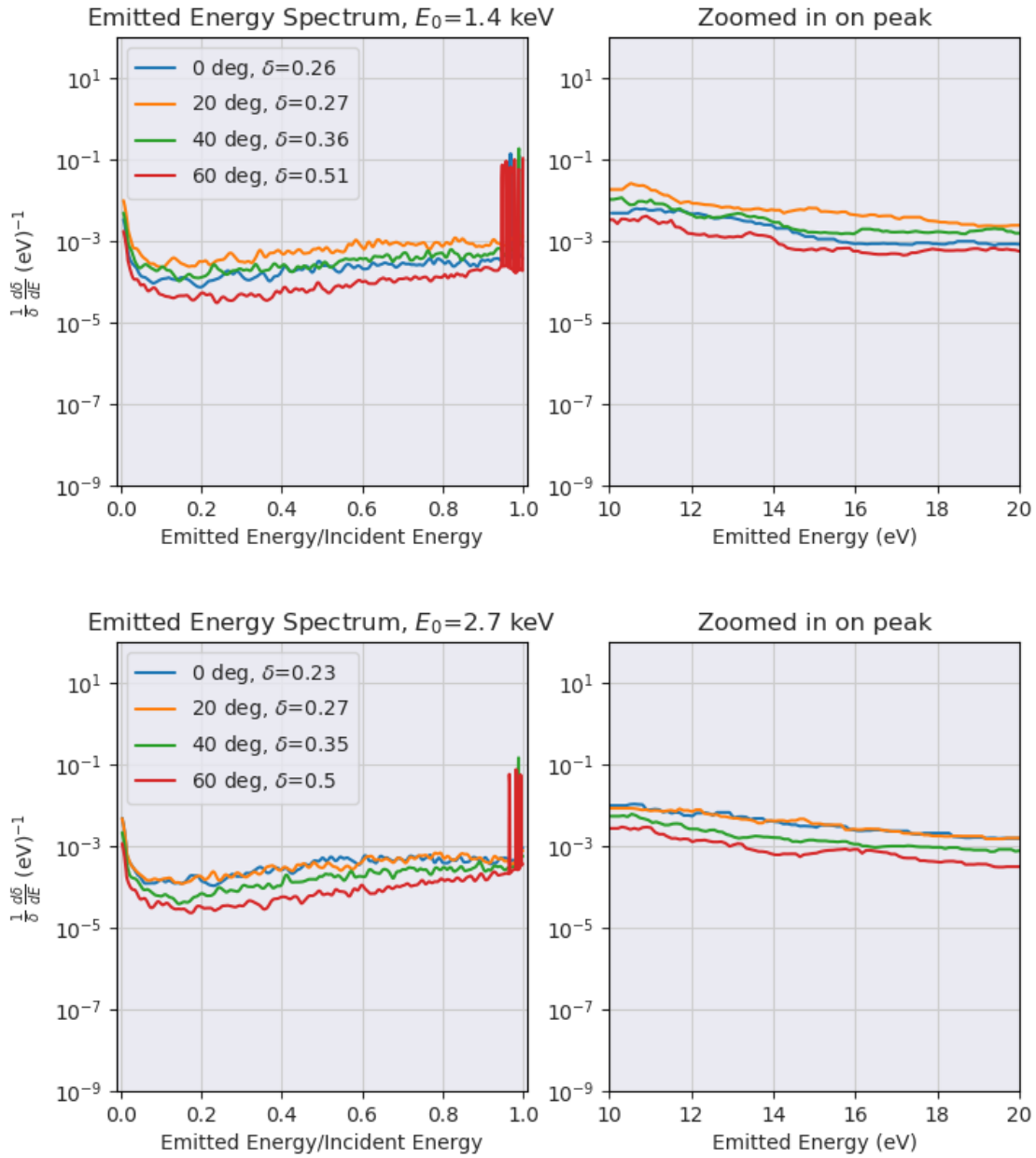


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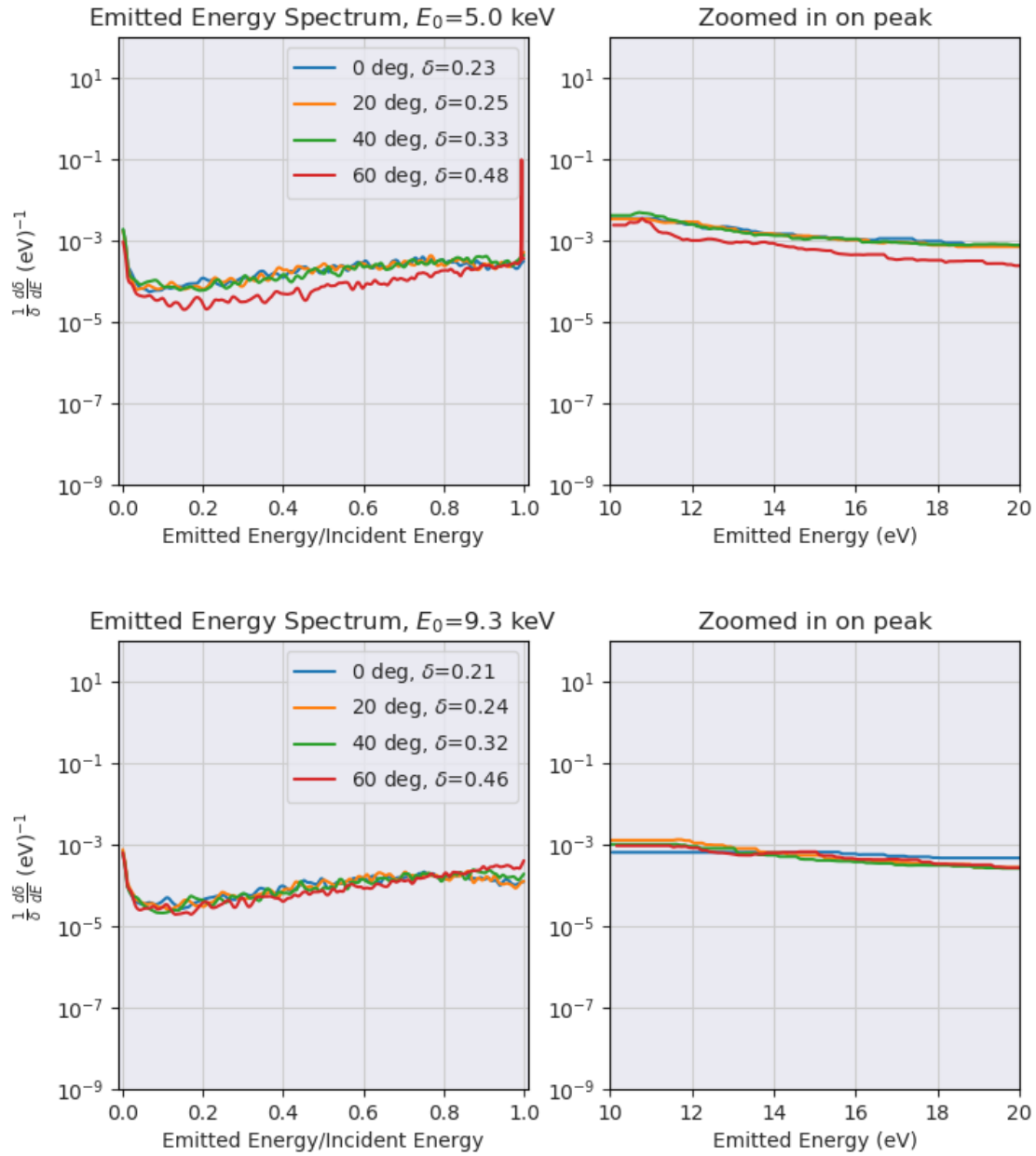


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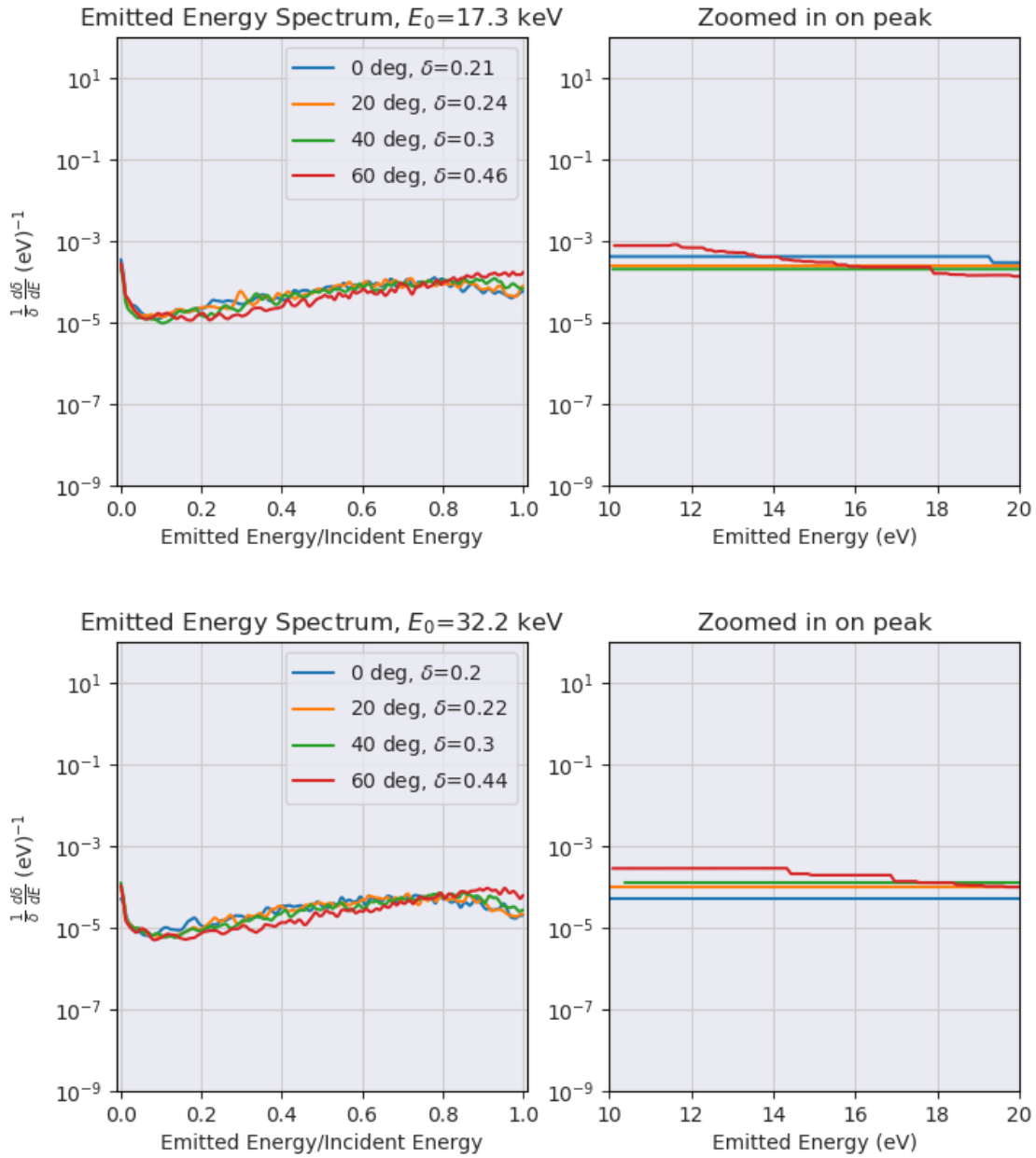


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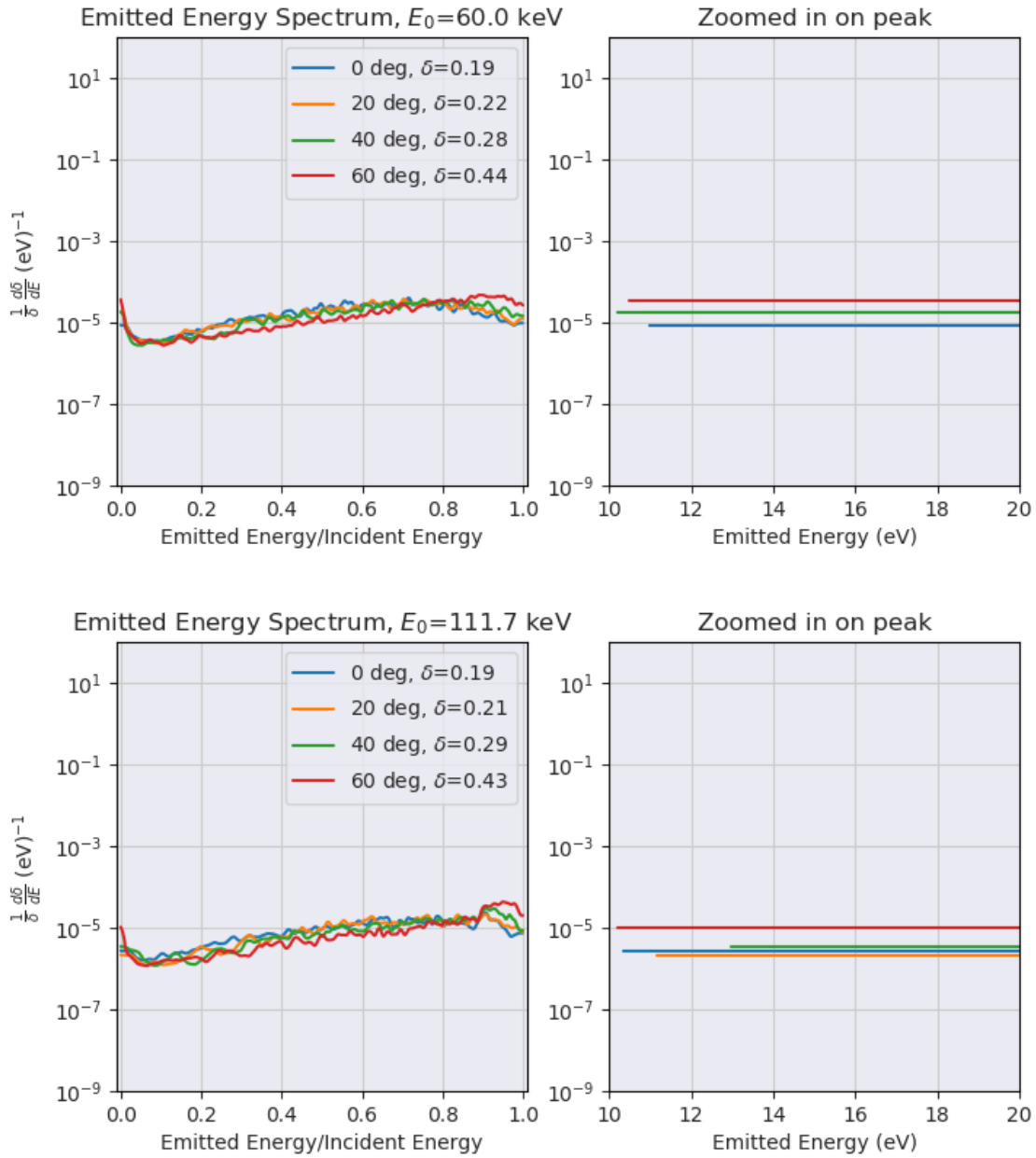


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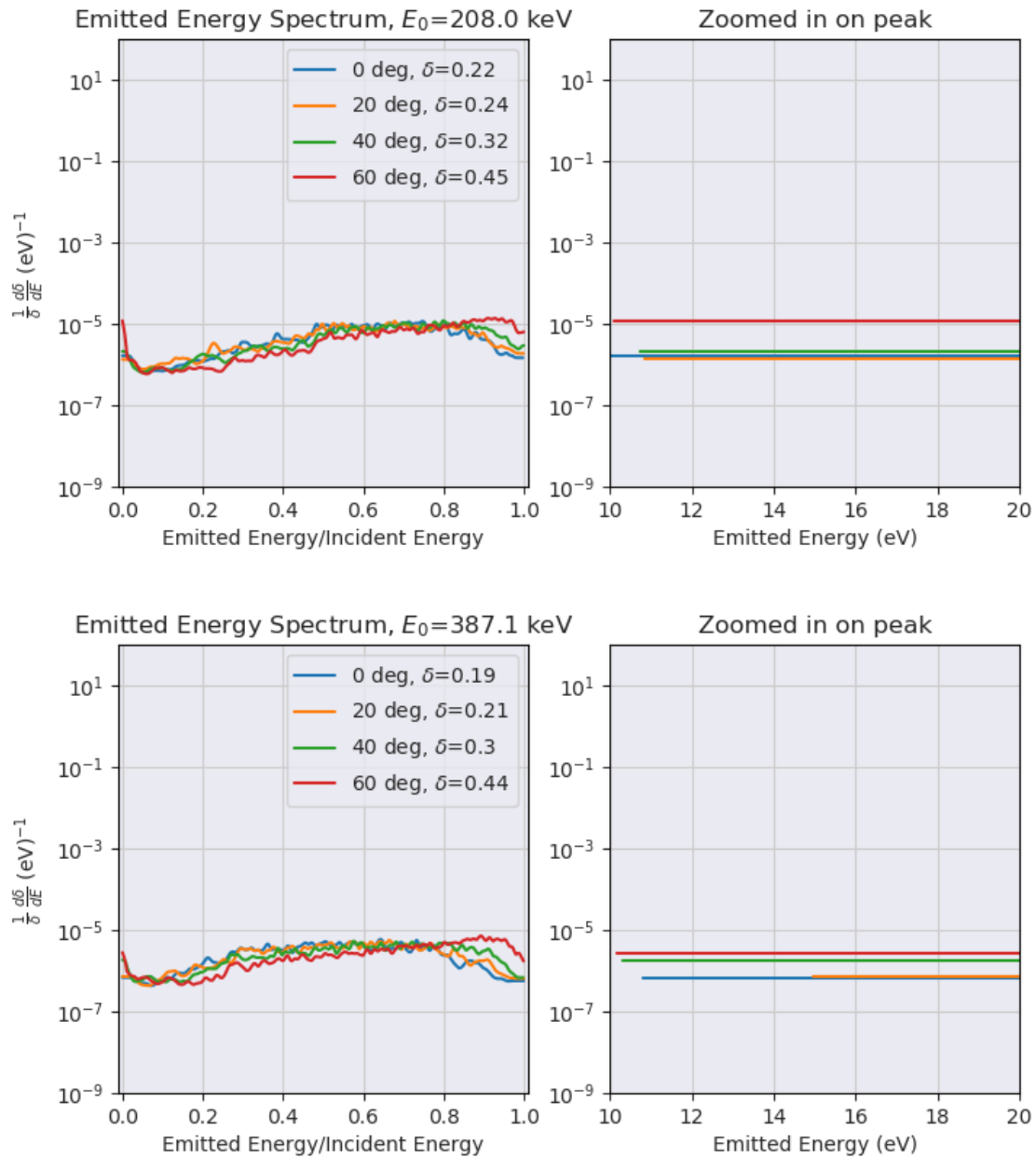


Figure B- 9: EES from GEANT4's Livermore Models for Electrons Incident on Aluminum with Energies E_0 of 208.0 keV and 387.1 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

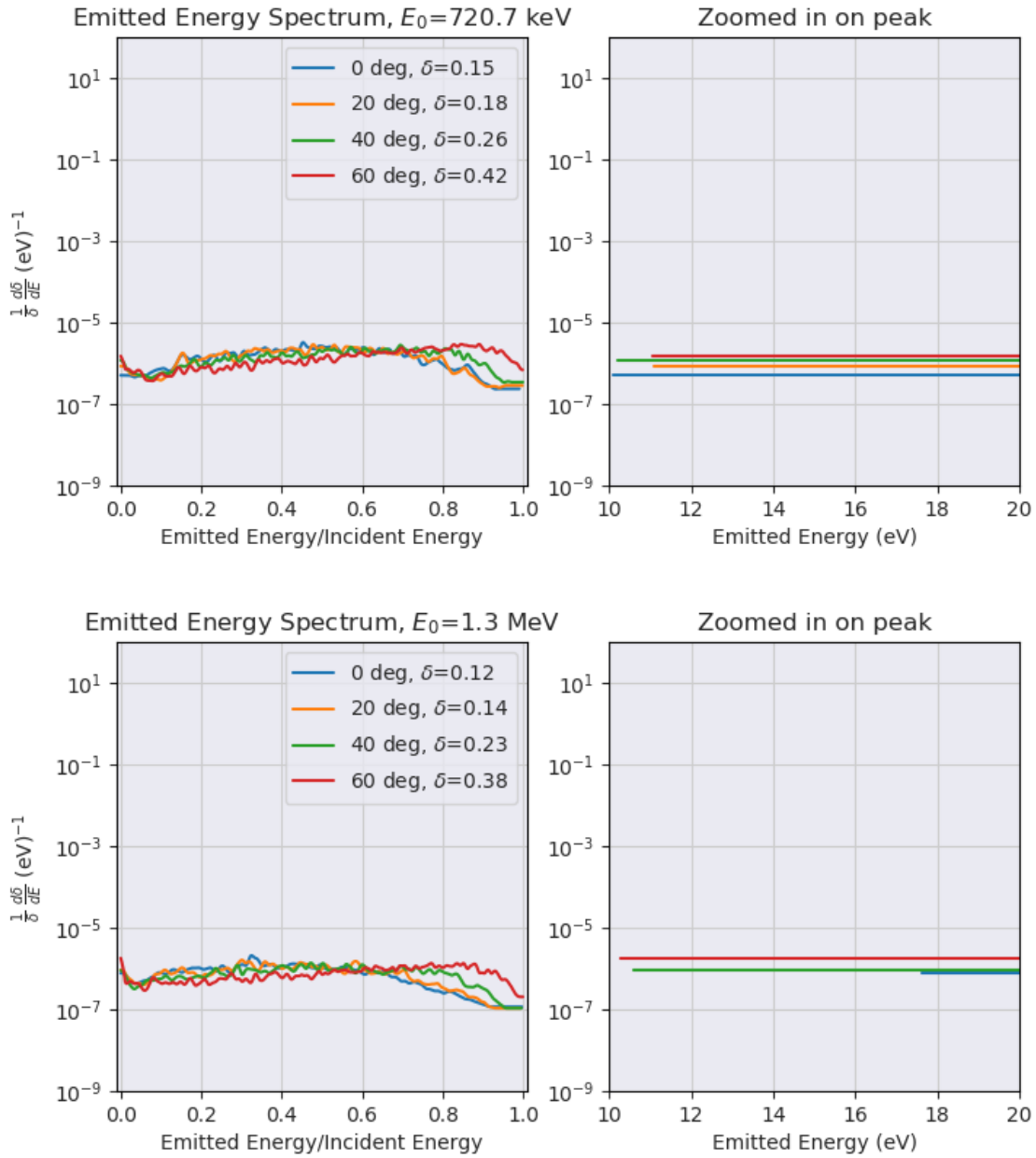


Figure B- 10: EES from GEANT4's Livermore Models for Electrons Incident on Aluminum with Energies E_0 of 720.7 keV and 1.3 MeV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

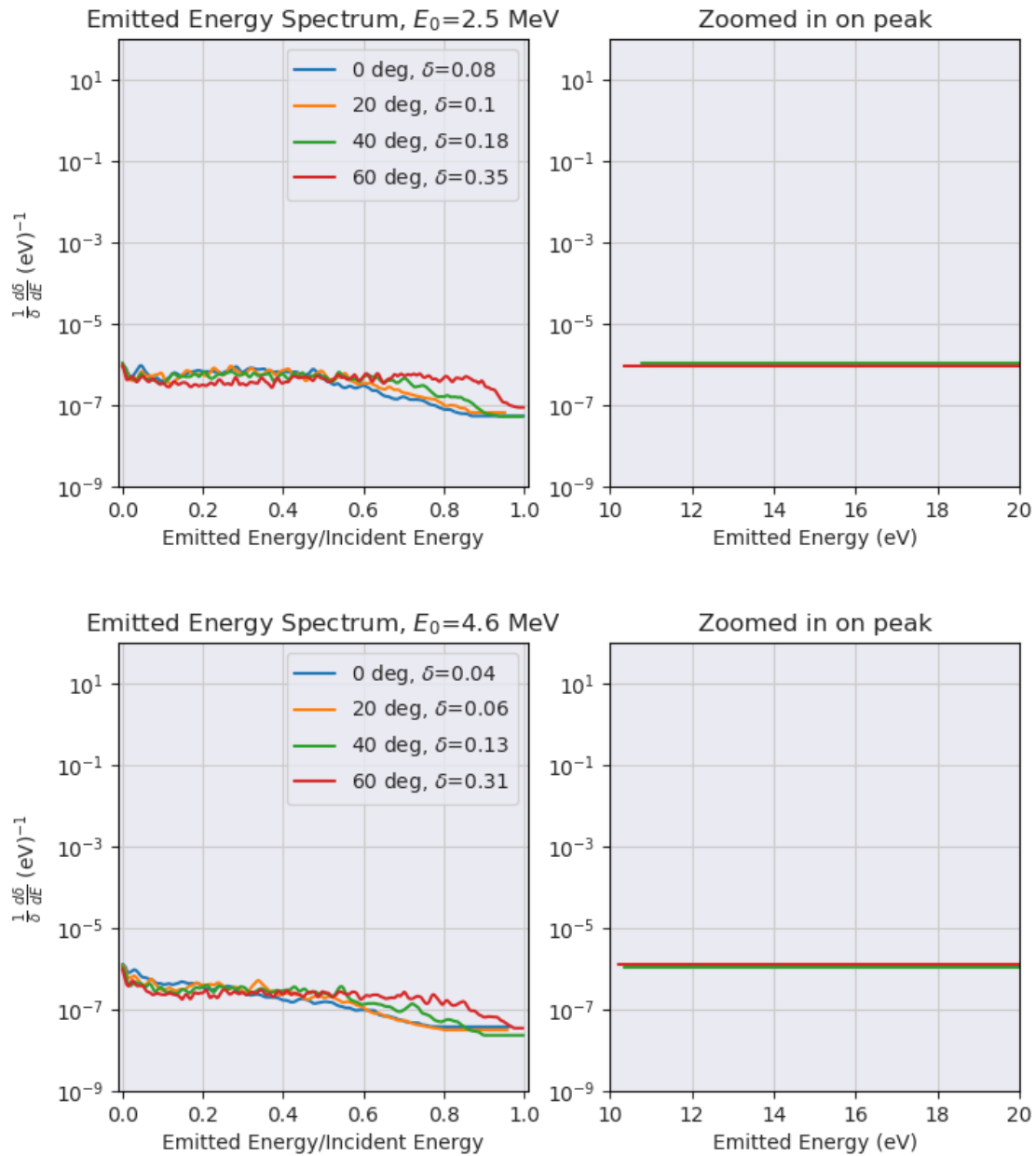


Figure B- 11: EES from GEANT4’s Livermore Models for Electrons Incident on Aluminum with Energies E_0 of 2.5 MeV and 4.6 MeV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

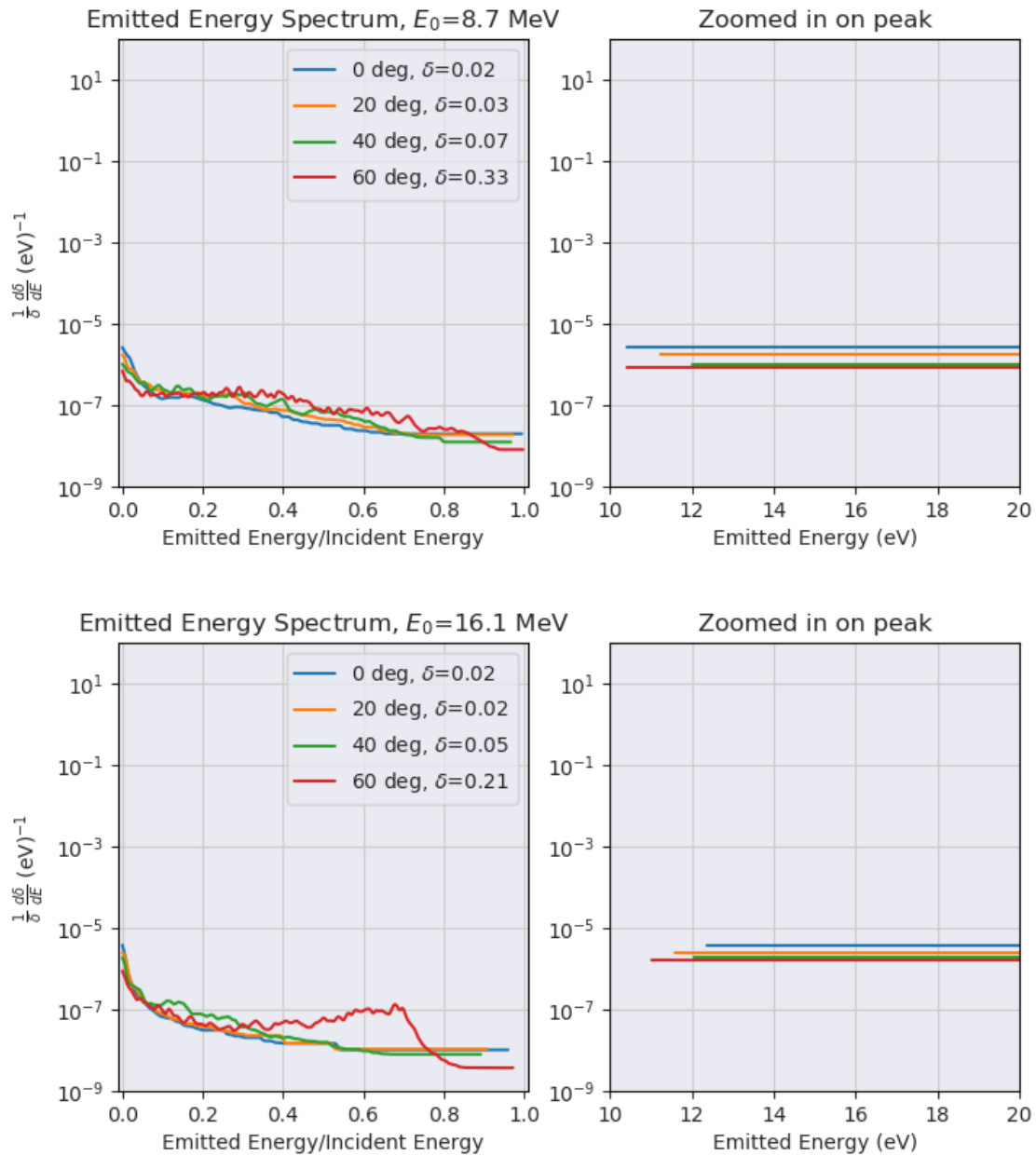


Figure B- 12: EES from GEANT4's Livermore Models for Electrons Incident on Aluminum with Energies E_0 of 8.7 MeV and 16.1 MeV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

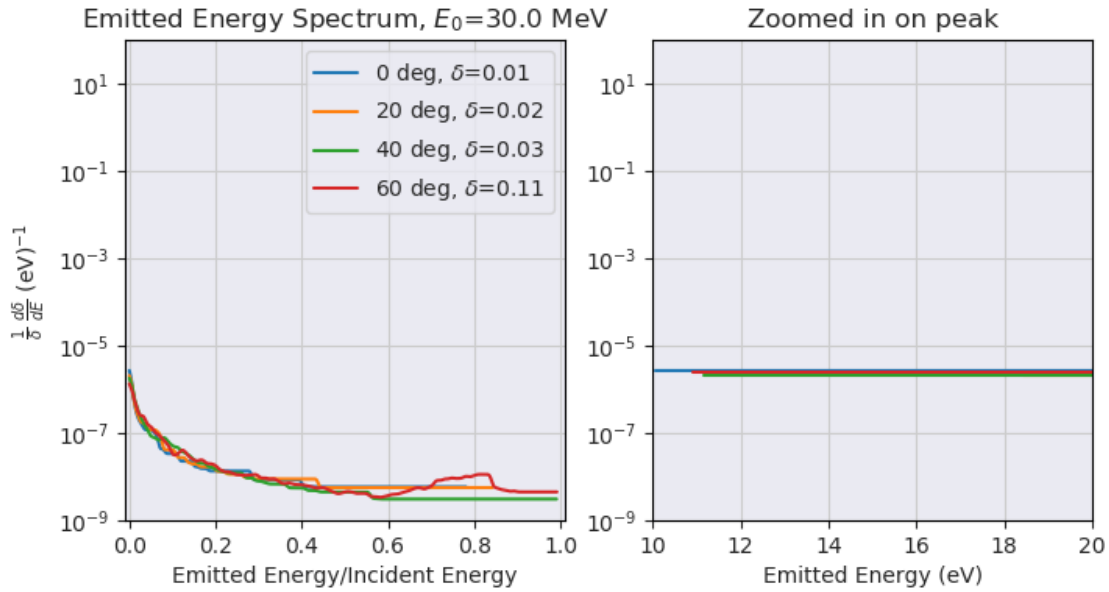


Figure B- 13: EES from GEANT4's Livermore Models for Electrons Incident on Aluminum with Energy E_0 of 30.0 MeV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

B.3 Niobium

In this section we provide the EES of niobium, as simulated using the built-in GEANT4 niobium material definition. The results are as shown in Figure B-14 through Figure B-25 . Like stainless steel and aluminum, the niobium EES lack an emission peak between 10-12 eV. Discrete spikes appear in some EES curves, likely due to quantum mechanical processes occurring at discrete transition energies.

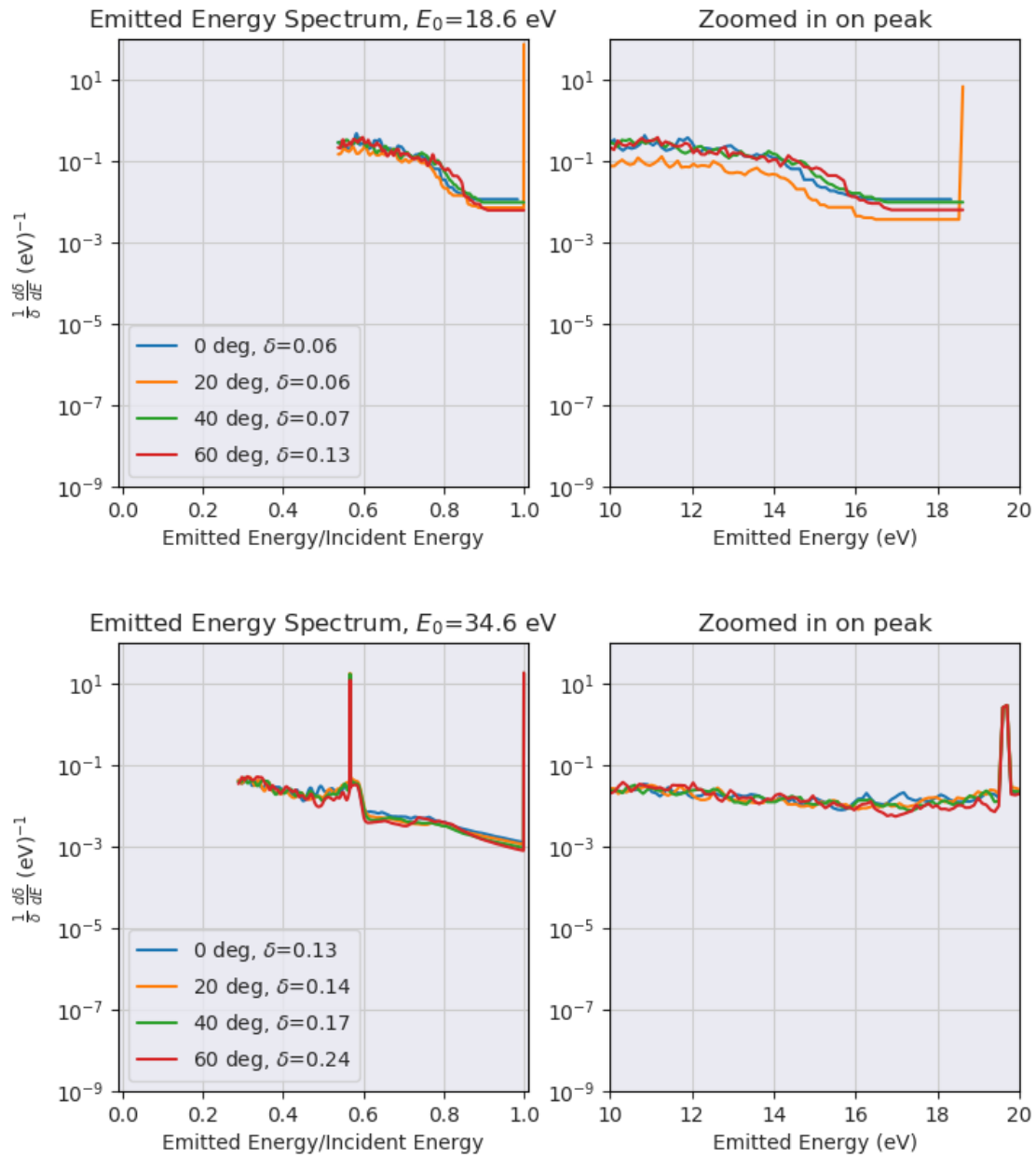


Figure B- 14: EES from GEANT4's Livermore Models for Electrons Incident on Niobium with Energies E_0 of 18.6 eV and 34.6 eV (left), and over the Emitted Energy Range 10-20 eV (right).

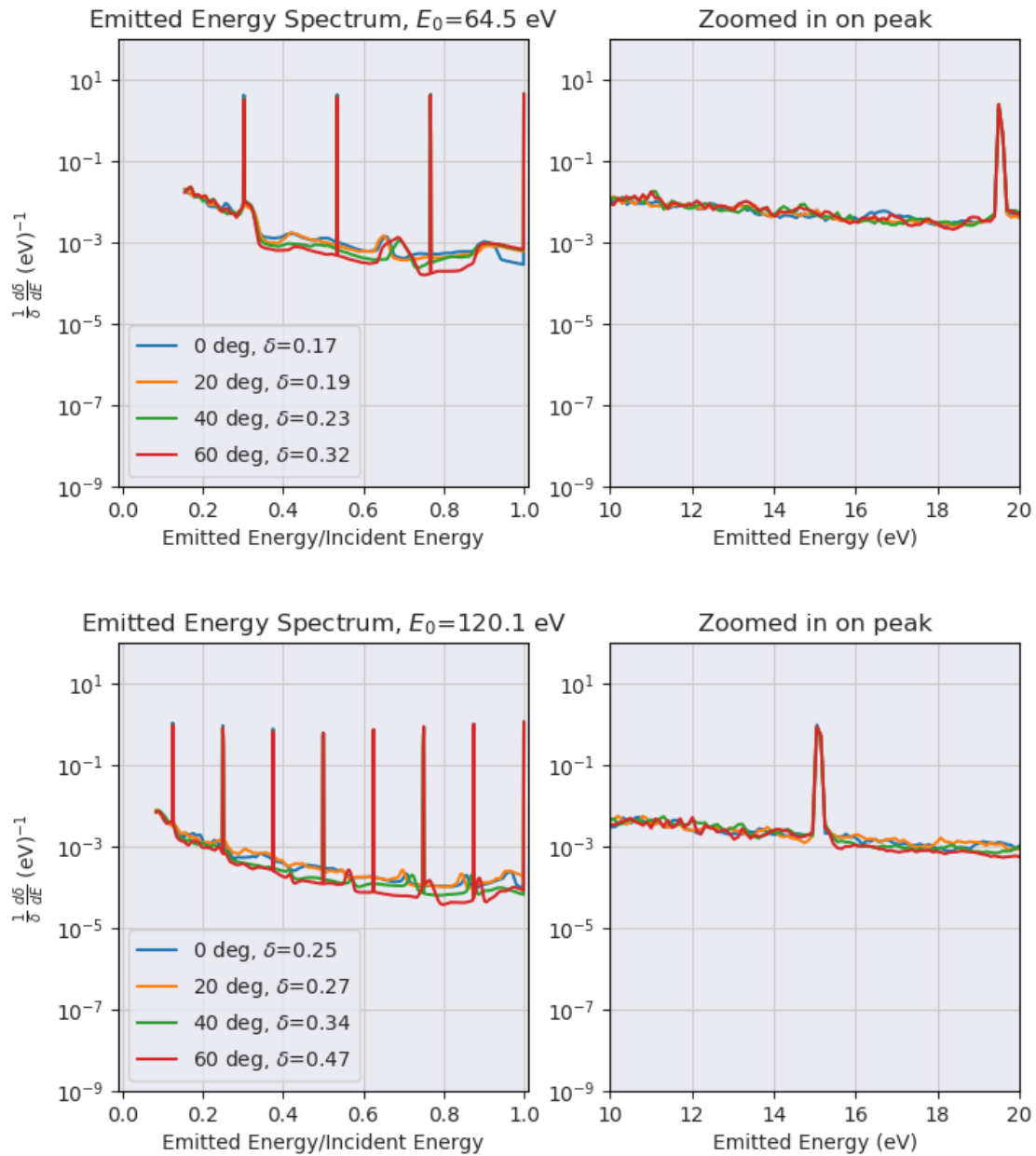


Figure B- 15: EES from GEANT4’s Livermore Models for Electrons Incident on Niobium with Energies E_0 of 64.5 eV and 120.1 eV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

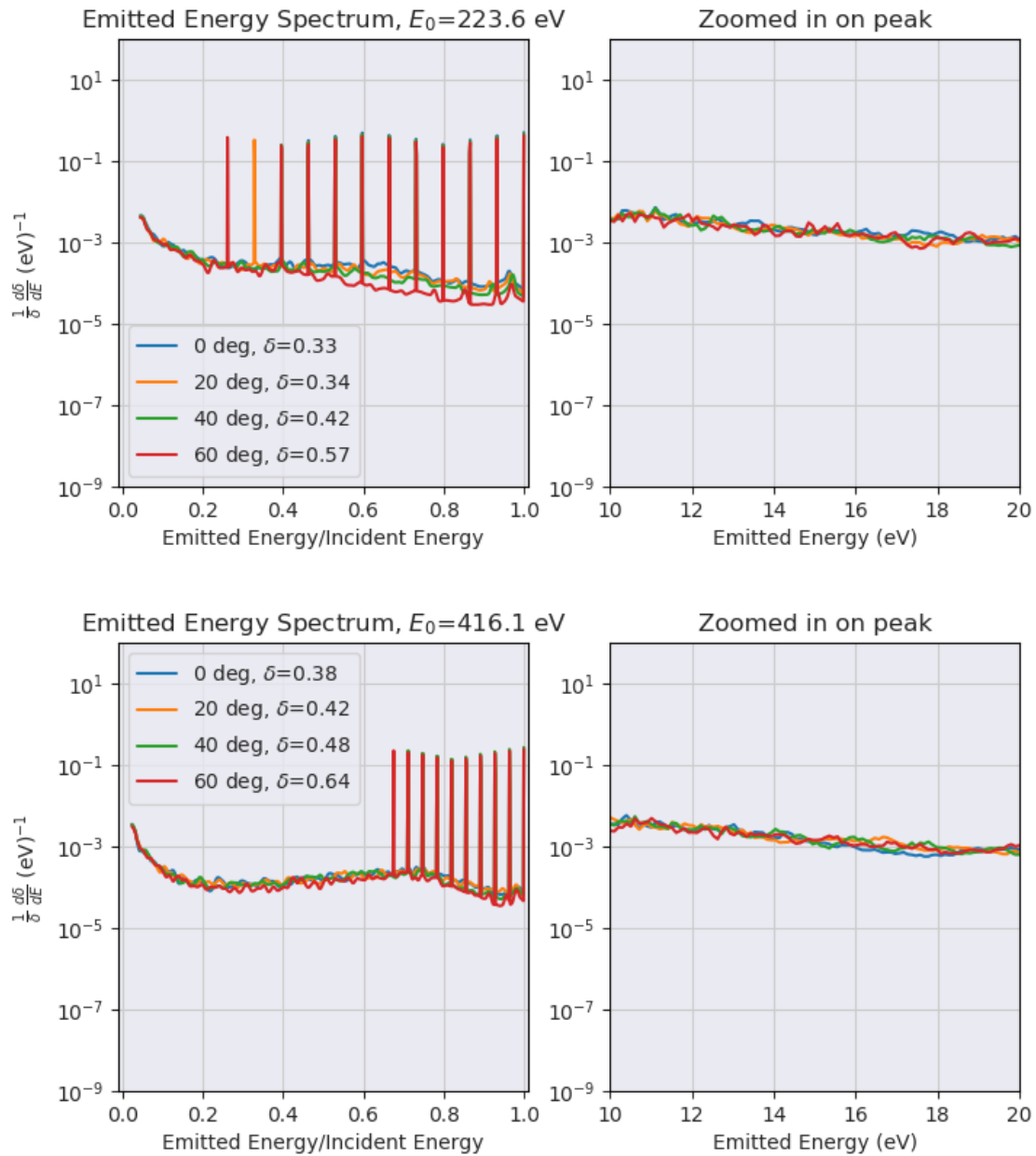


Figure B- 16: EES from GEANT4's Livermore Models for Electrons Incident on Niobium with Energies E_0 of 223.6 eV and 416.1 eV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

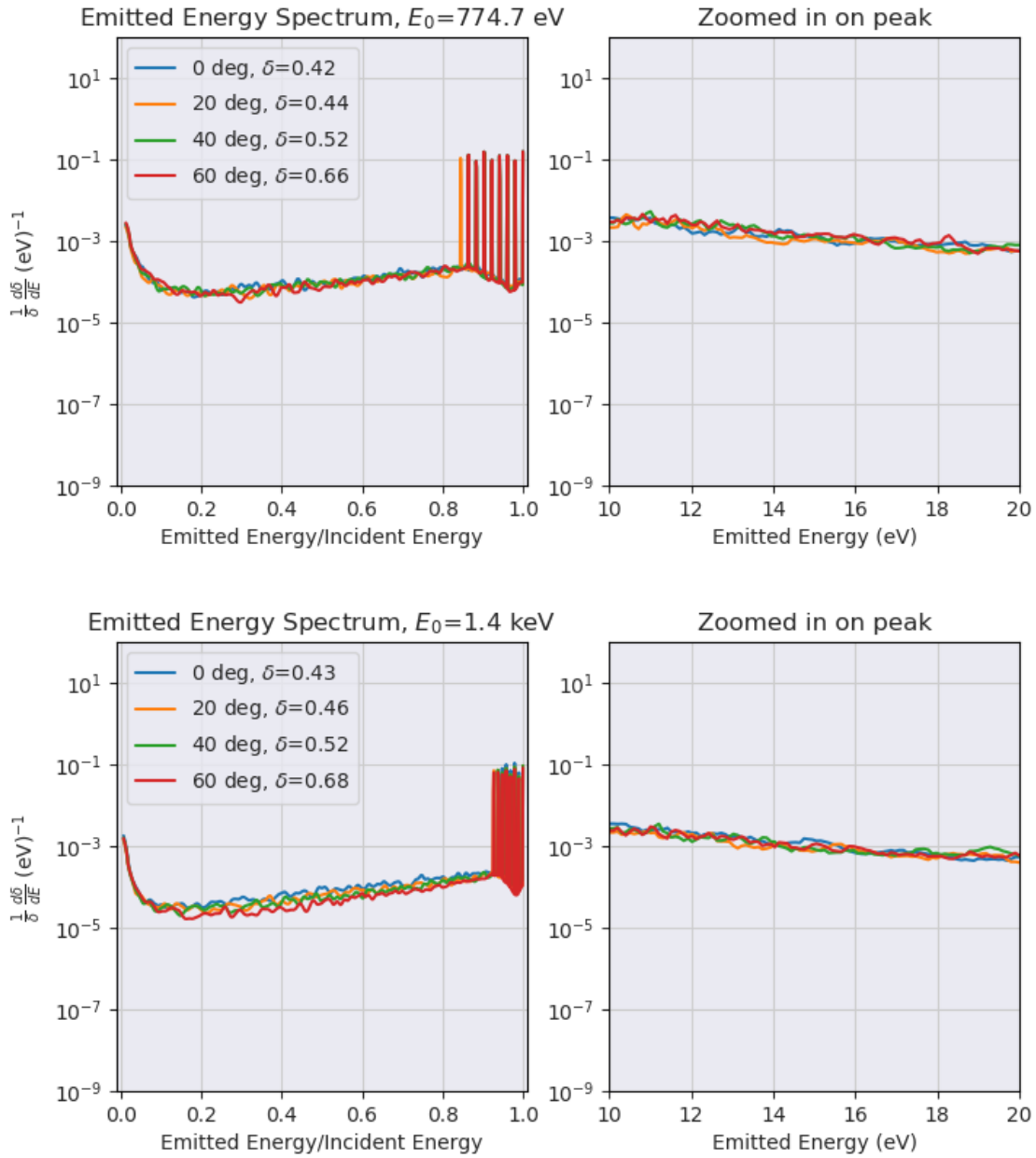


Figure B- 17: EES from GEANT4's Livermore Models for Electrons Incident on Niobium with Energies E_0 of 774.7 eV and 1.4 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

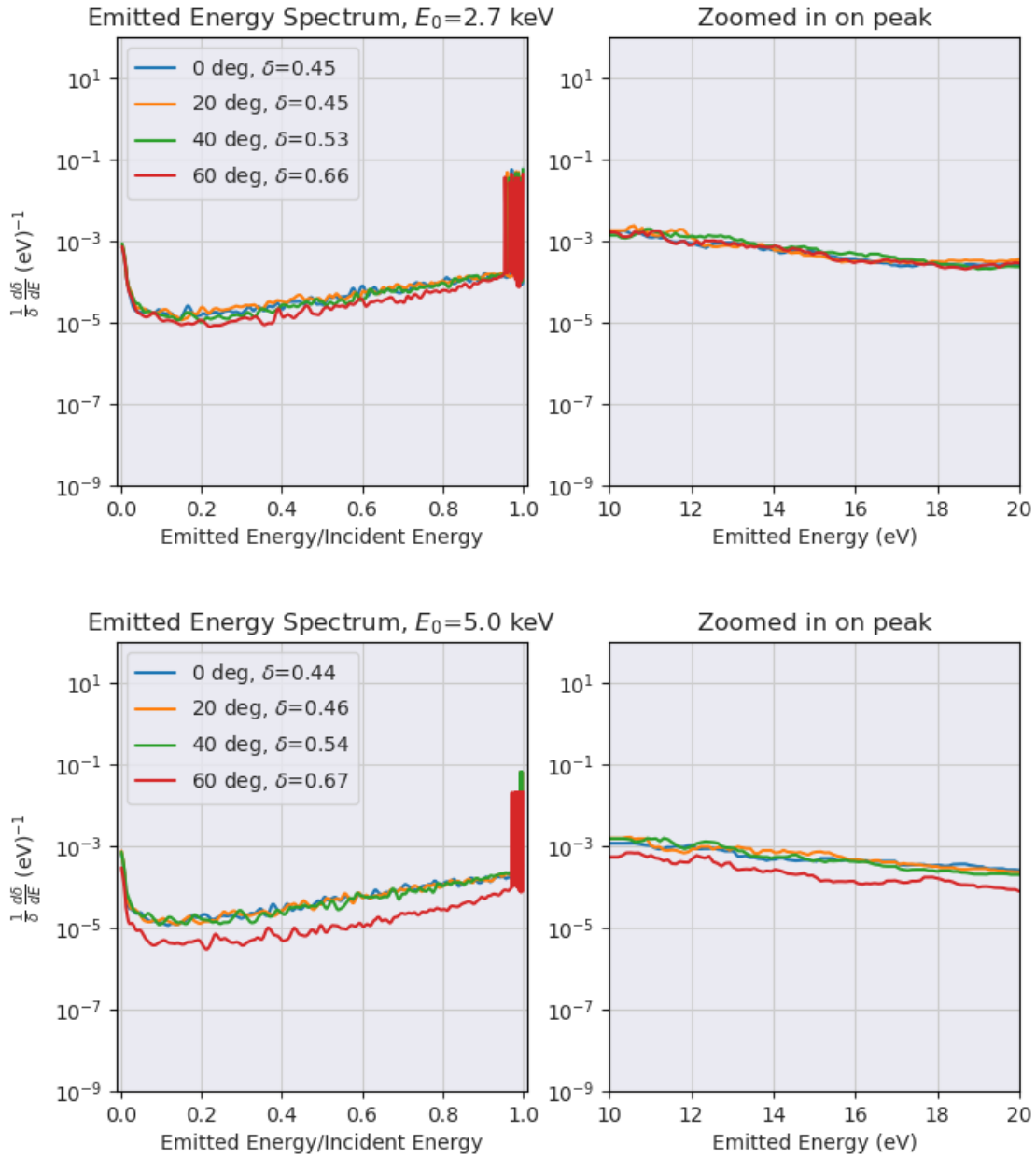


Figure B- 18: EES from GEANT4's Livermore Models for Electrons Incident on Niobium with Energies E_0 of 2.7 keV and 5.0 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

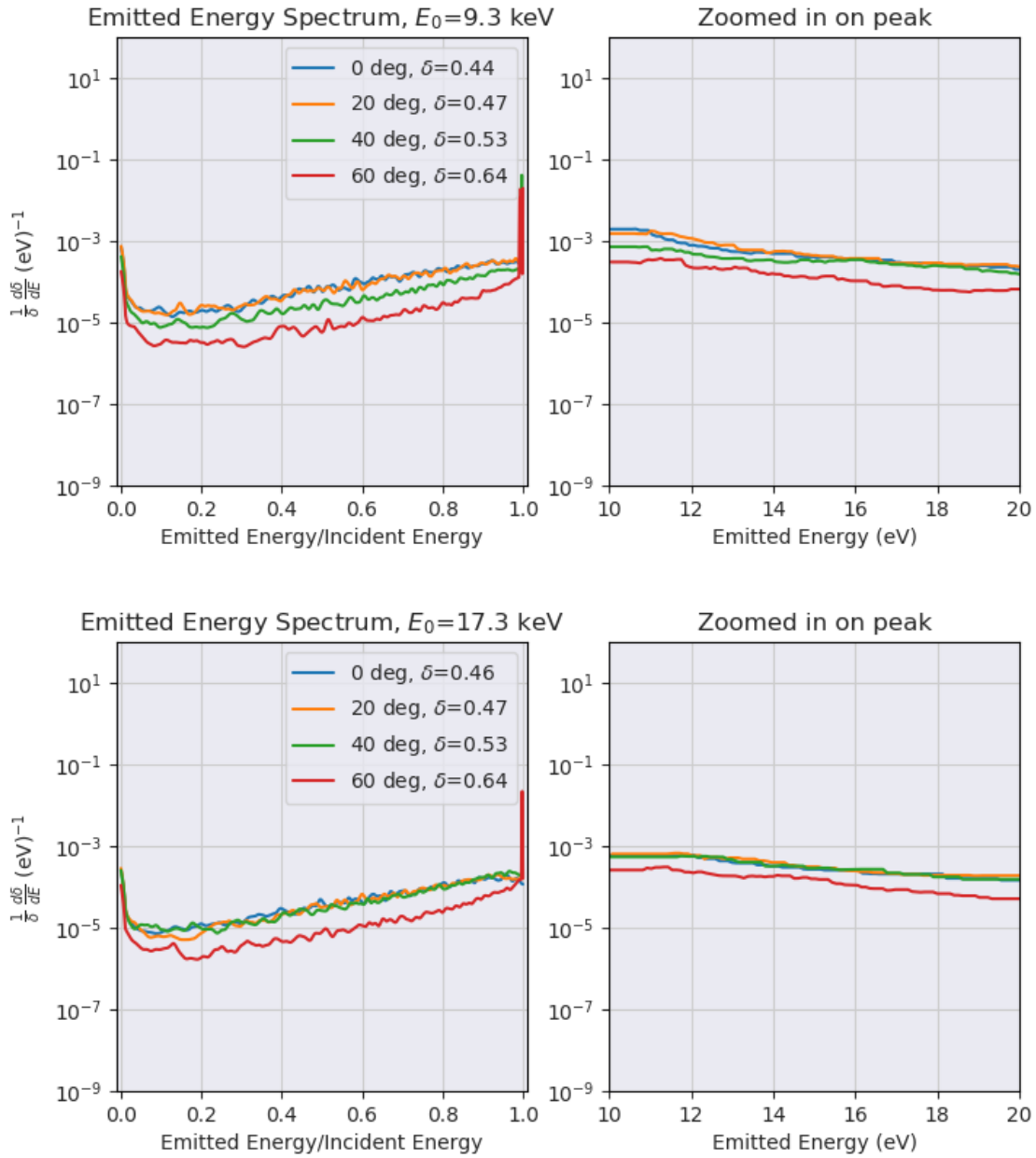


Figure B- 19: EES from GEANT4's Livermore Models for Electrons Incident on Niobium with Energies E_0 of 9.3 keV and 17.3 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

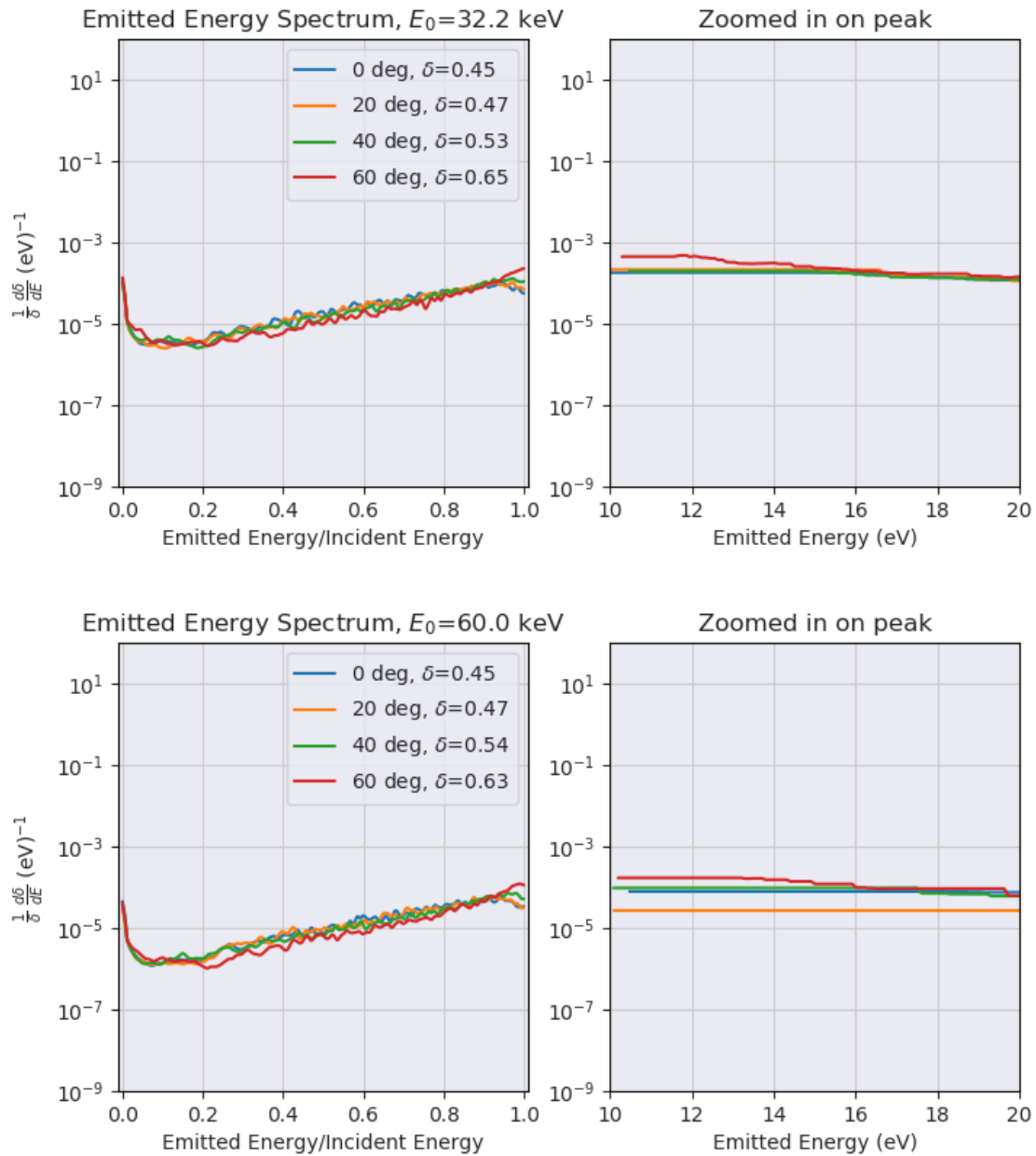


Figure B- 20: EES from GEANT4's Livermore Models for Electrons Incident on Niobium with Energies E_0 of 32.2 keV and 60.0 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

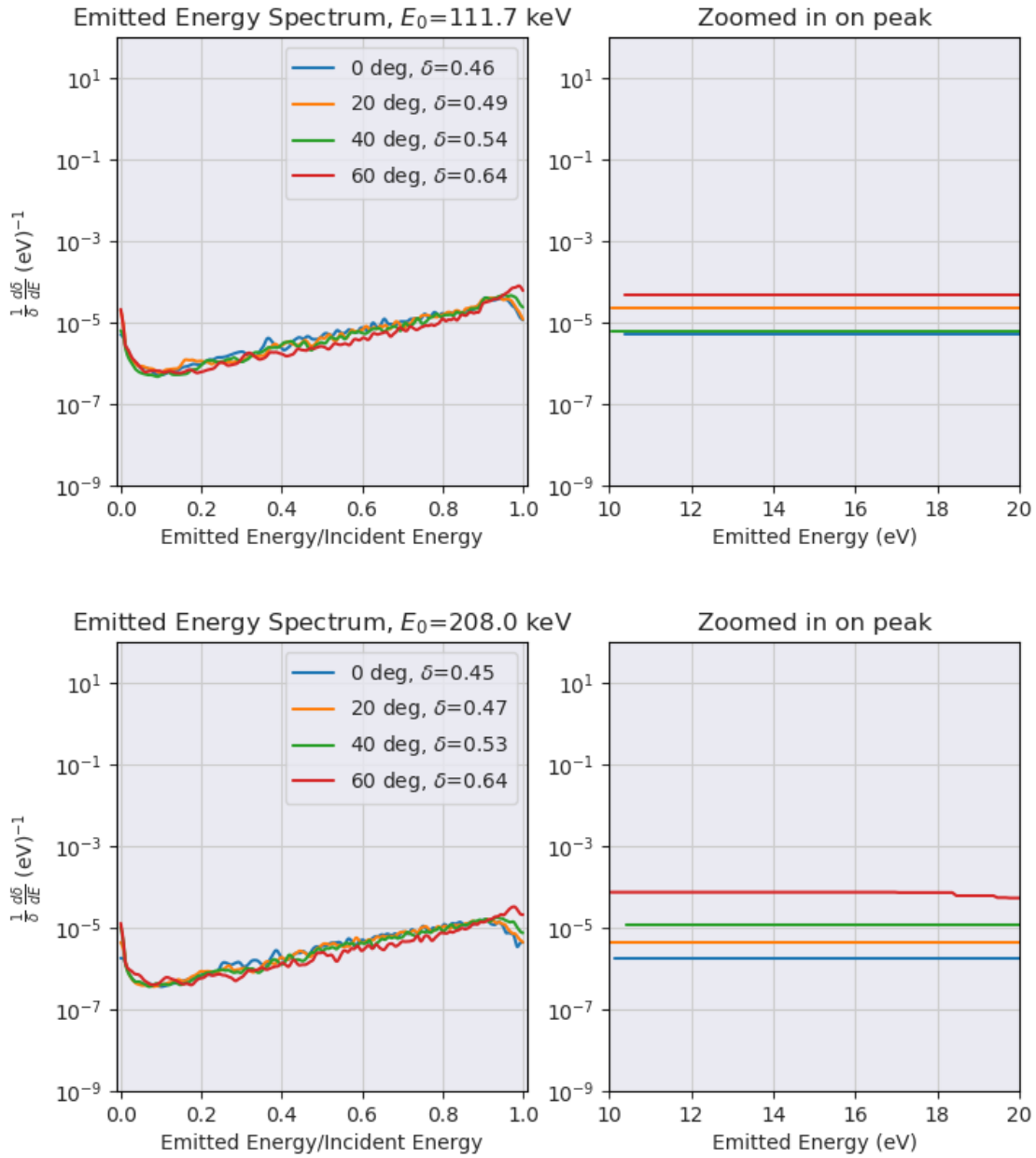


Figure B- 21: EES from GEANT4's Livermore Models for Electrons Incident on Niobium with Energies E_0 of 111.7 keV and 208.0 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

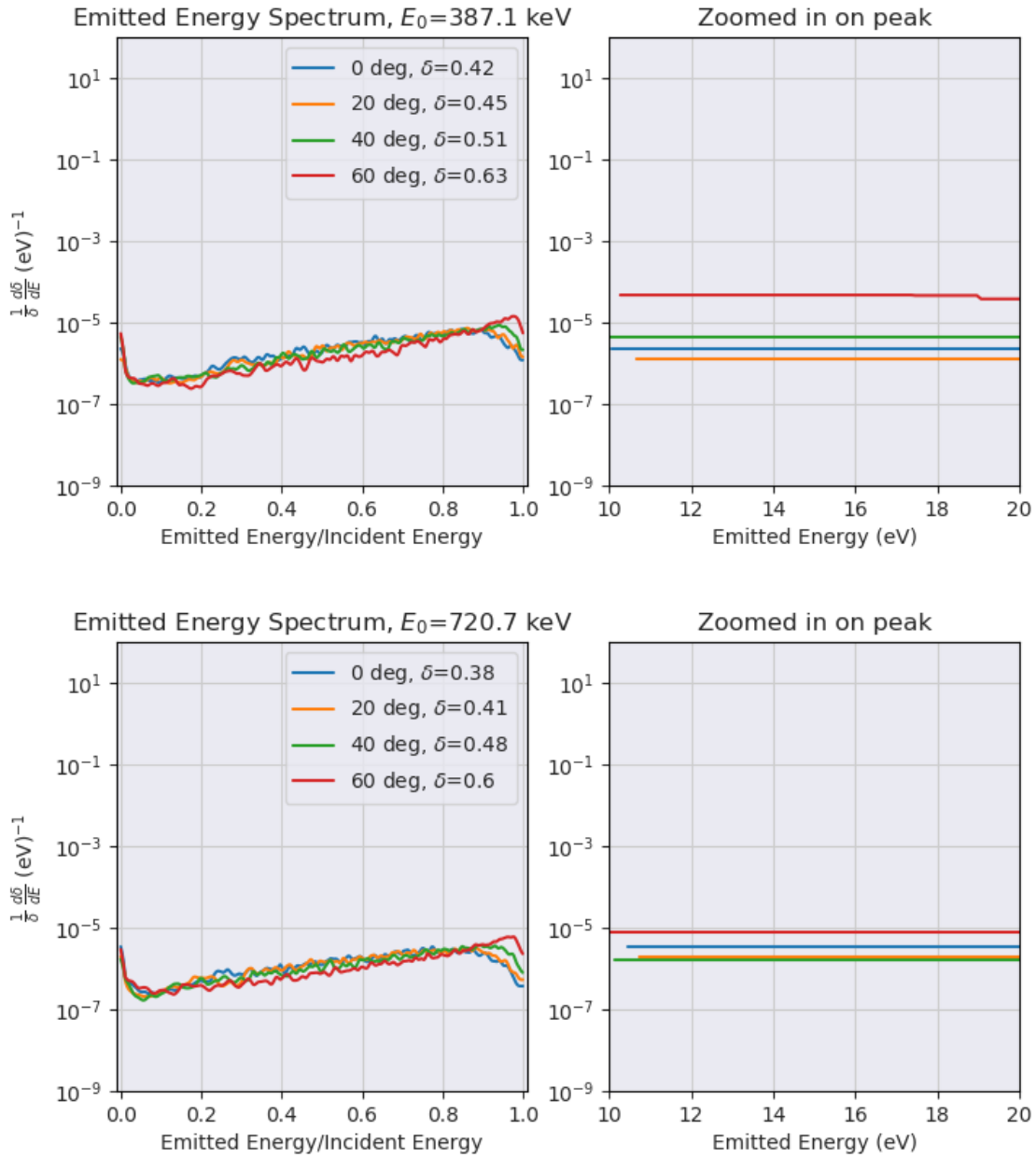


Figure B- 22: EES from GEANT4's Livermore Models for Electrons Incident on Niobium with Energies E_0 of 387.1 keV and 720.7 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

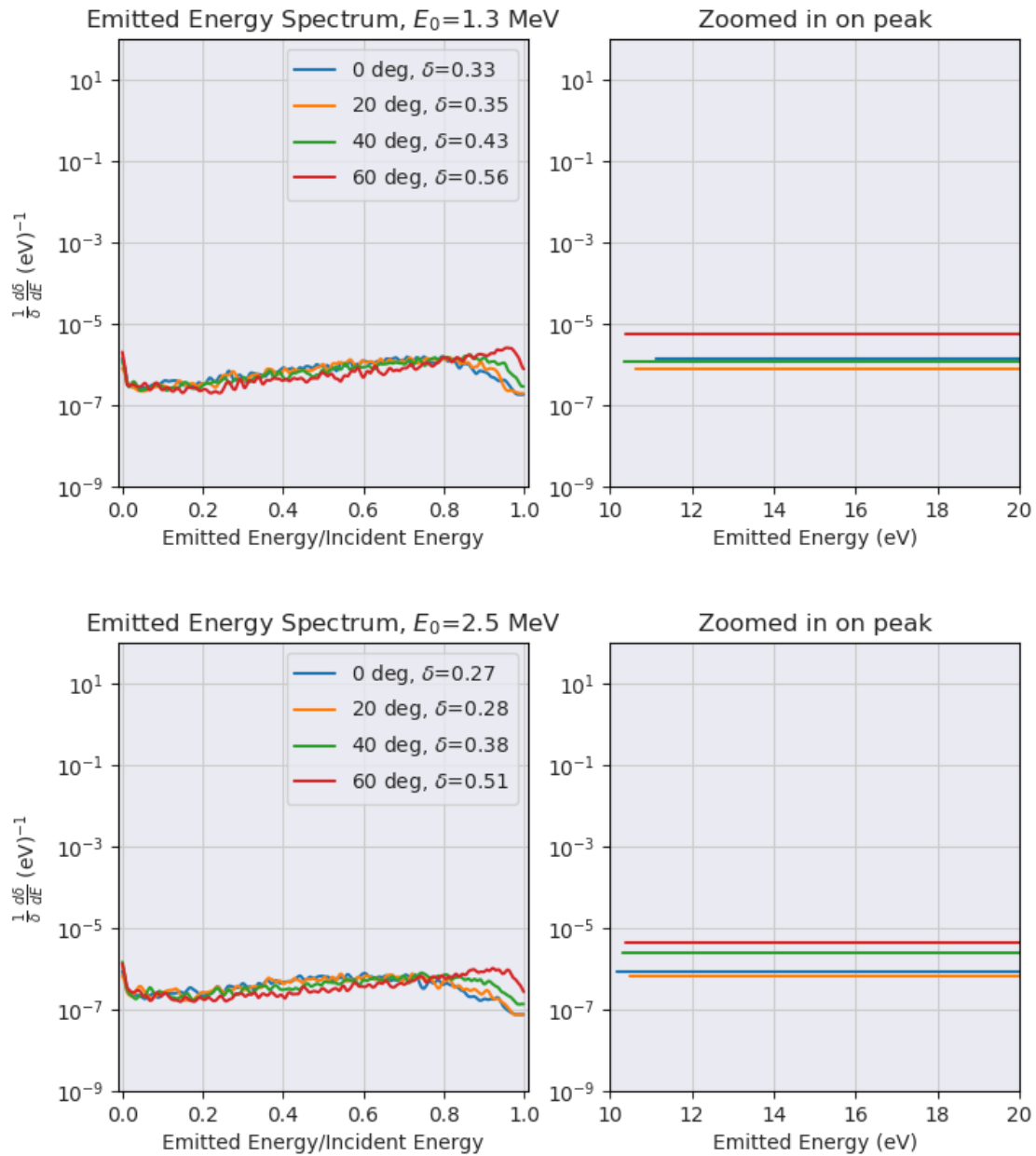


Figure B- 23: EES from GEANT4's Livermore Models for Electrons Incident on Niobium with Energies E_0 of 1.3 MeV and 2.5 MeV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

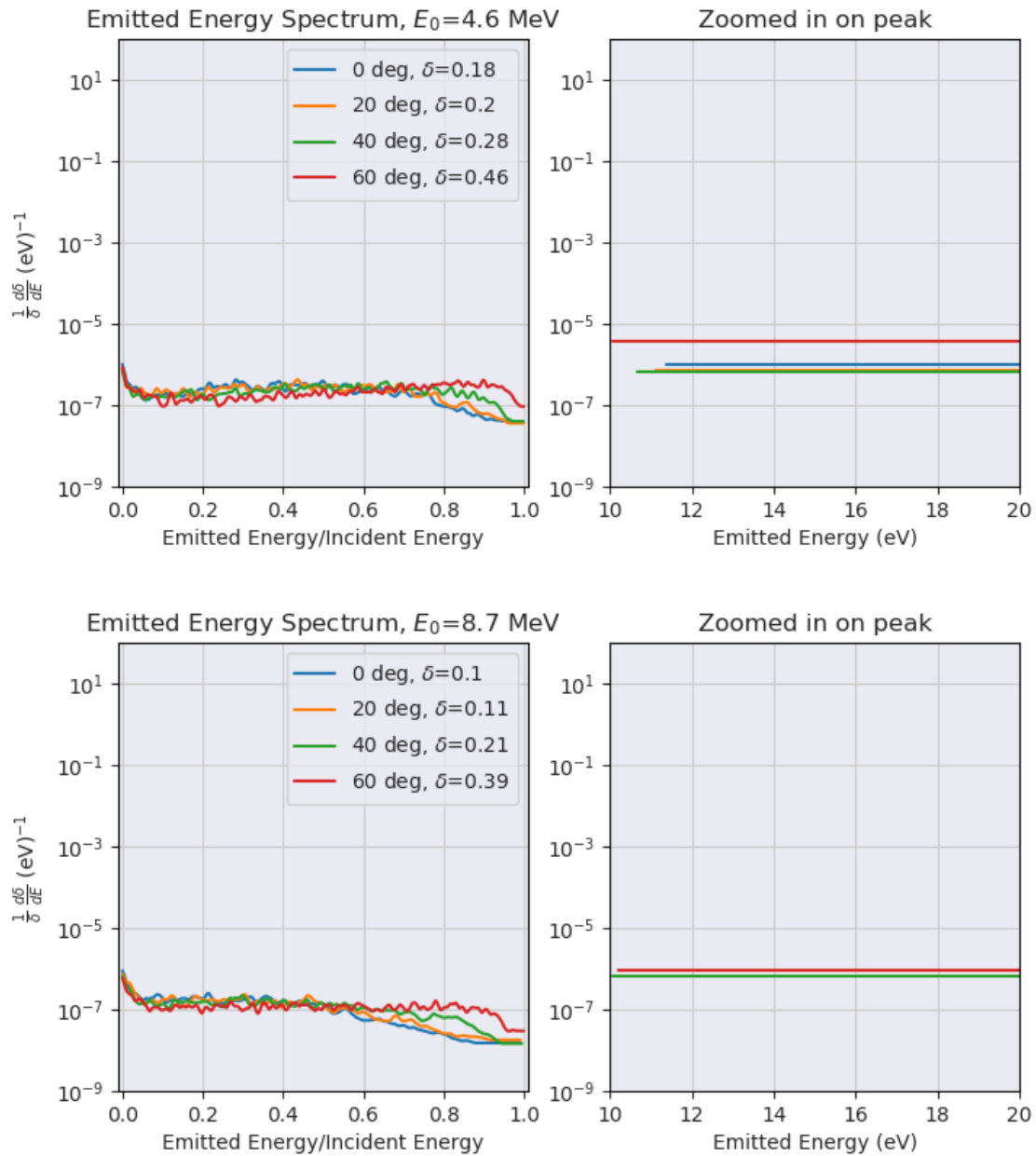


Figure B- 24: EES from GEANT4’s Livermore Models for Electrons Incident on Niobium with Energies E_0 of 4.6 MeV and 8.7 MeV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

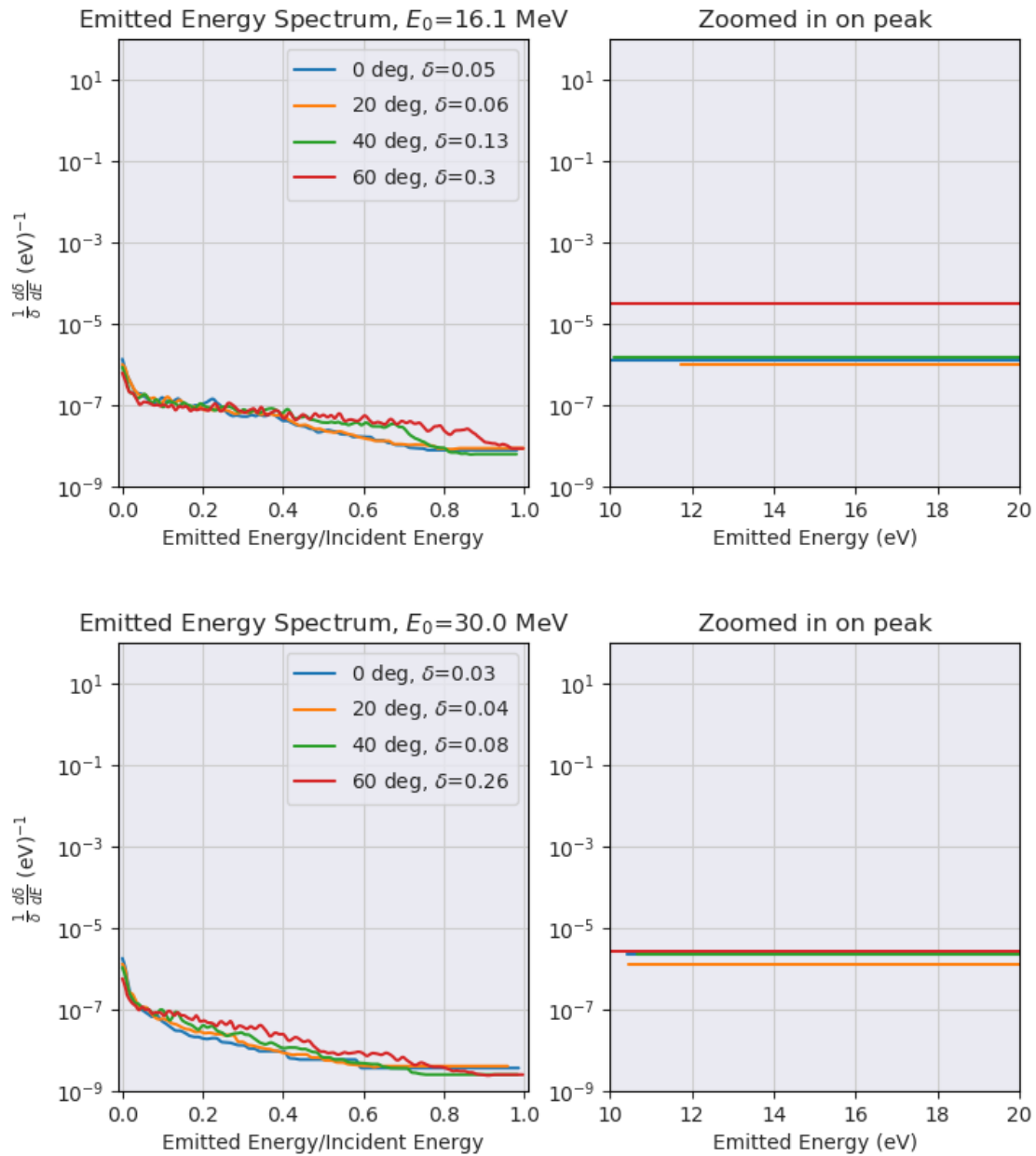


Figure B- 25: EES from GEANT4's Livermore Models for Electrons Incident on Niobium with Energies E_0 of 16.1 MeV and 30.0 MeV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

B.4 Graphite

In this section we provide the EES of graphite, as simulated using the built-in GEANT4 graphite material definition. The results are as shown in Figure B-26 through B-37, along with a zoomed view for emission energies between 10-20 eV.

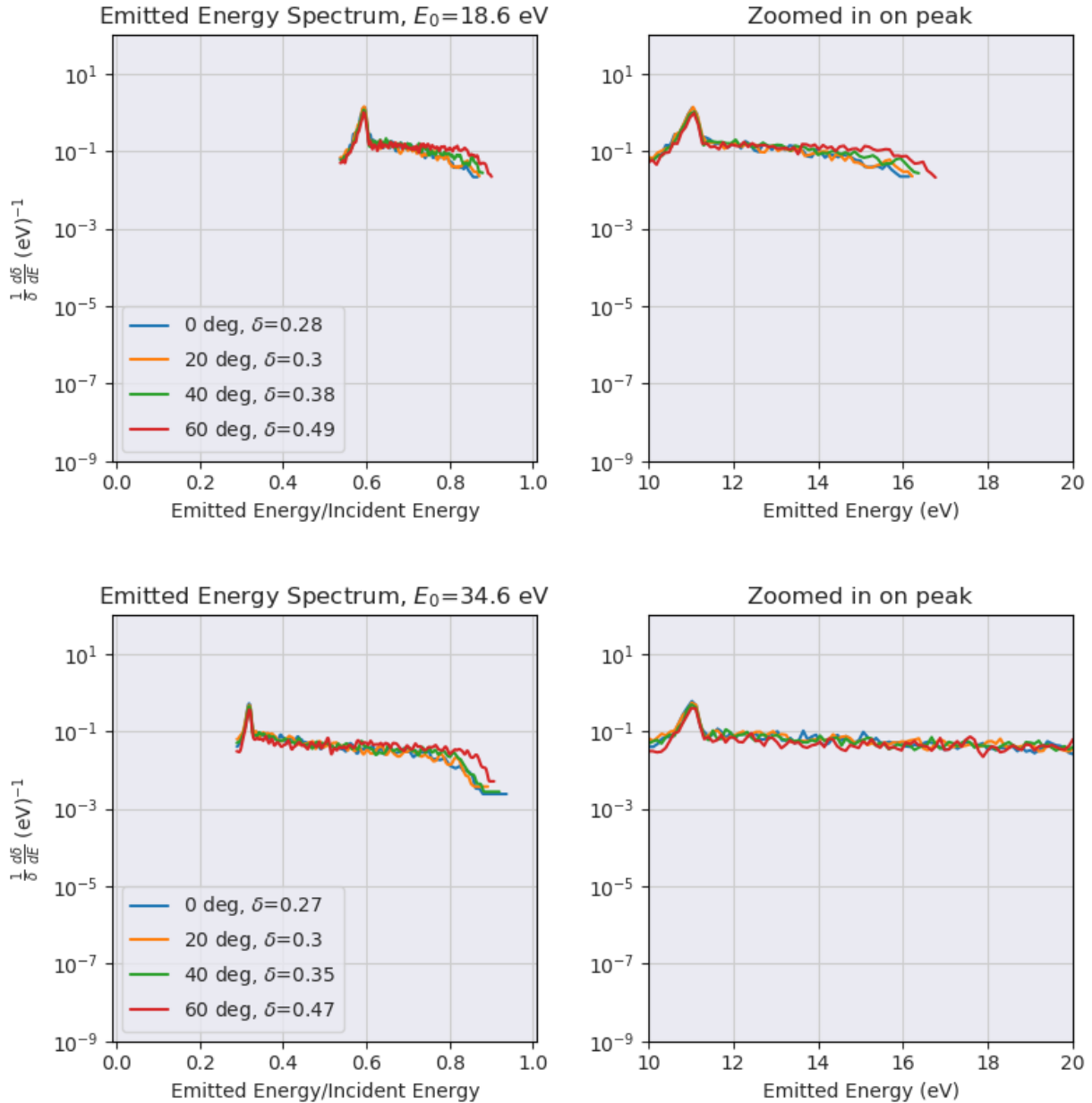


Figure B- 26: EES from GEANT4's Livermore Models for Electrons Incident on Graphite with Energies E_0 of 18.6 eV and 34.6 eV (left), and over the Emitted Energy Range 10-20 eV (right).

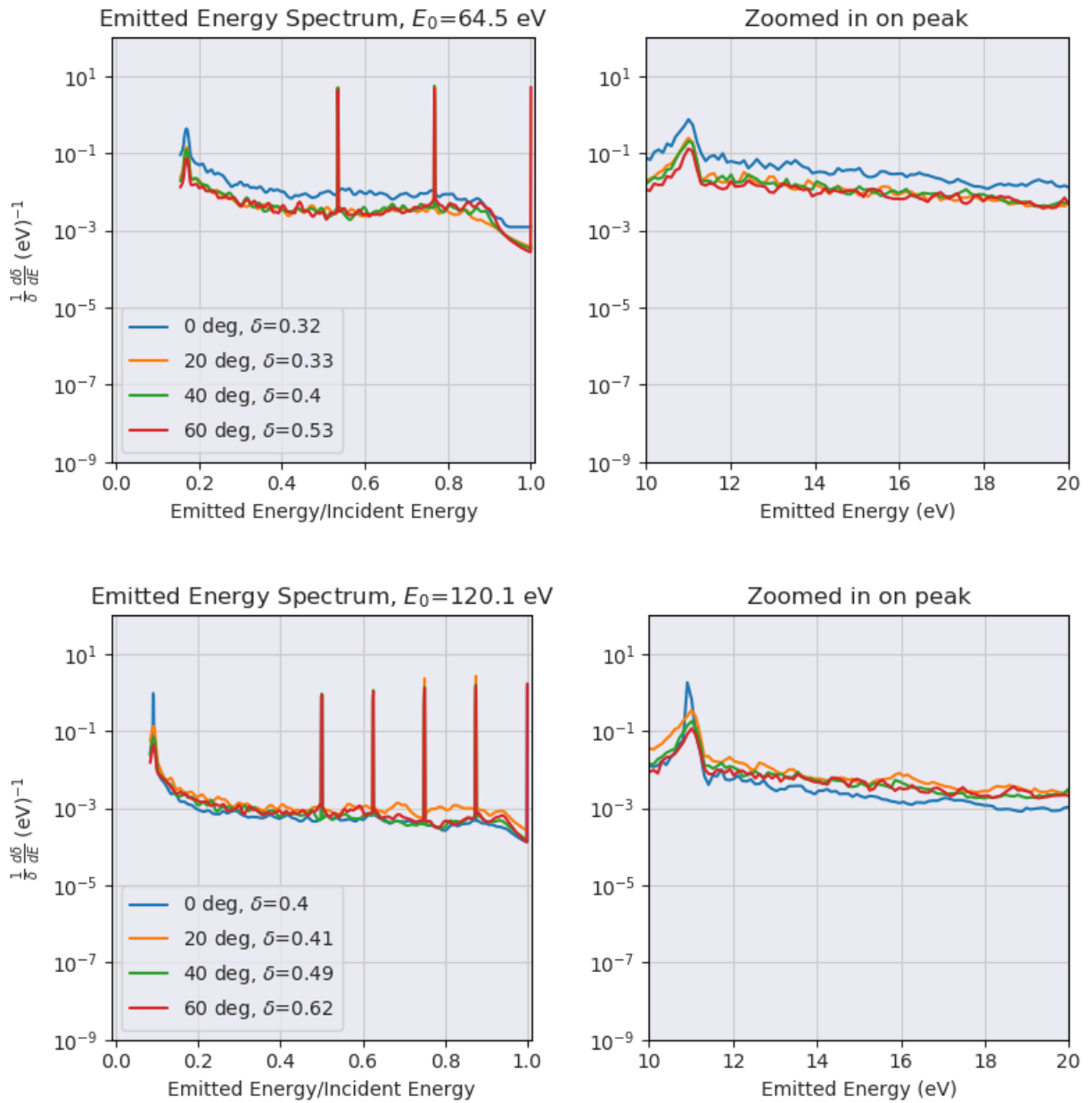


Figure B- 27: EES from GEANT4’s Livermore Models for Electrons Incident on Graphite with Energies E_0 of 64.5 eV and 120.1 eV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

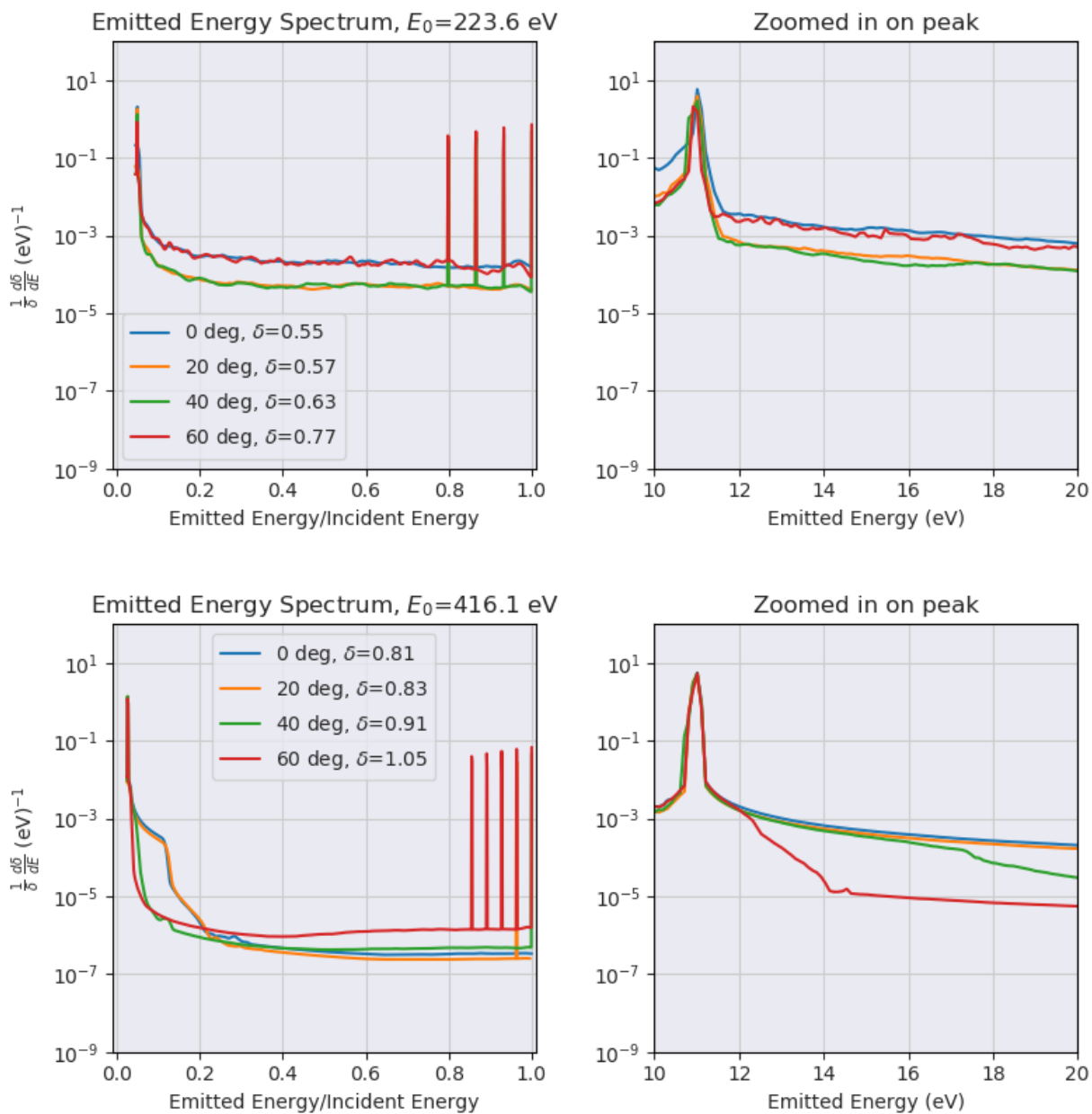


Figure B- 28: EES from GEANT4's Livermore Models for Electrons Incident on Graphite with Energies E_0 of 223.6 eV and 416.1 eV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

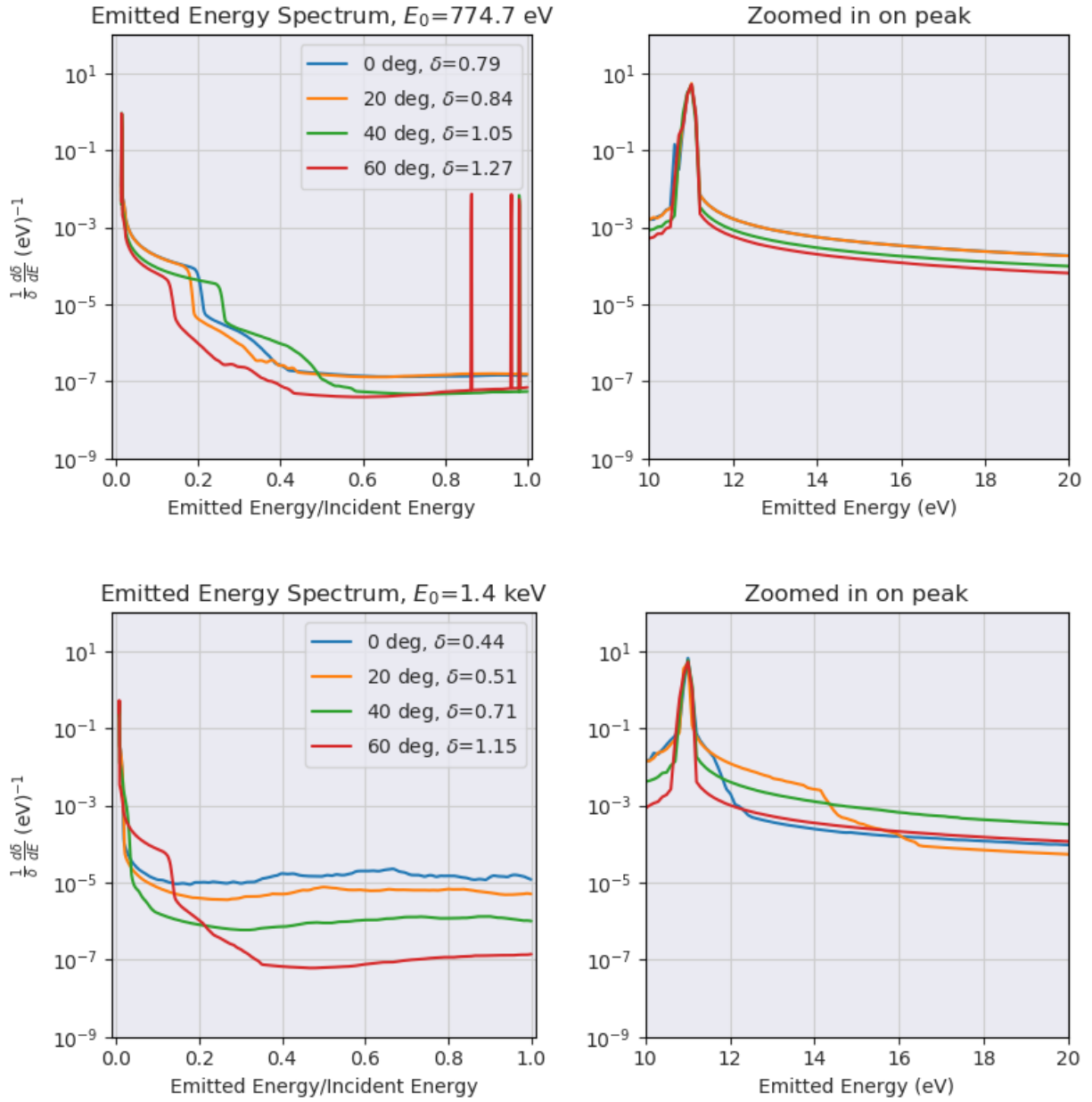


Figure B- 29: EES from GEANT4's Livermore Models for Electrons Incident on Graphite with Energies E_0 of 774.7 eV and 1.4 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

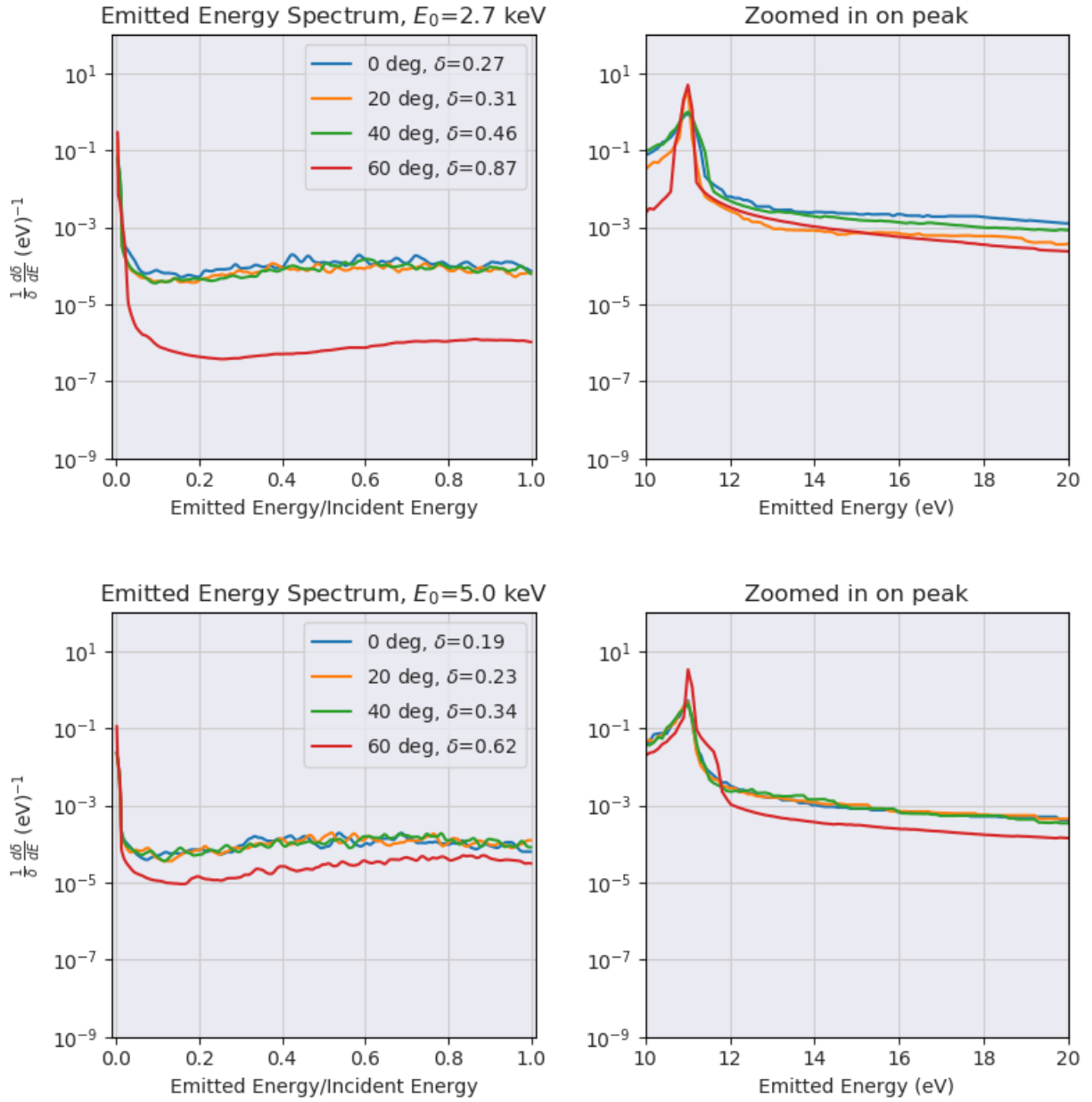


Figure B- 30: EES from GEANT4’s Livermore Models for Electrons Incident on Graphite with Energies E_0 of 2.7 keV and 5.0 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

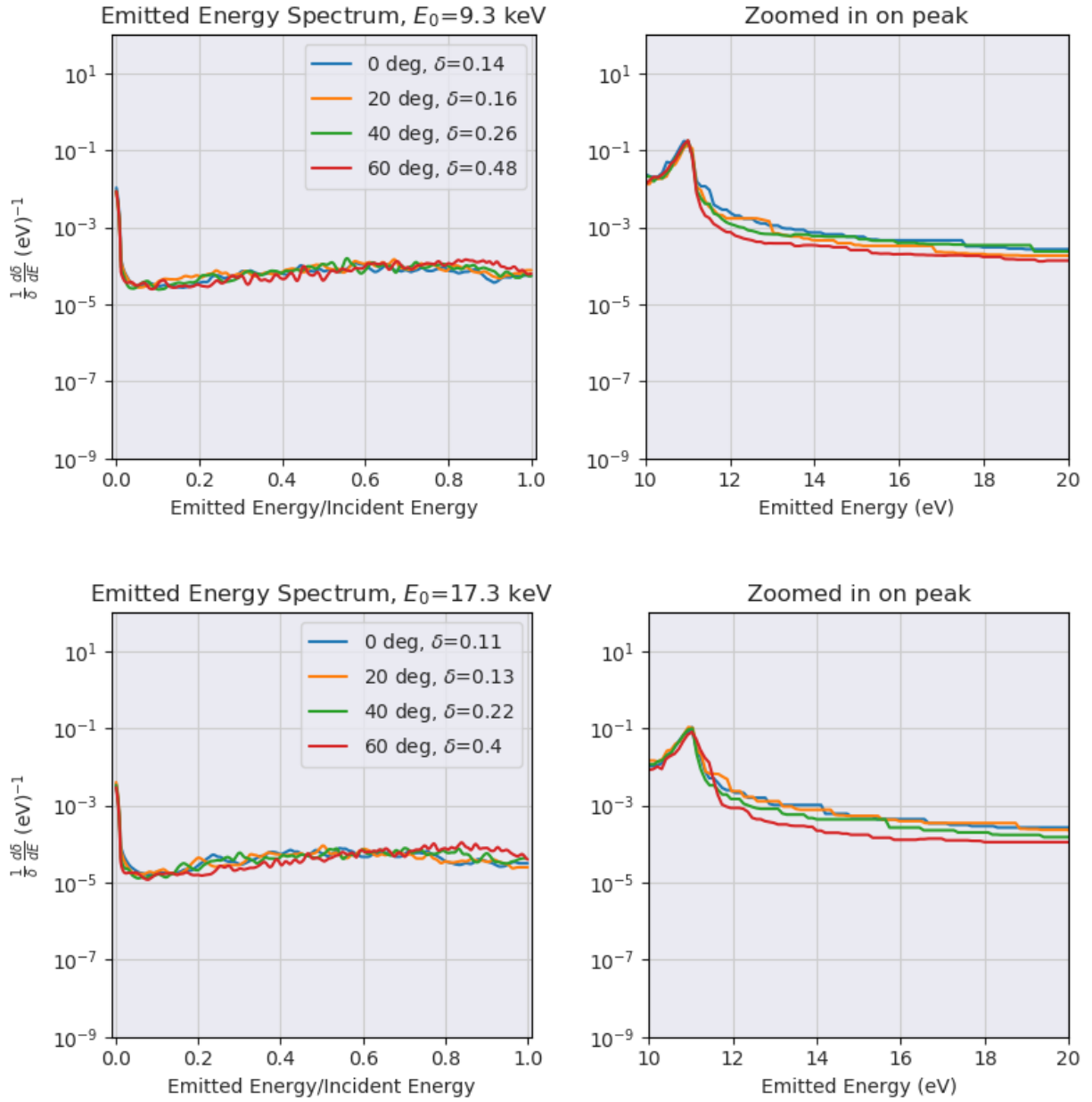


Figure B- 31: EES from GEANT4’s Livermore Models for Electrons Incident on Graphite with Energies E_0 of 9.3 keV and 17.3 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

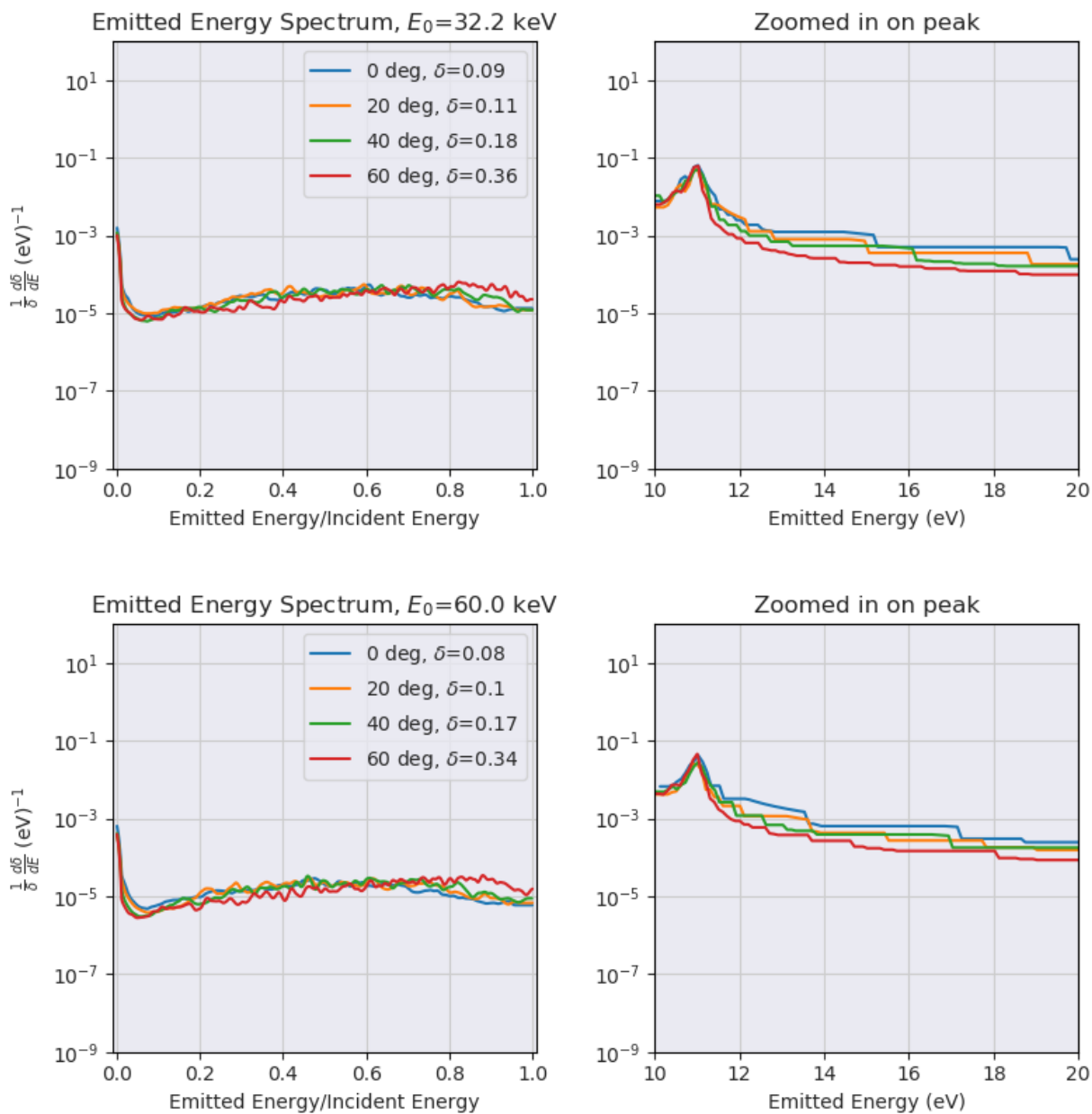


Figure B- 32: EES from GEANT4’s Livermore Models for Electrons Incident on Graphite with Energies E_0 of 32.2 keV and 60.0 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

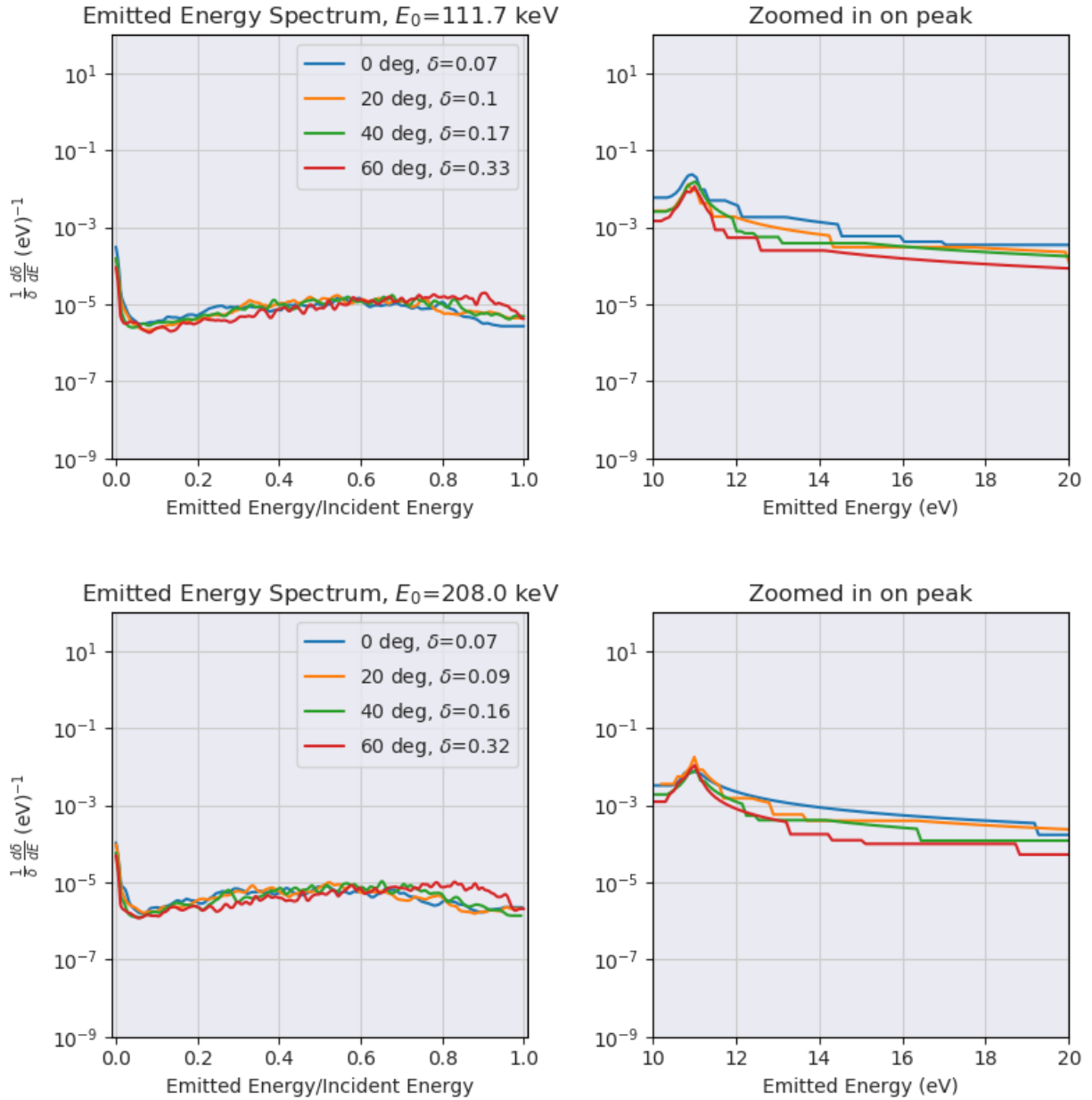


Figure B- 33: EES from GEANT4's Livermore Models for Electrons Incident on Graphite with Energies E_0 of 111.7 keV and 208.0 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

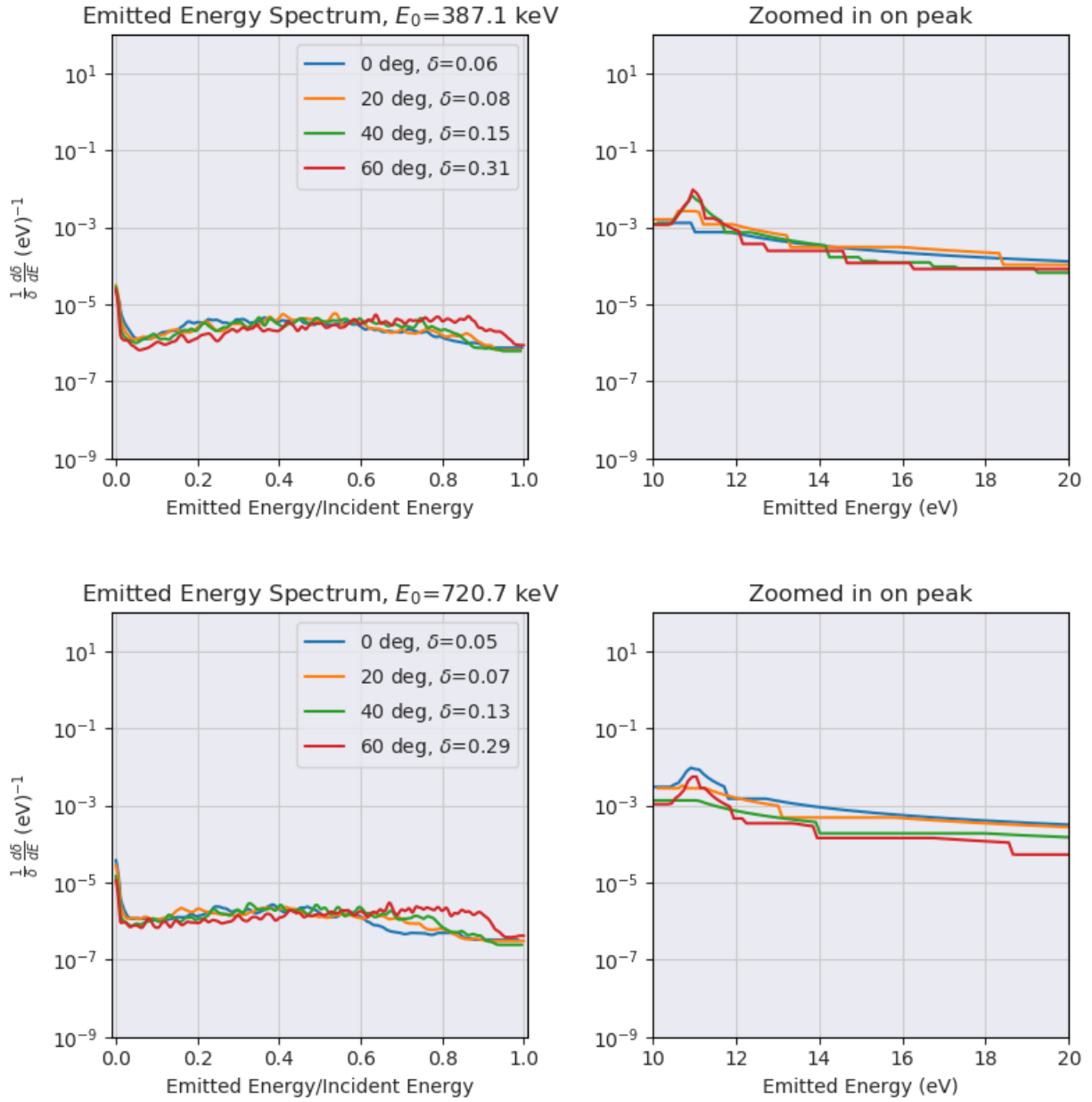


Figure B- 34: EES from GEANT4’s Livermore Models for Electrons Incident on Graphite with Energies E_0 of 387.1 keV and 720.7 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

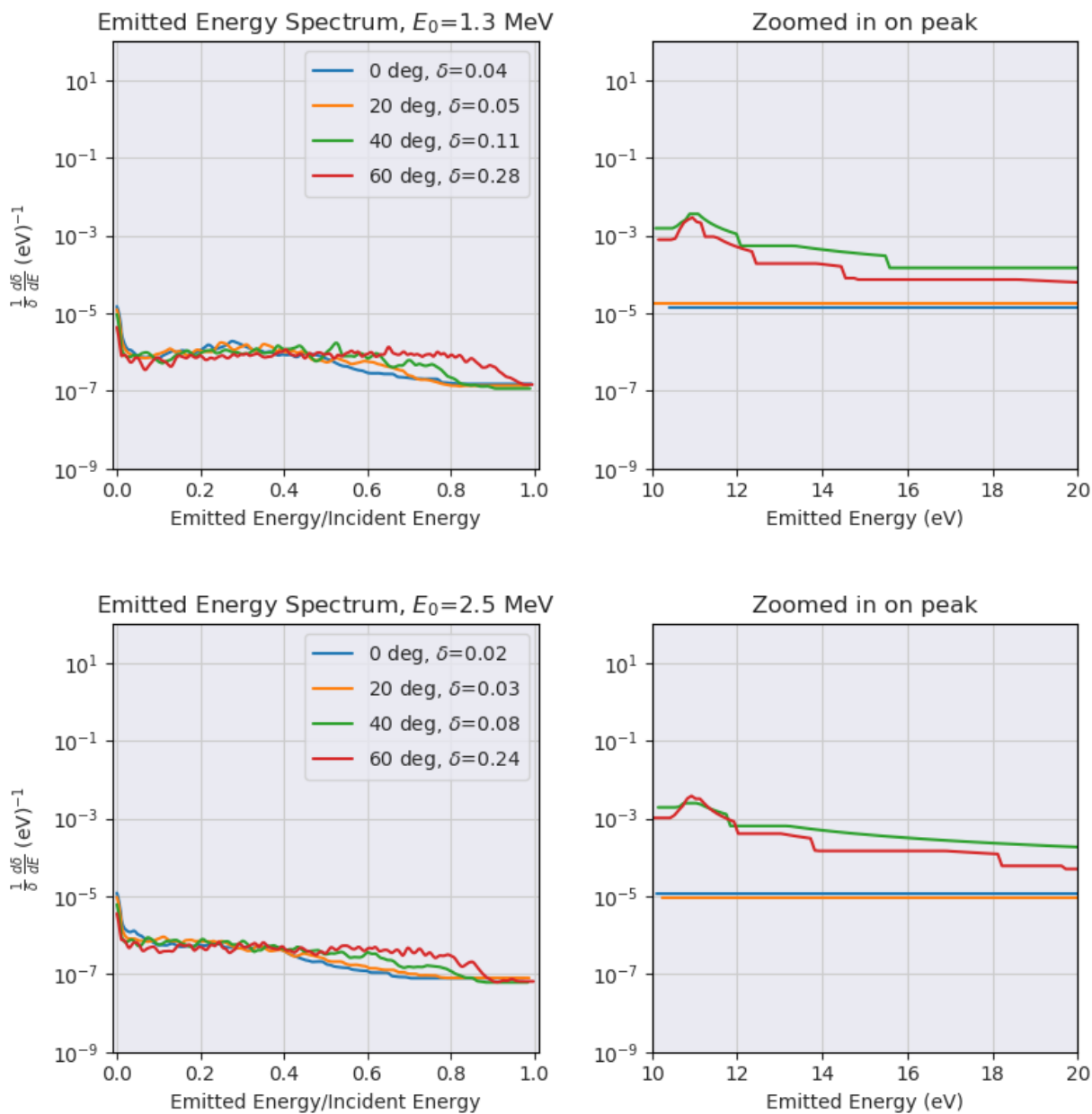


Figure B- 35: EES from GEANT4's Livermore Models for Electrons Incident on Graphite with Energies E_0 of 1.3 MeV and 2.5 MeV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

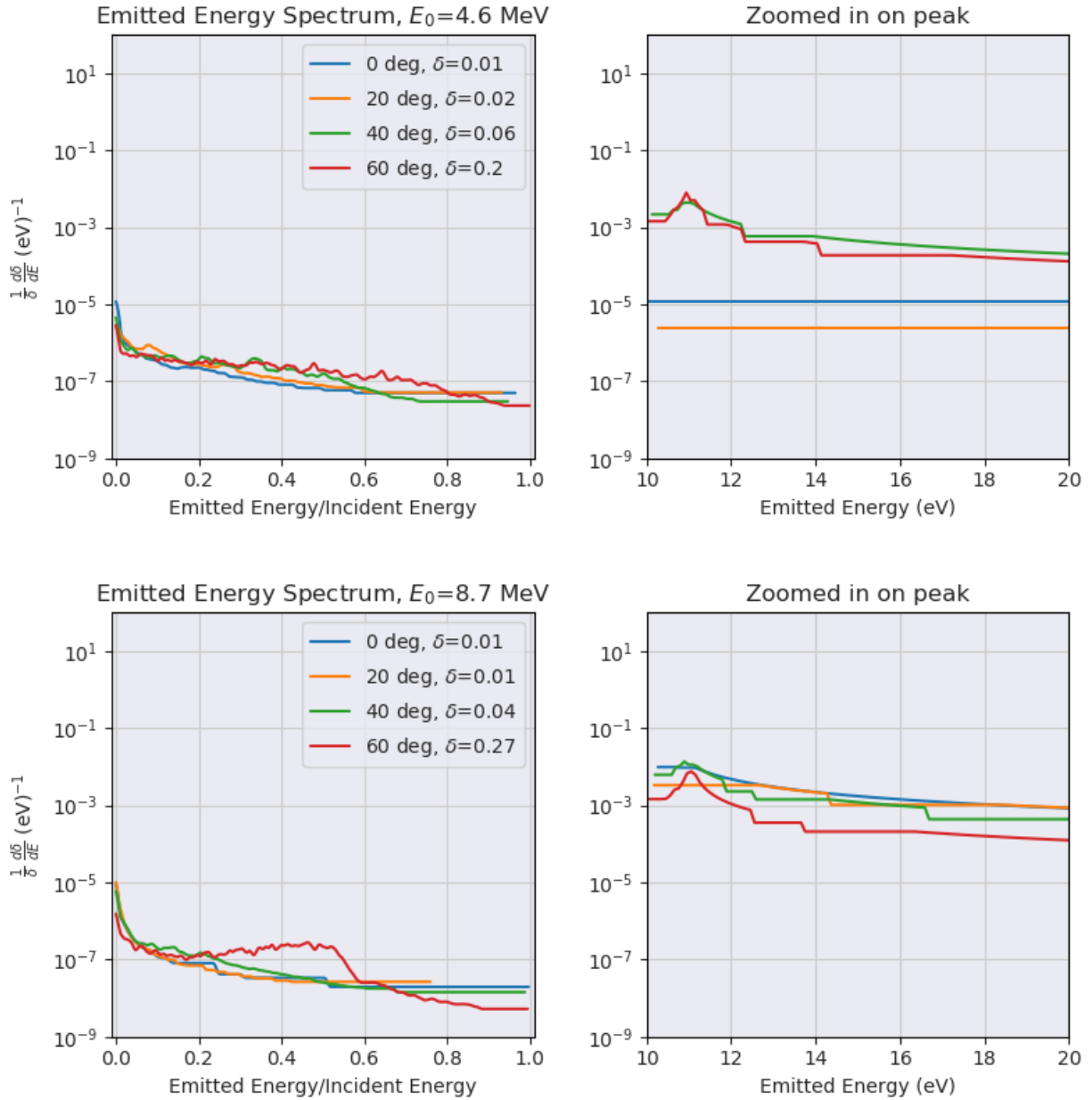


Figure B- 36: EES from GEANT4's Livermore Models for Electrons Incident on Graphite with Energies E_0 of 4.6 MeV and 8.7 MeV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

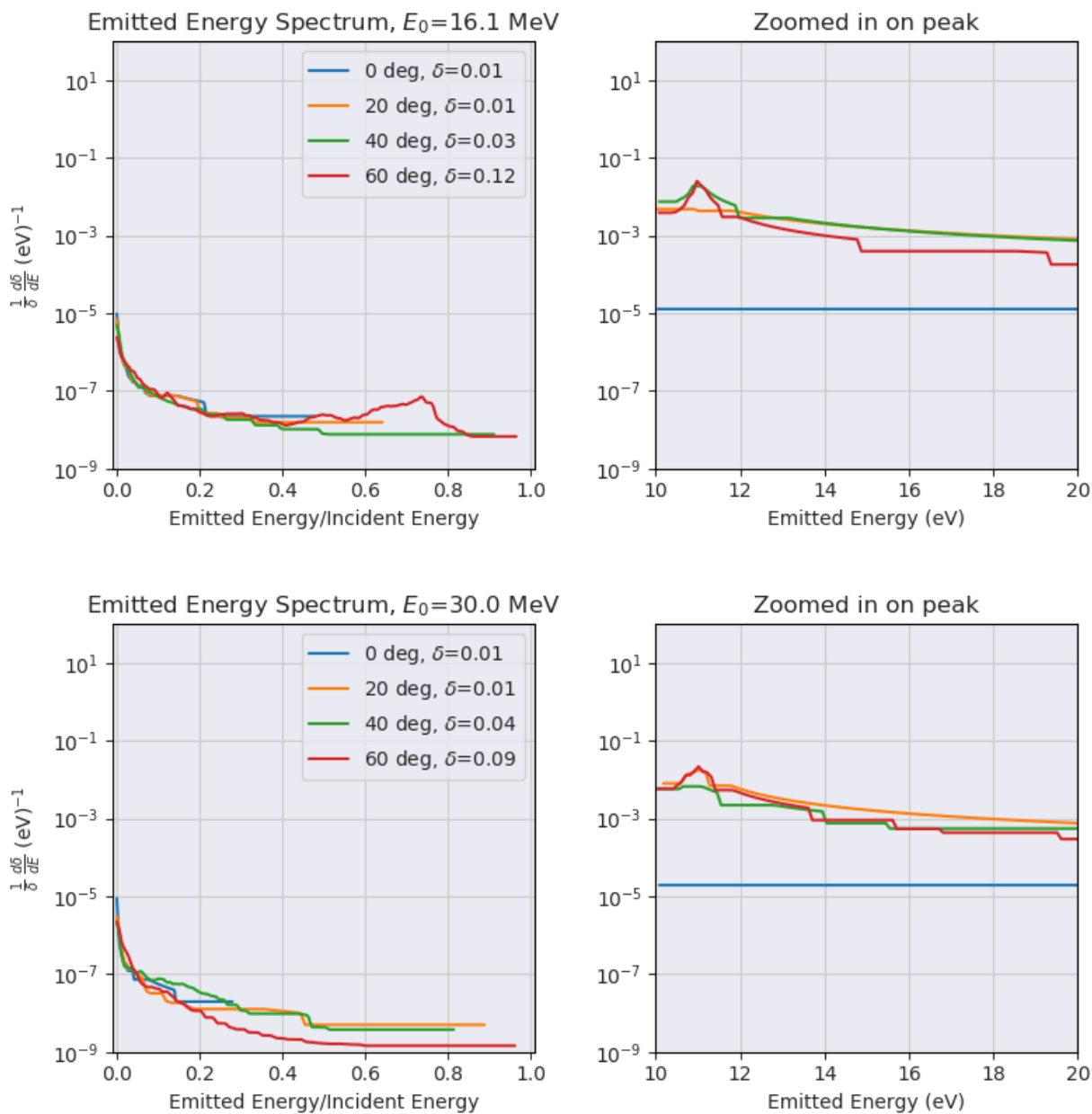


Figure B- 37: EES from GEANT4's Livermore Models for Electrons Incident on Graphite with Energies E_0 of 16.1 MeV and 30.0 MeV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

B.5 Aluminum Oxide

In this section we provide the EES of aluminum oxide (alumina), as simulated using the built-in GEANT4 aluminum oxide (alumina) material definition. The results are as shown in Figure B-38 through Figure B-49, along with a zoomed view for emission energies between 10-20 eV.

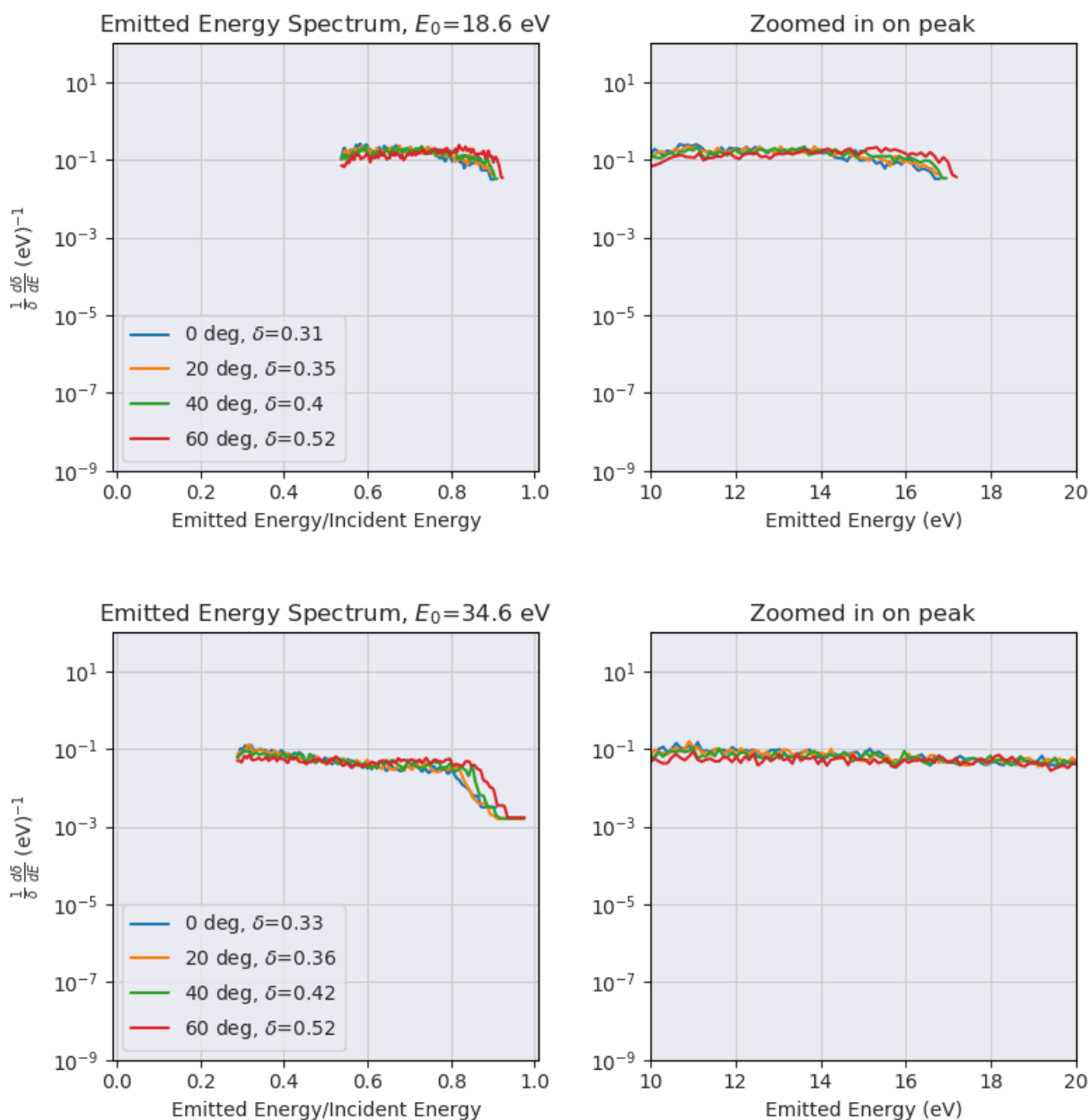


Figure B- 38: EES from GEANT4’s Livermore Models for Electrons Incident on Aluminum Oxide with Energies E_0 of 18.6 eV and 34.6 eV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

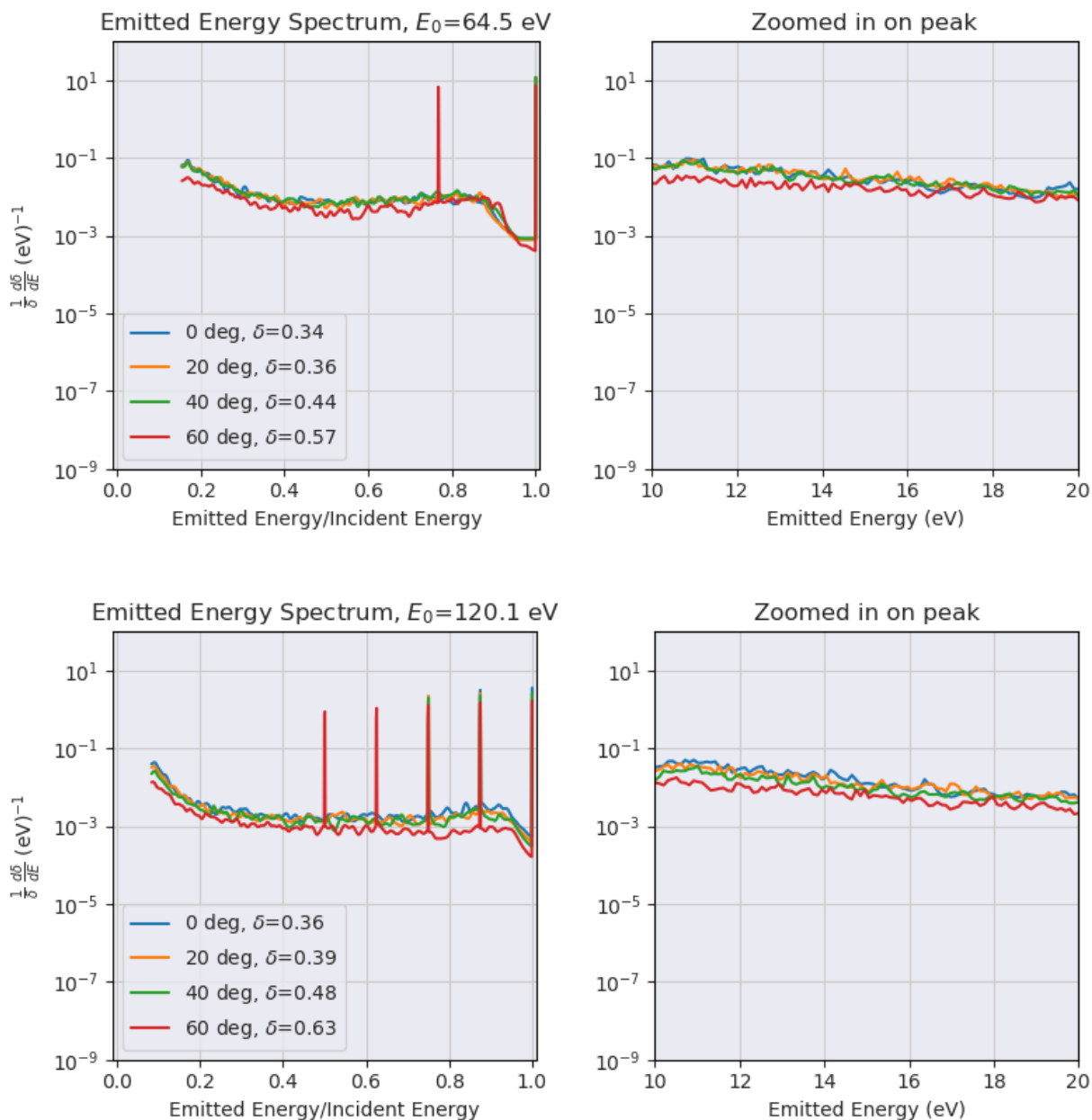


Figure B- 39: EES from GEANT4's Livermore Models for Electrons Incident on Aluminum Oxide with Energies E_0 of 64.5 eV and 120.1 eV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

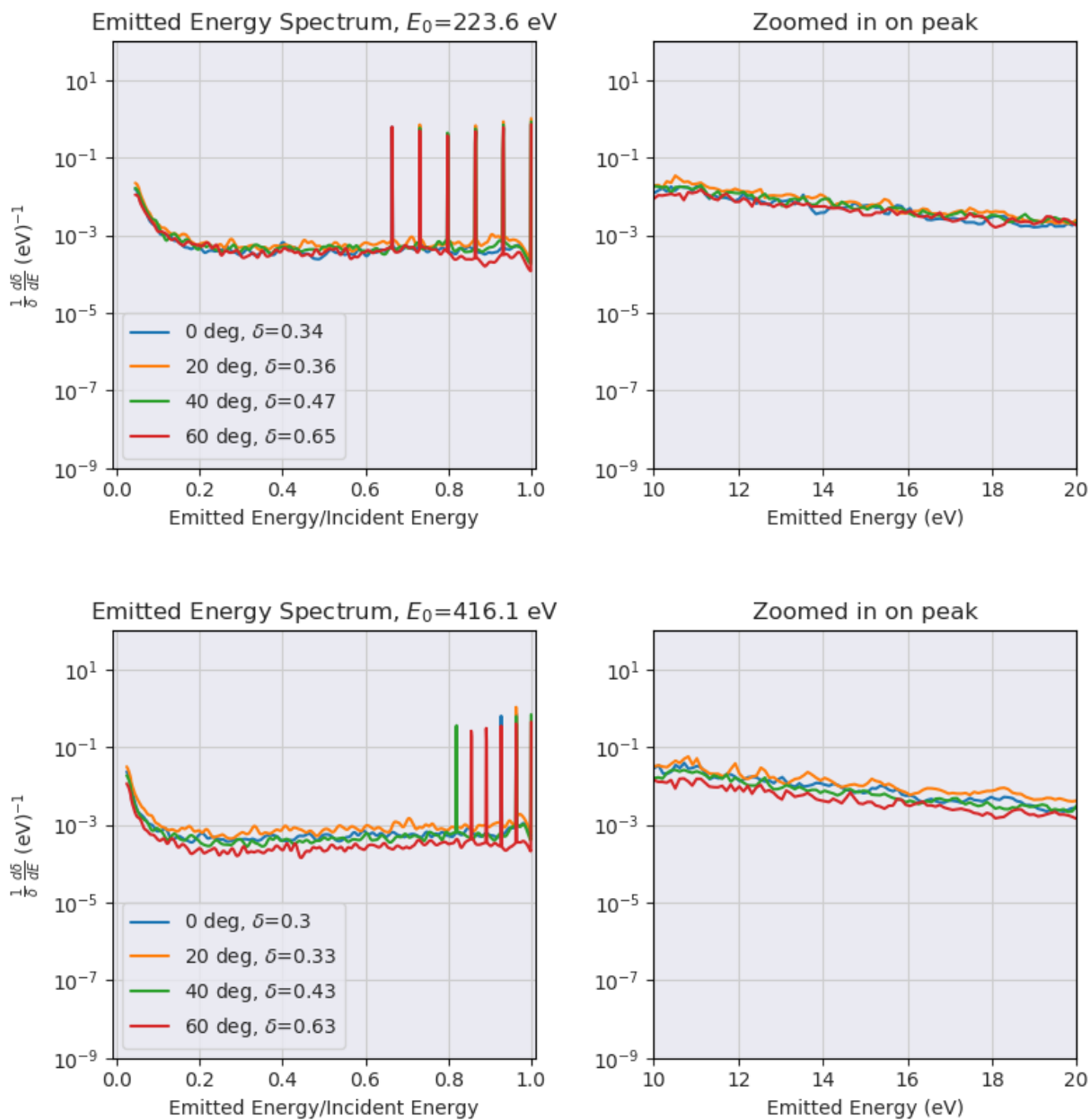


Figure B- 40: EES from GEANT4's Livermore Models for Electrons Incident on Aluminum Oxide with Energies E_0 of 223.6 eV and 416.1 eV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

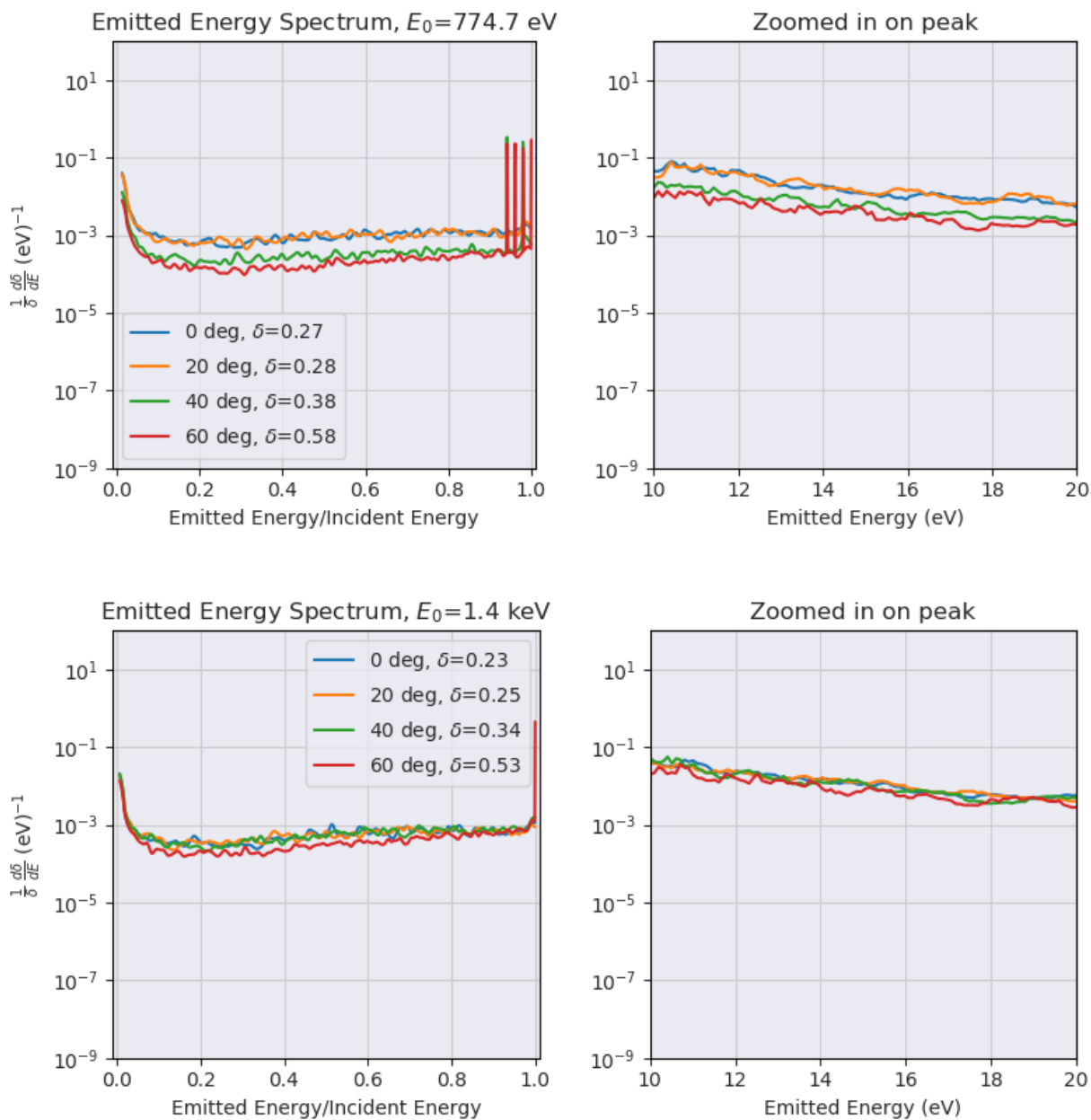


Figure B- 41: EES from GEANT4’s Livermore Models for Electrons Incident on Aluminum Oxide with Energies E_0 of 774.7 eV and 1.4 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

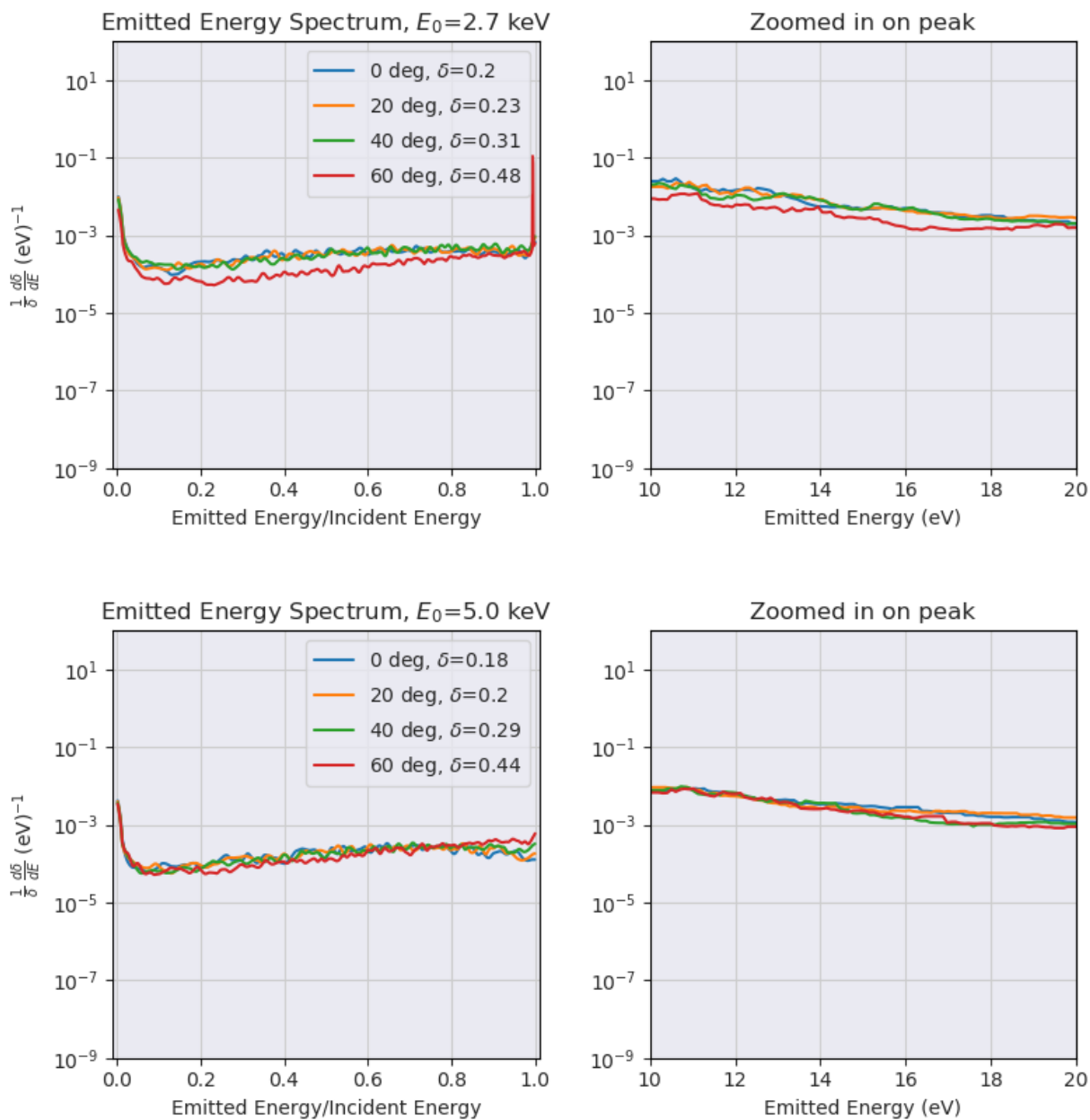


Figure B- 42: EES from GEANT4's Livermore Models for Electrons Incident on Aluminum Oxide with Energies E_0 of 2.7 keV and 5.0 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

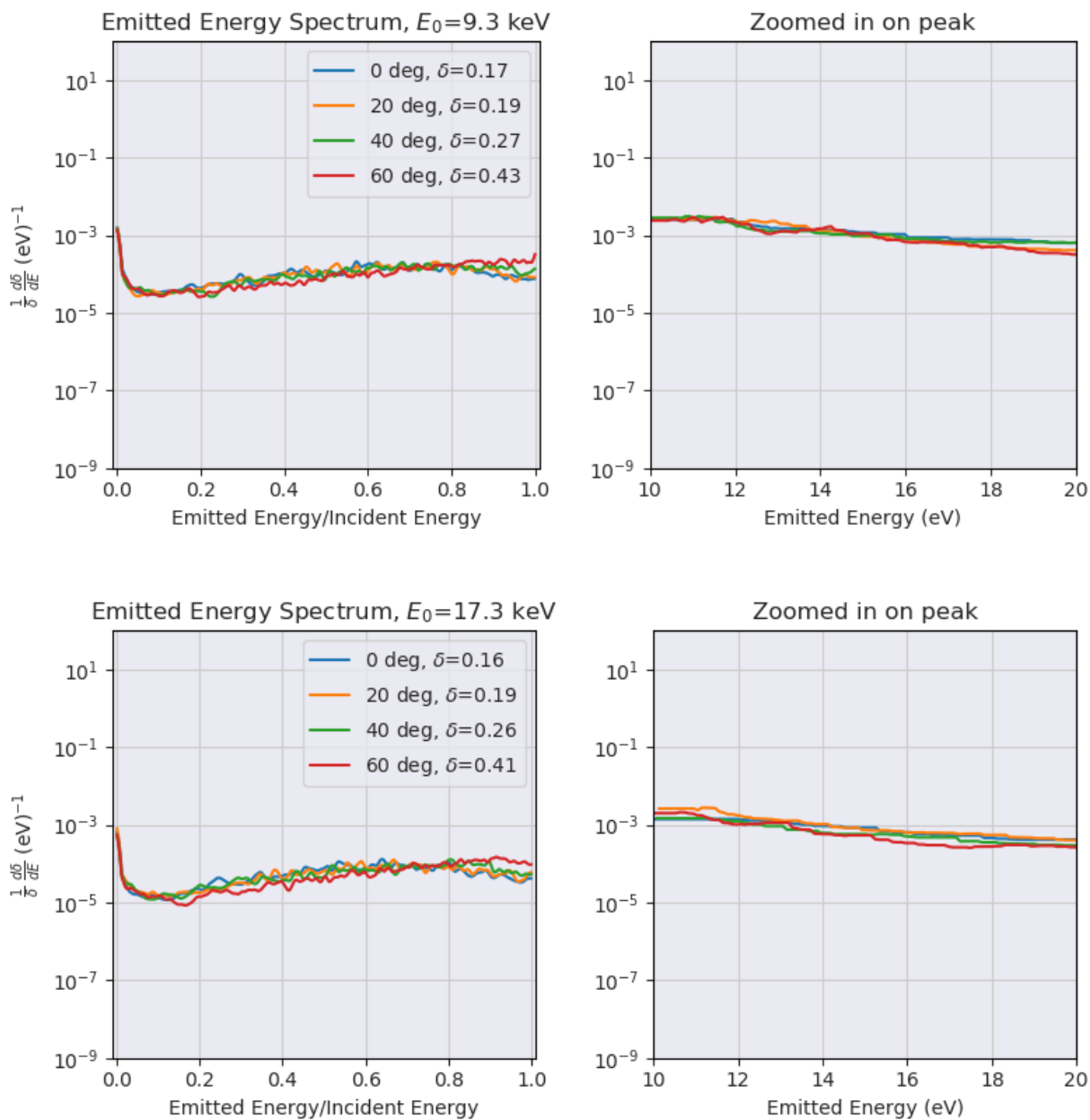


Figure B- 43: EES from GEANT4's Livermore Models for Electrons Incident on Aluminum Oxide with Energies E_0 of 9.3 keV and 17.3 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

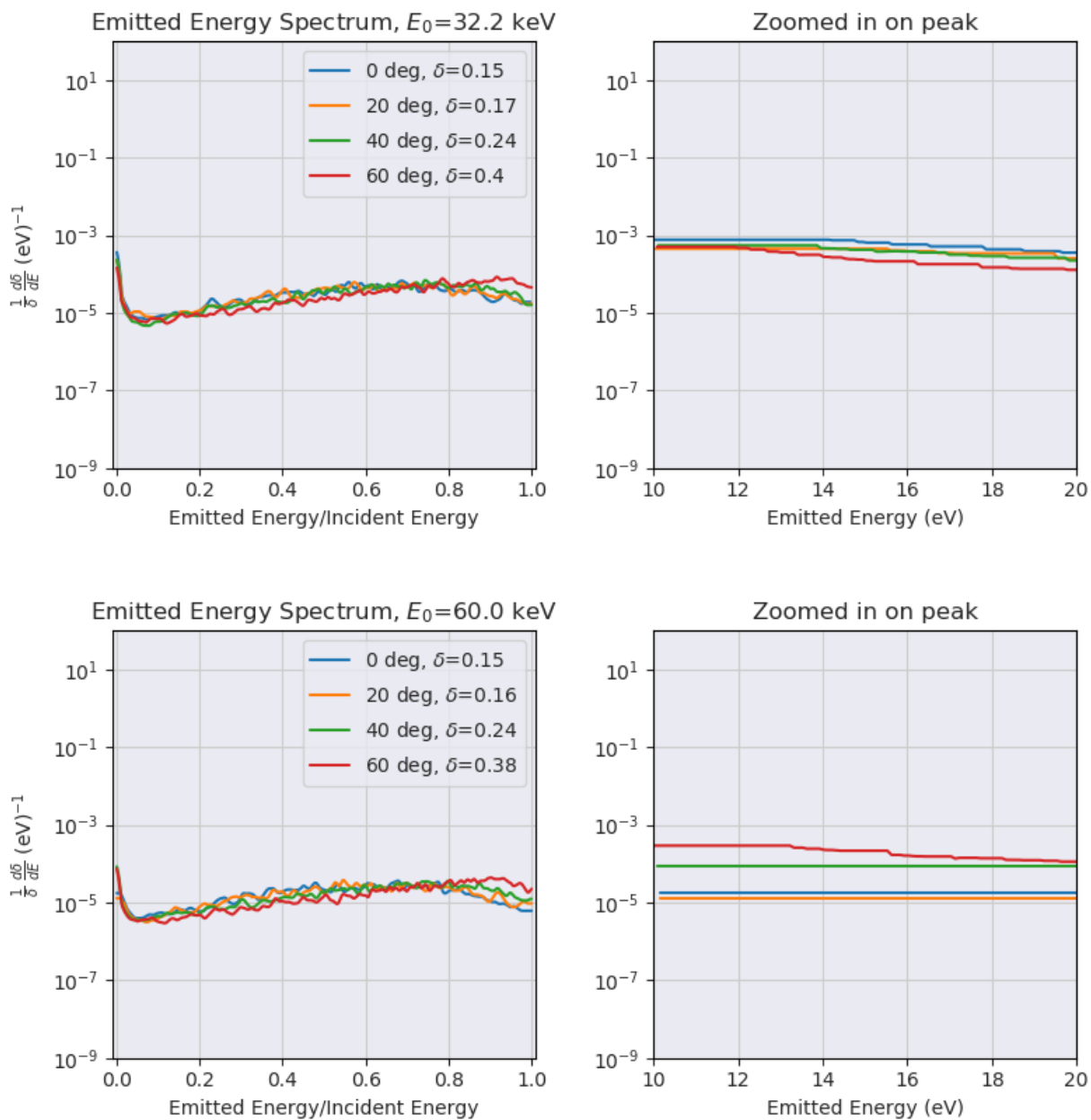


Figure B- 44: EES from GEANT4's Livermore Models for Electrons Incident on Aluminum Oxide with Energies E_0 of 32.2 keV and 60.0 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

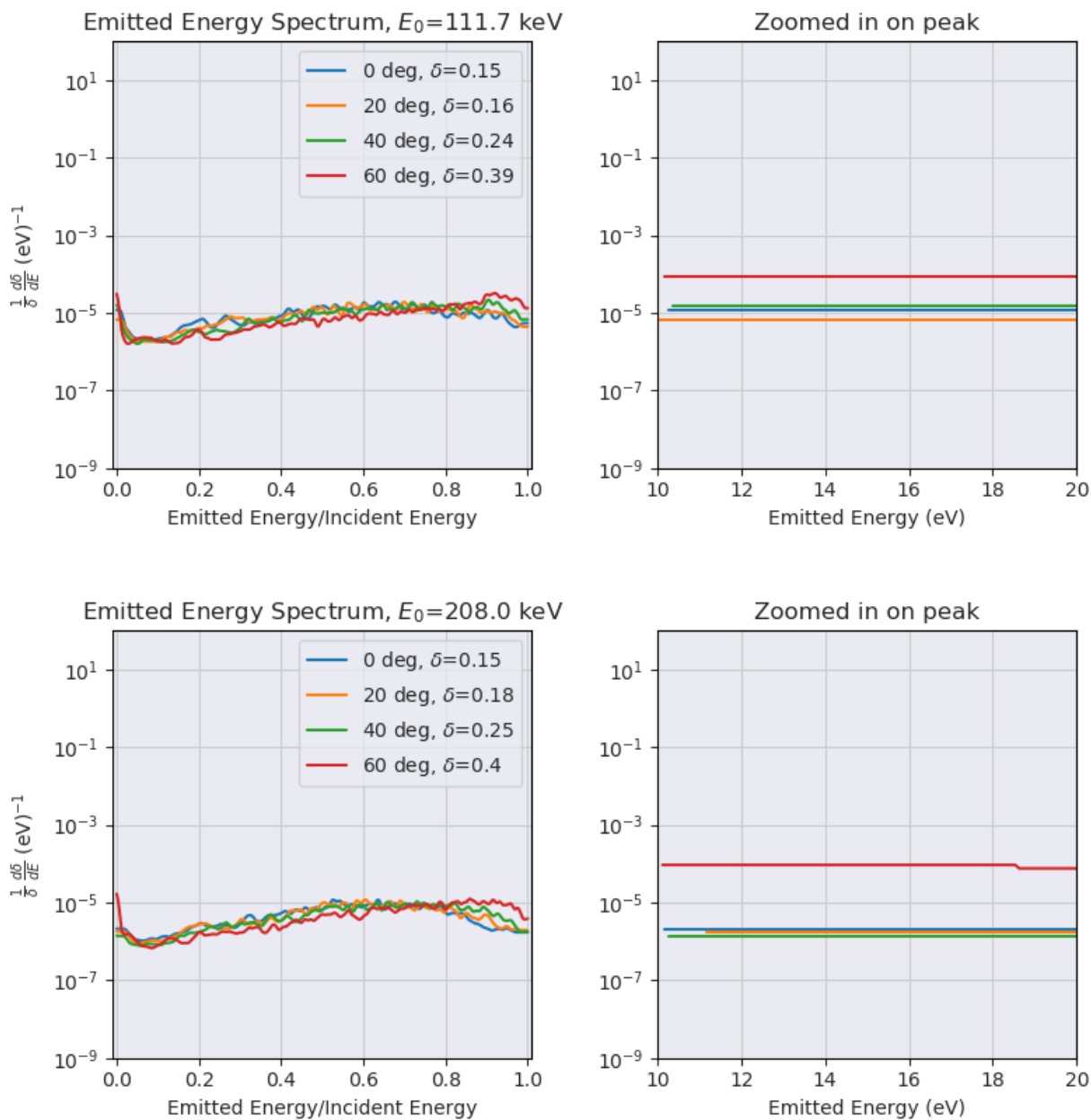


Figure B- 45: EES from GEANT4's Livermore Models for Electrons Incident on Aluminum Oxide with Energies E_0 of 111.7 keV and 208.0 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

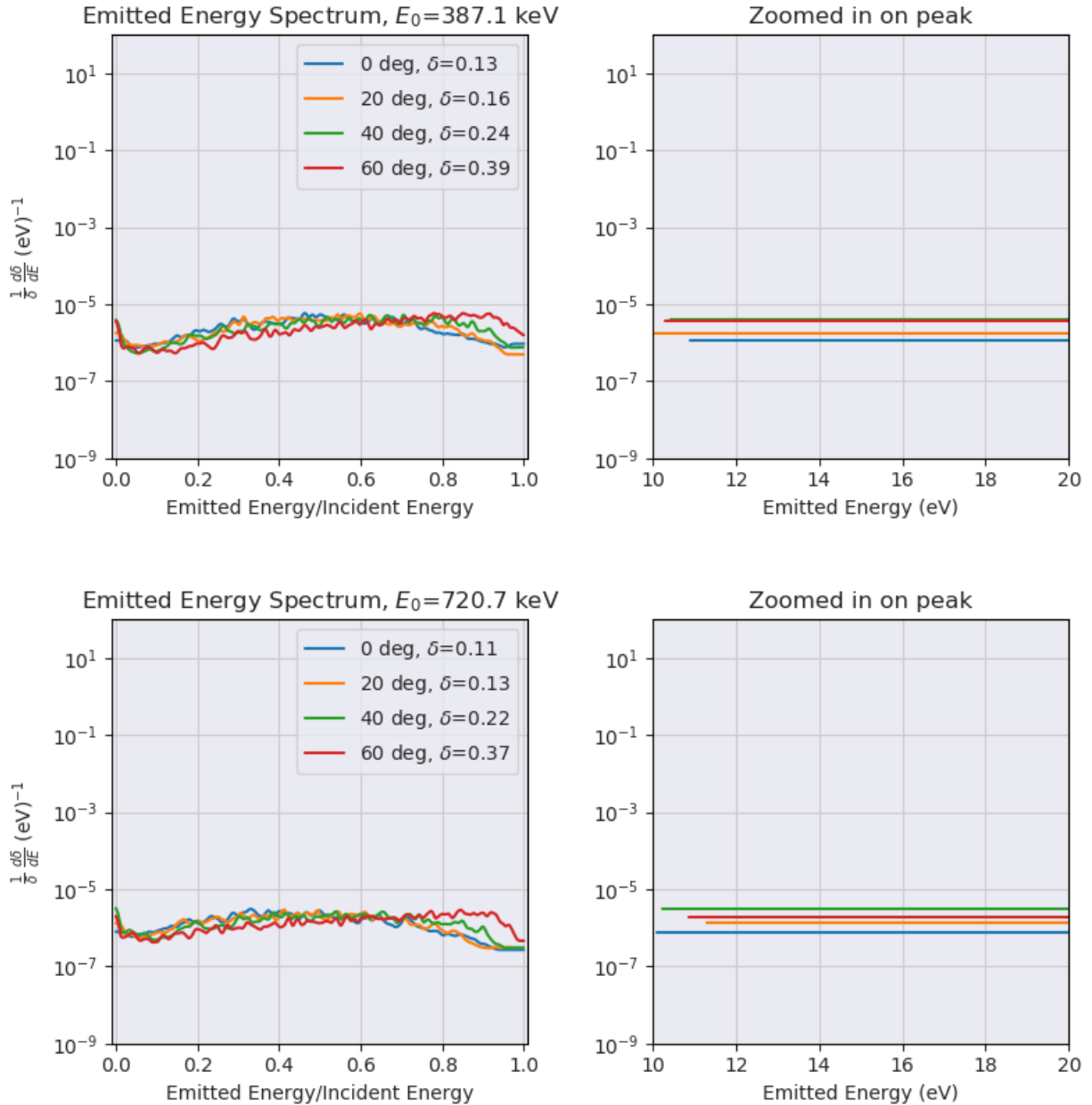


Figure B- 46: EES from GEANT4's Livermore Models for Electrons Incident on Aluminum Oxide with Energies E_0 of 387.1 keV and 720.7 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

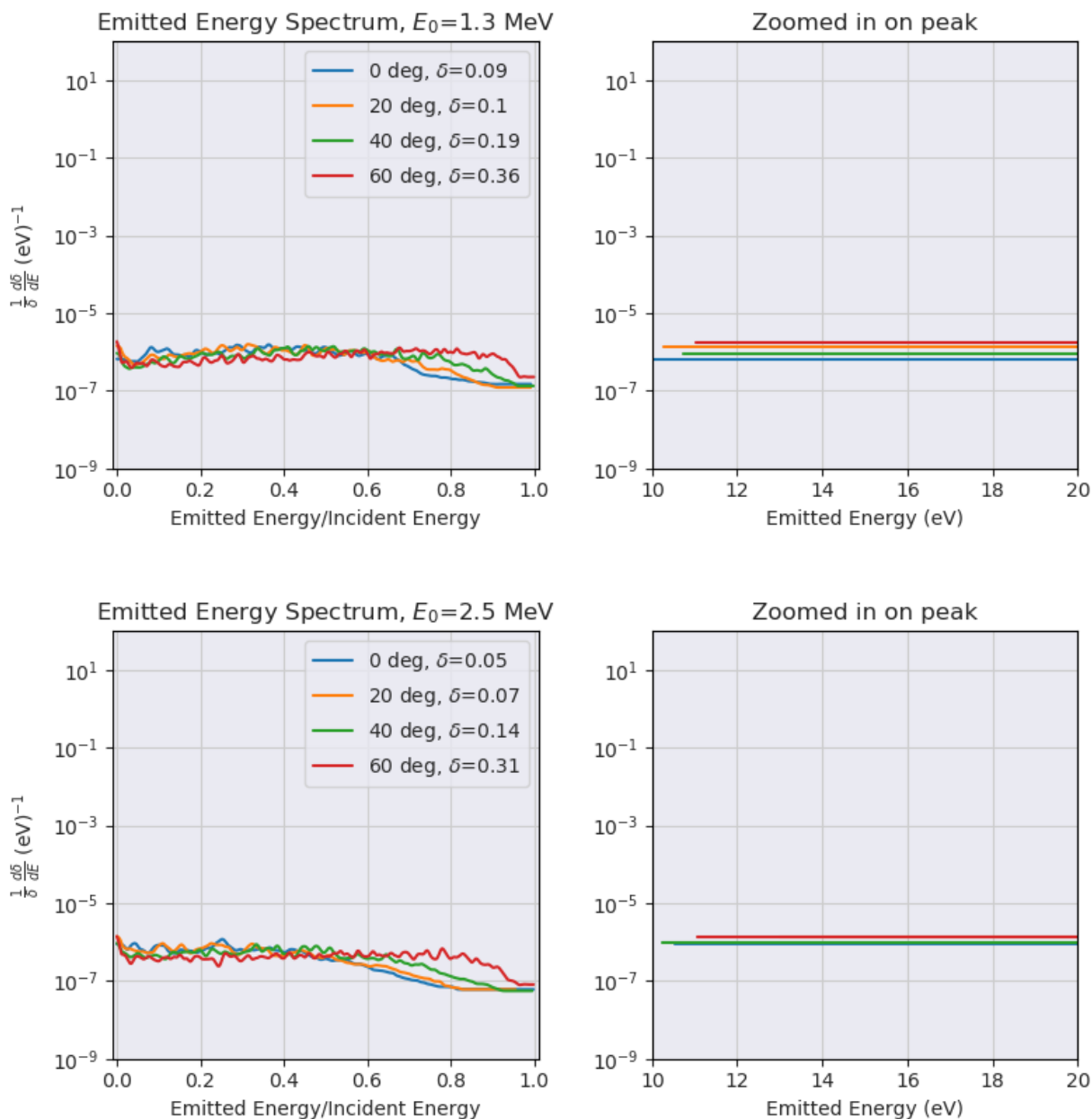


Figure B- 47 : EES from GEANT4's Livermore Models for Electrons Incident on Aluminum Oxide with Energies E_0 of 1.3 MeV and 2.5 MeV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

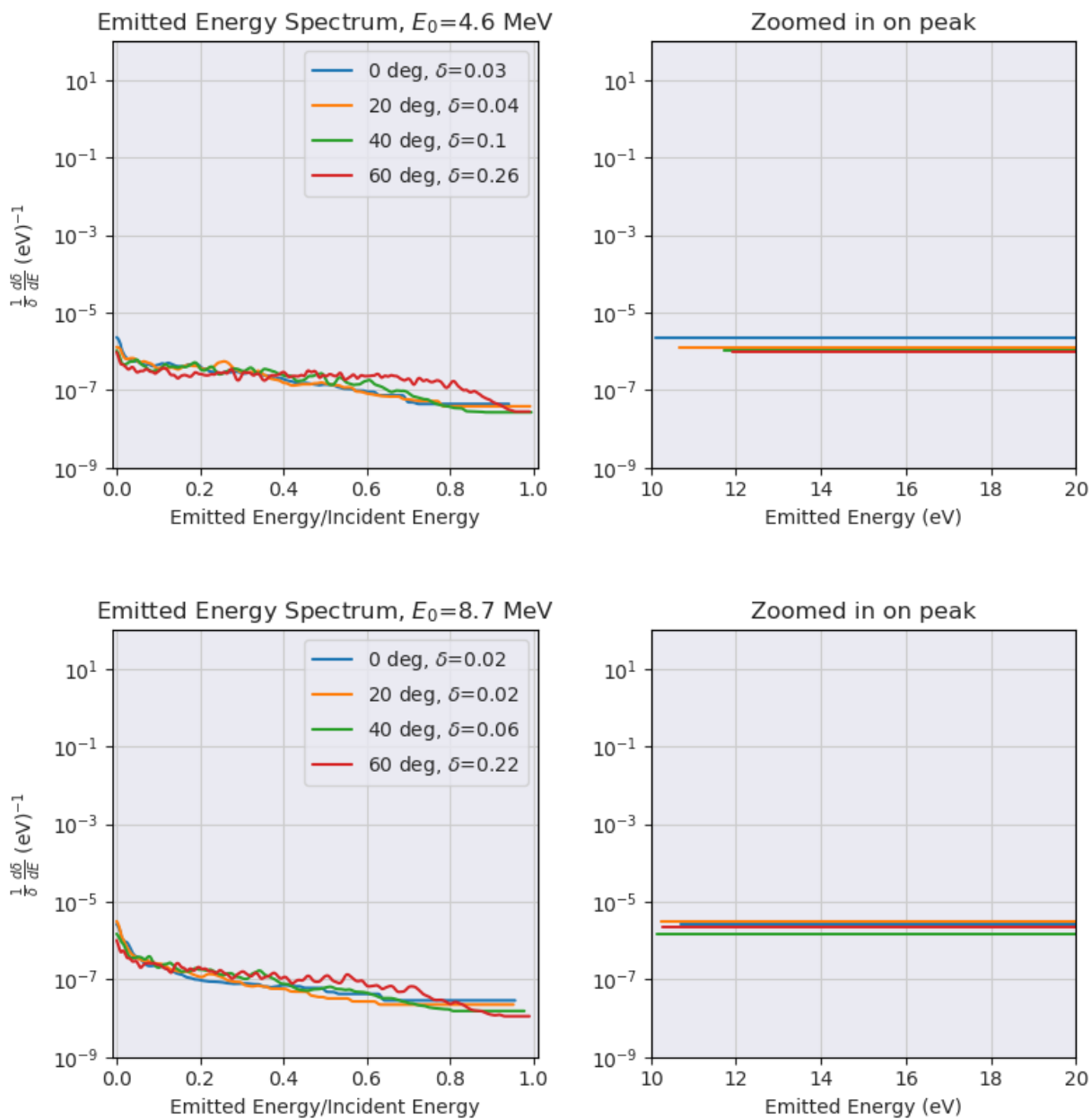


Figure B- 48: EES from GEANT4's Livermore Models for Electrons Incident on Aluminum Oxide with Energies E_0 of 4.6 MeV and 8.7 MeV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

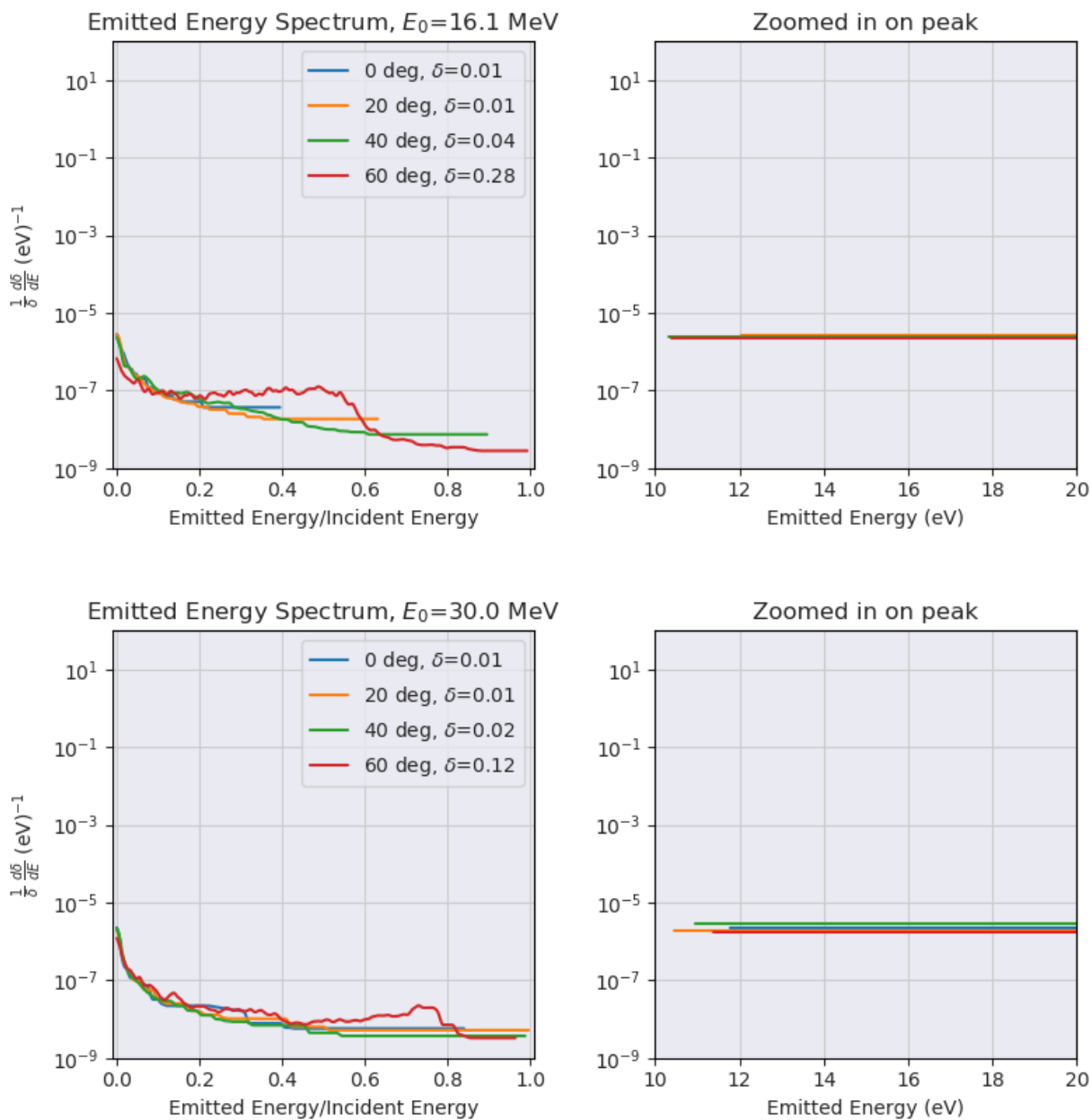


Figure B- 49: EES from GEANT4's Livermore Models for Electrons Incident on Aluminum Oxide with Energies E_0 of 16.1 MeV and 30.0 MeV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

B.6 Beryllium Oxide

In this section we provide the EES of beryllium oxide (BeO), as simulated using the built-in GEANT4 beryllium oxide material definition. The results are as shown in Figure B-50 through B-61, along with a zoomed view for emission energies between 10-20 eV.

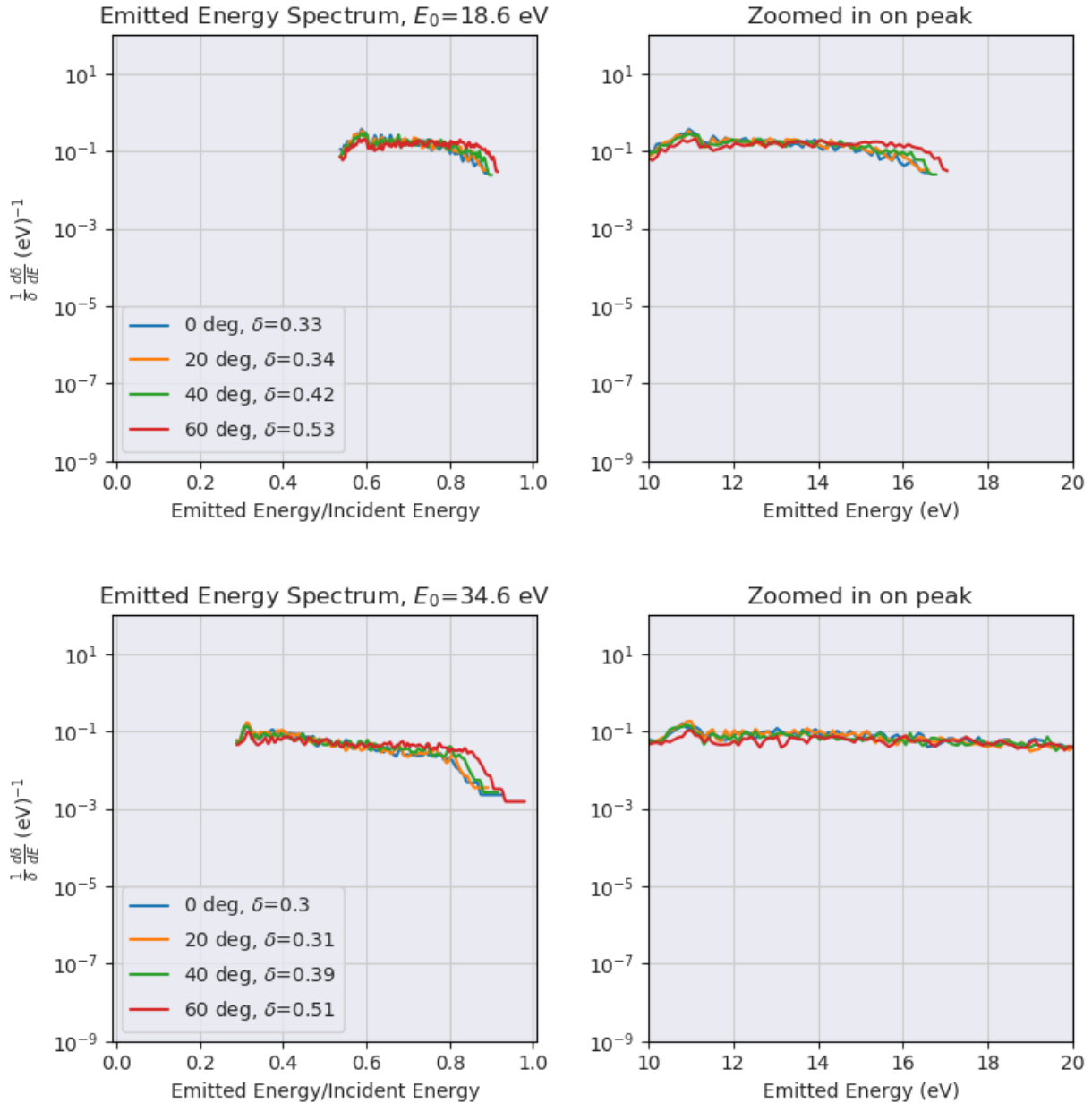


Figure B- 50: EES from GEANT4's Livermore Models for Electrons Incident on Beryllium Oxide with Energies E_0 of 18.6 eV and 34.6 eV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

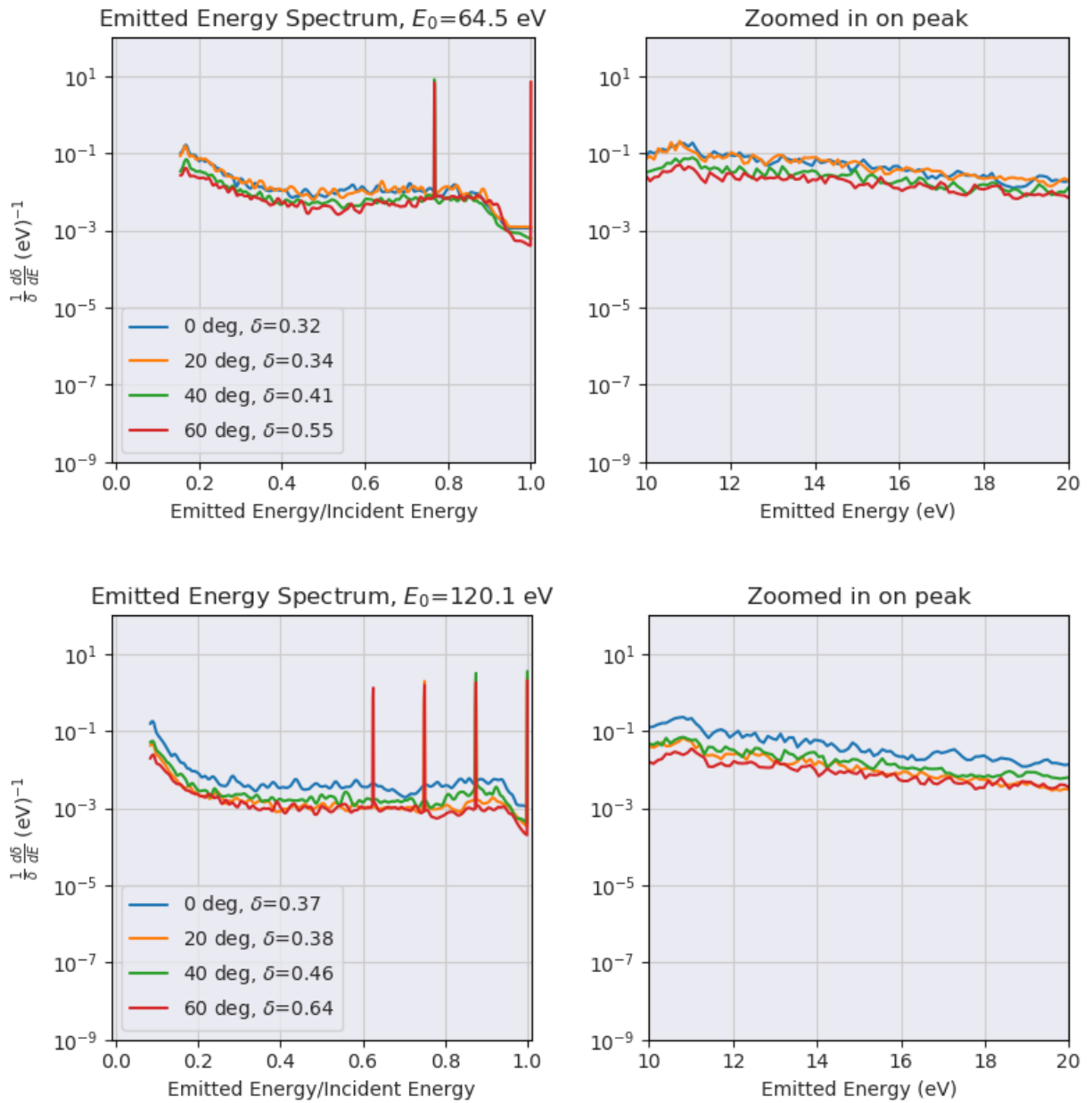


Figure B- 51: EES from GEANT4's Livermore Models for Electrons Incident on Beryllium Oxide with Energies E_0 of 64.5 eV and 120.1 eV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

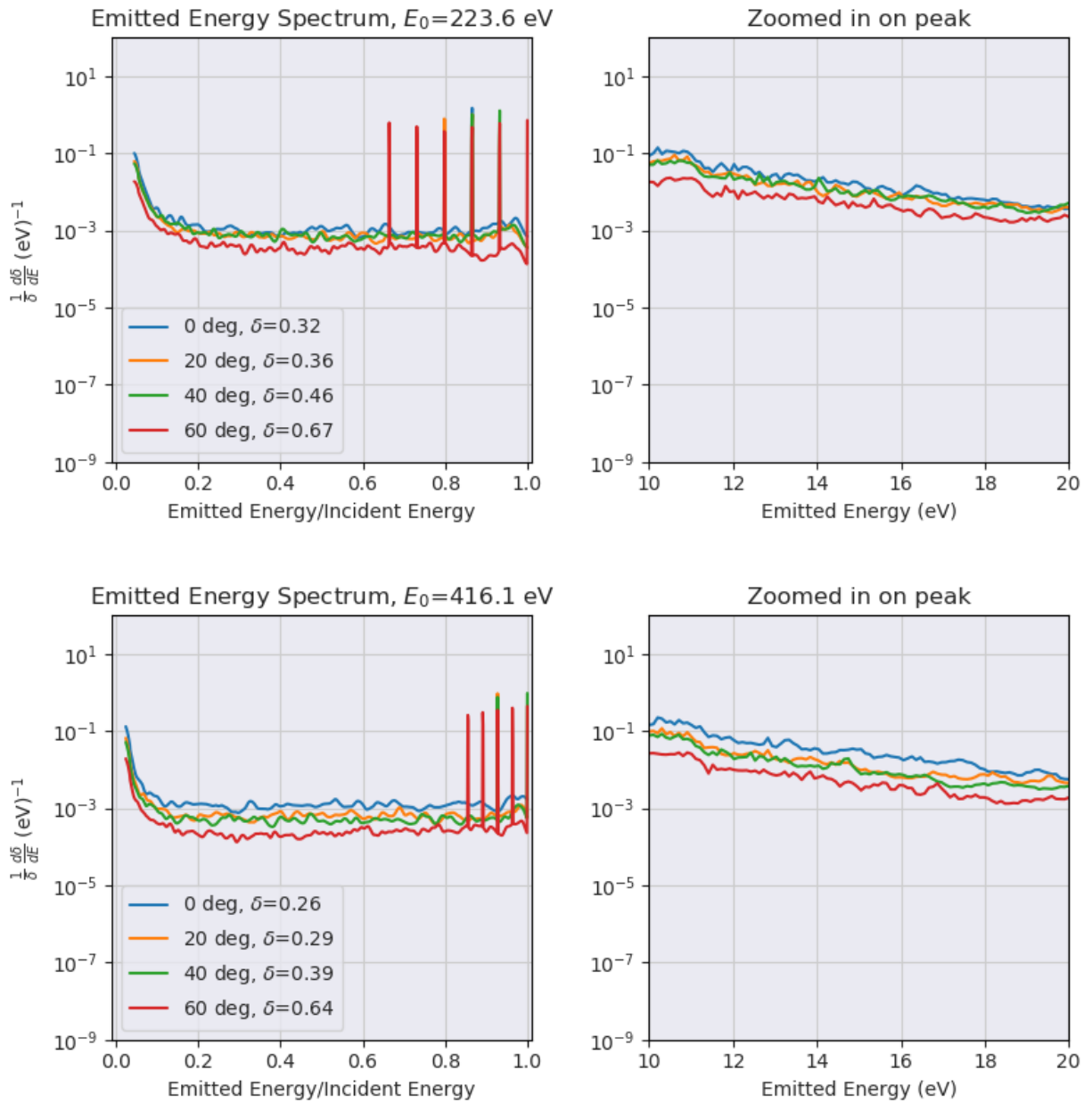


Figure B- 52: EES from GEANT4's Livermore Models for Electrons Incident on Beryllium Oxide with Energies E_0 of 223.6 eV and 416.1 eV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

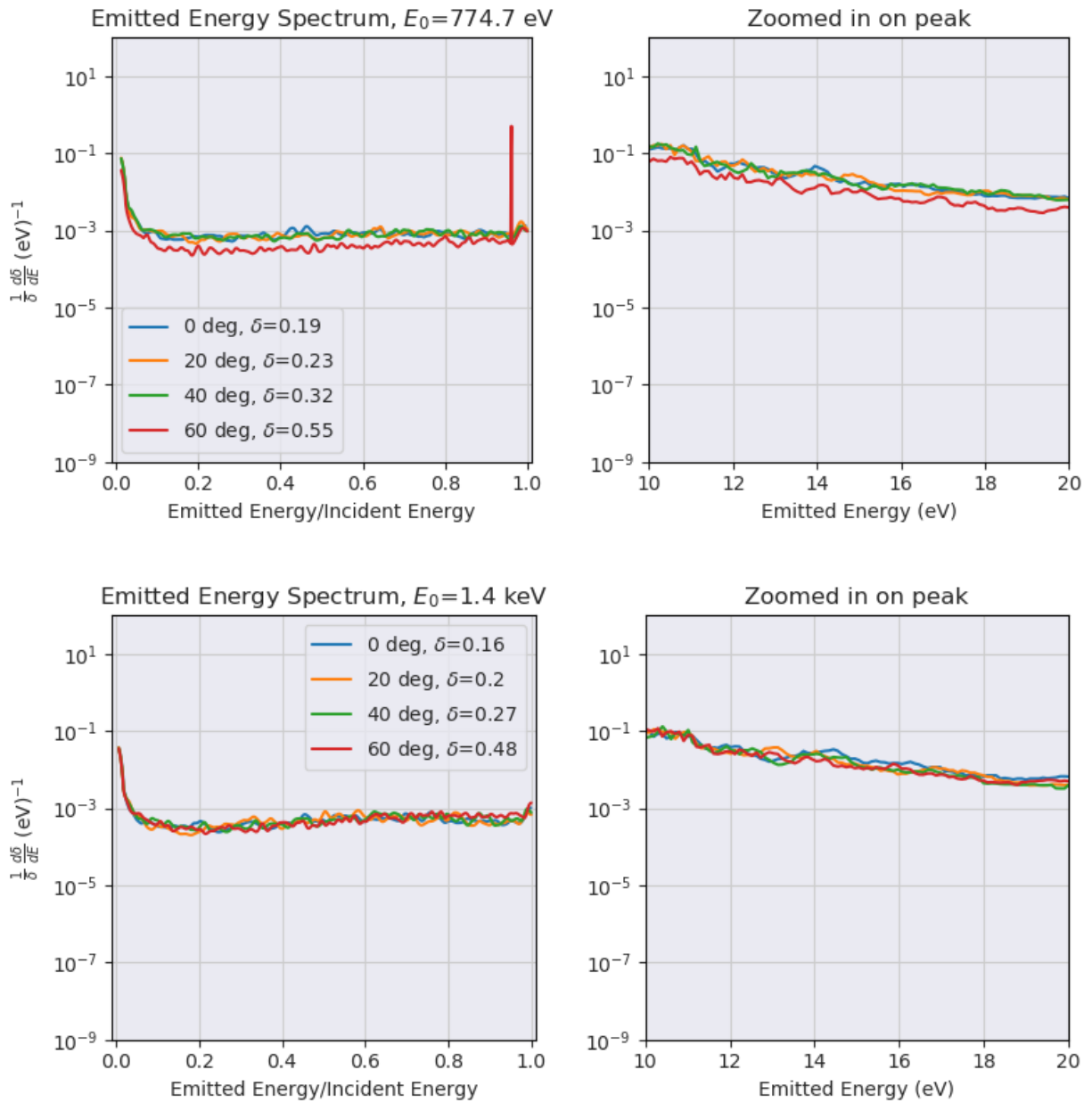


Figure B- 53: EES from GEANT4's Livermore Models for Electrons Incident on Beryllium Oxide with Energies E_0 of 774.7 eV and 1.4 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

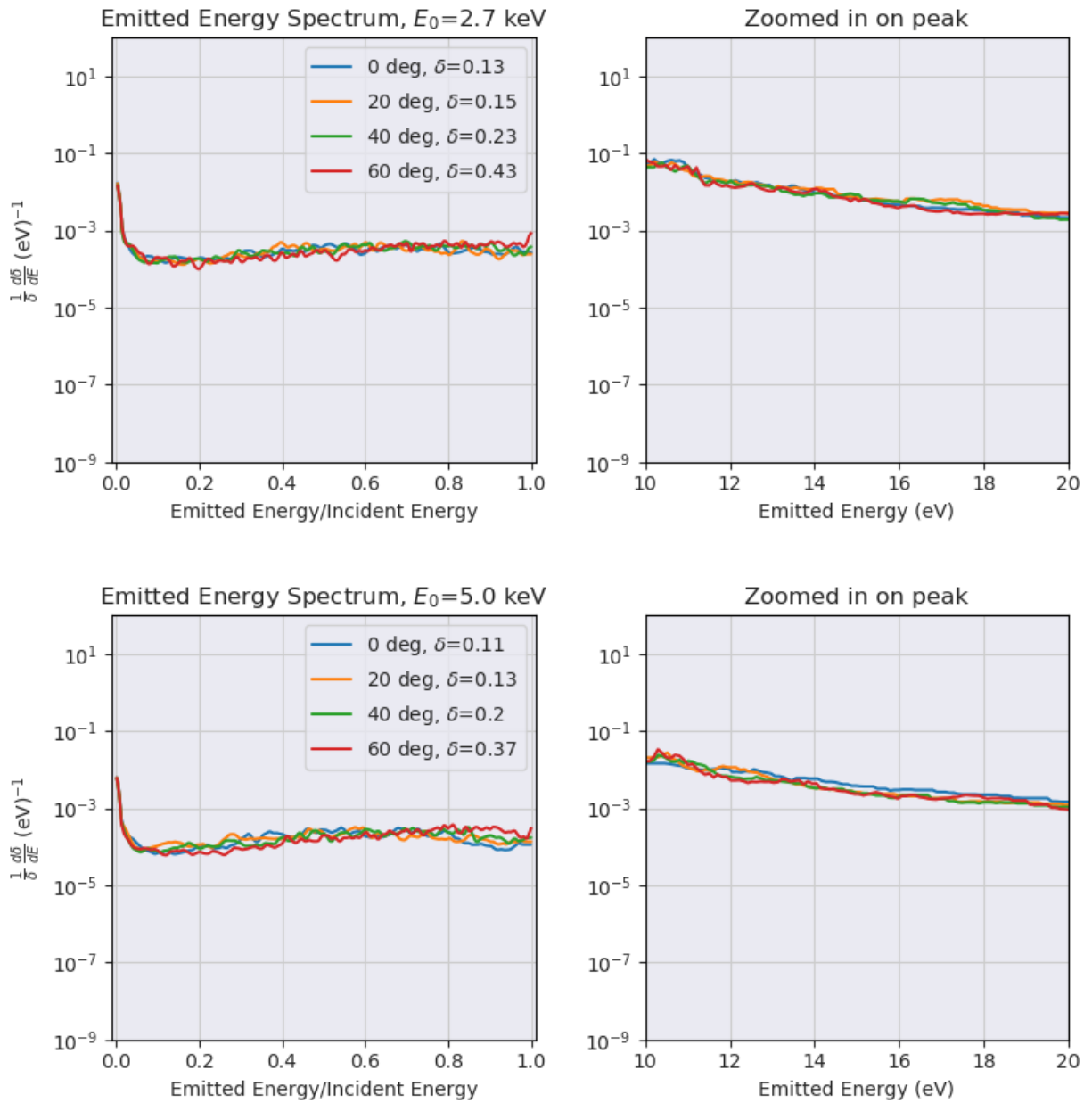


Figure B- 54: EES from GEANT4's Livermore Models for Electrons Incident on Beryllium Oxide with Energies E_0 of 2.7 keV and 5.0 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

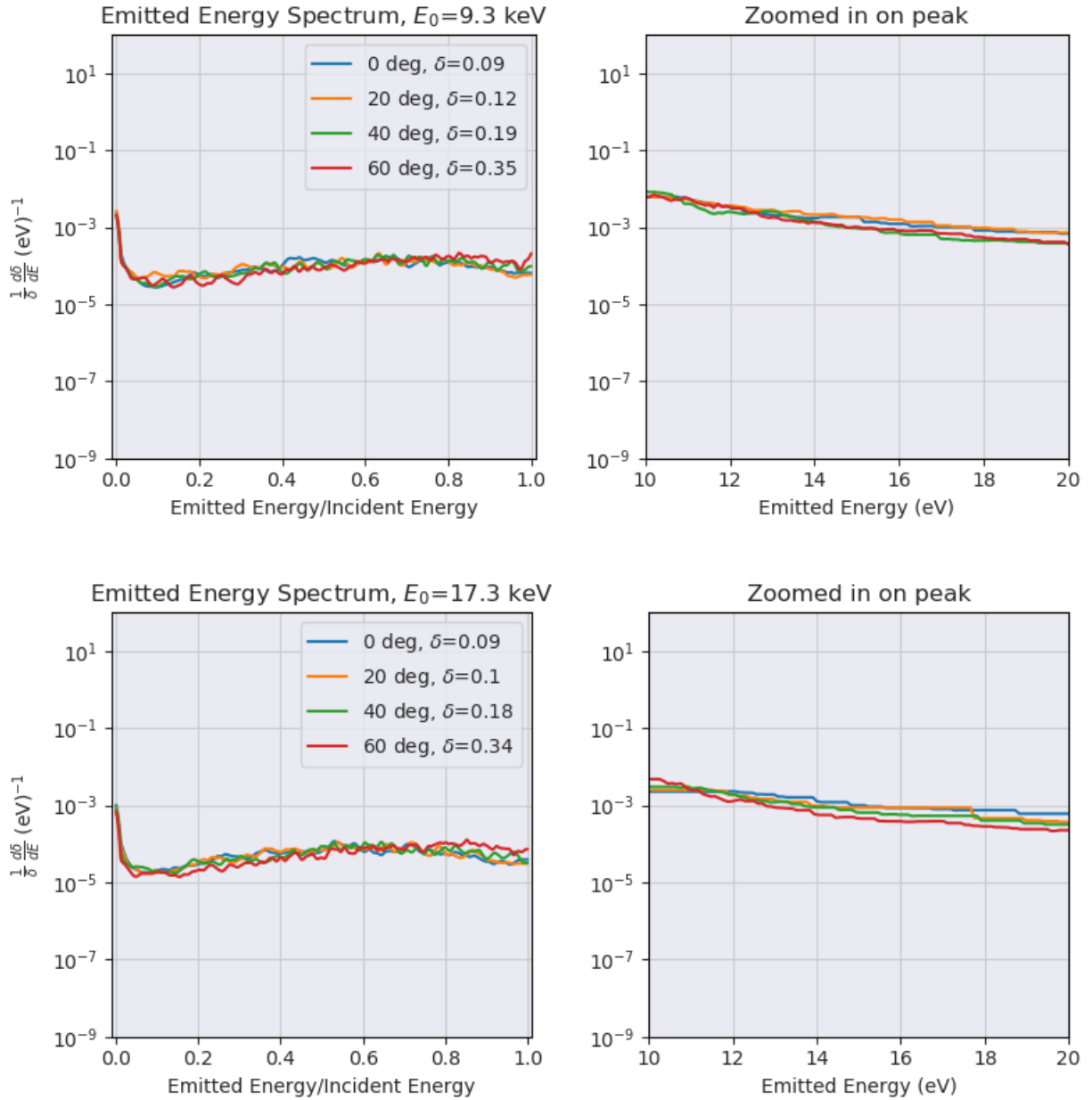


Figure B- 55: EES from GEANT4's Livermore Models for Electrons Incident on Beryllium Oxide with Energies E_0 of 9.3 keV and 17.3 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

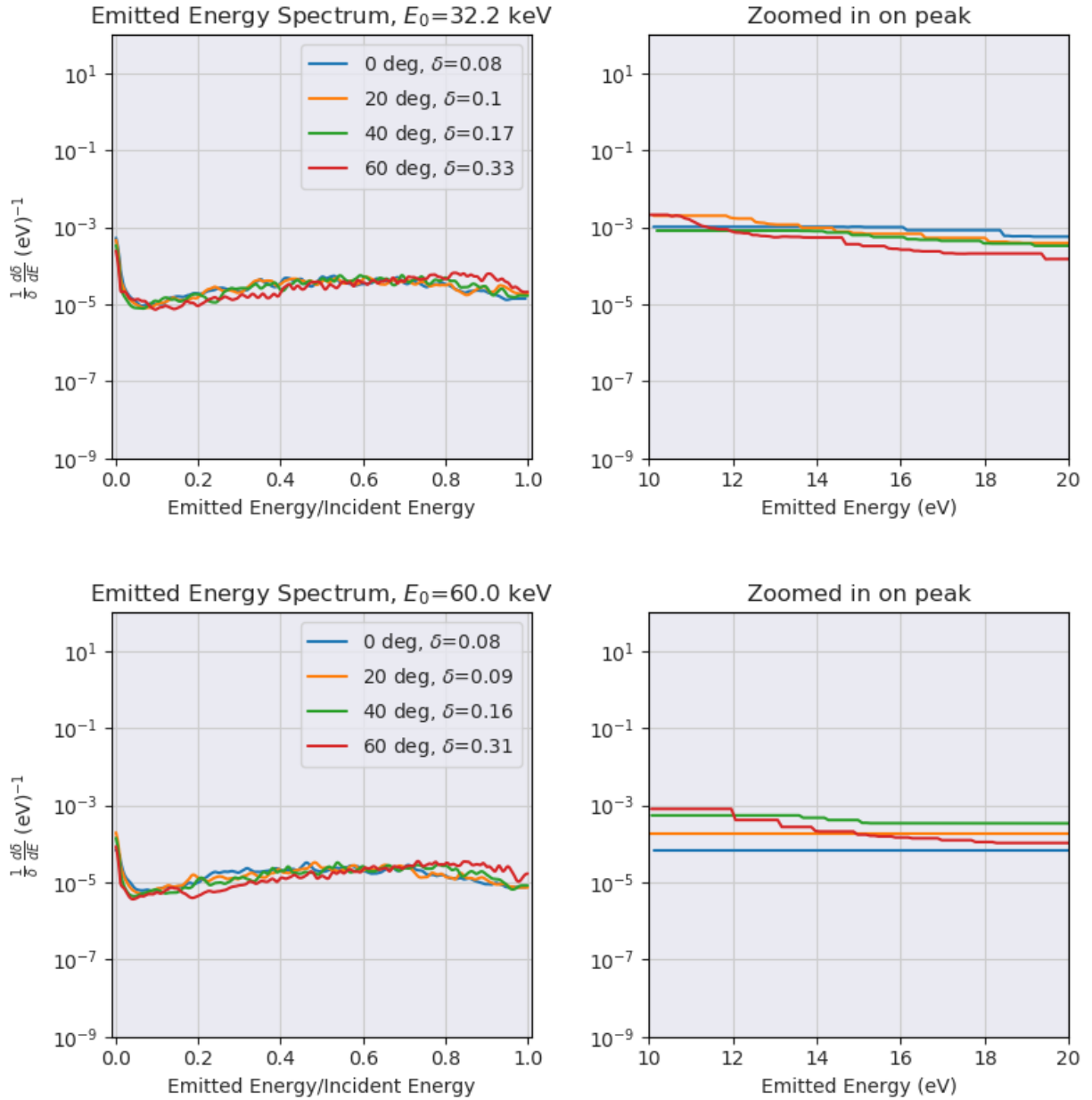


Figure B- 56: EES from GEANT4's Livermore Models for Electrons Incident on Beryllium Oxide with Energies E_0 of 32.2 keV and 60.0 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

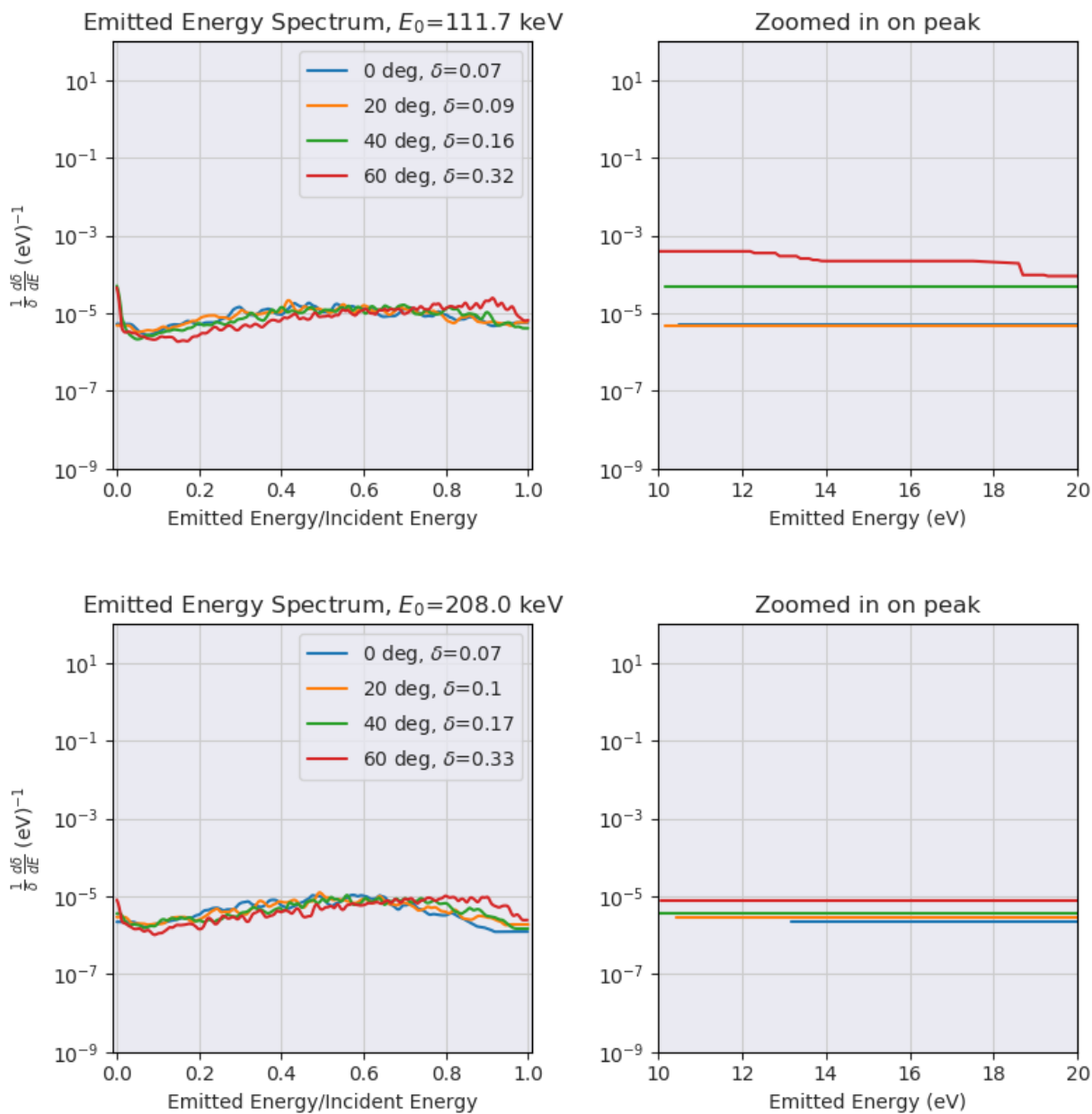


Figure B- 57: EES from GEANT4’s Livermore Models for Electrons Incident on Beryllium Oxide with Energies E_0 of 111.7 keV and 208.0 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

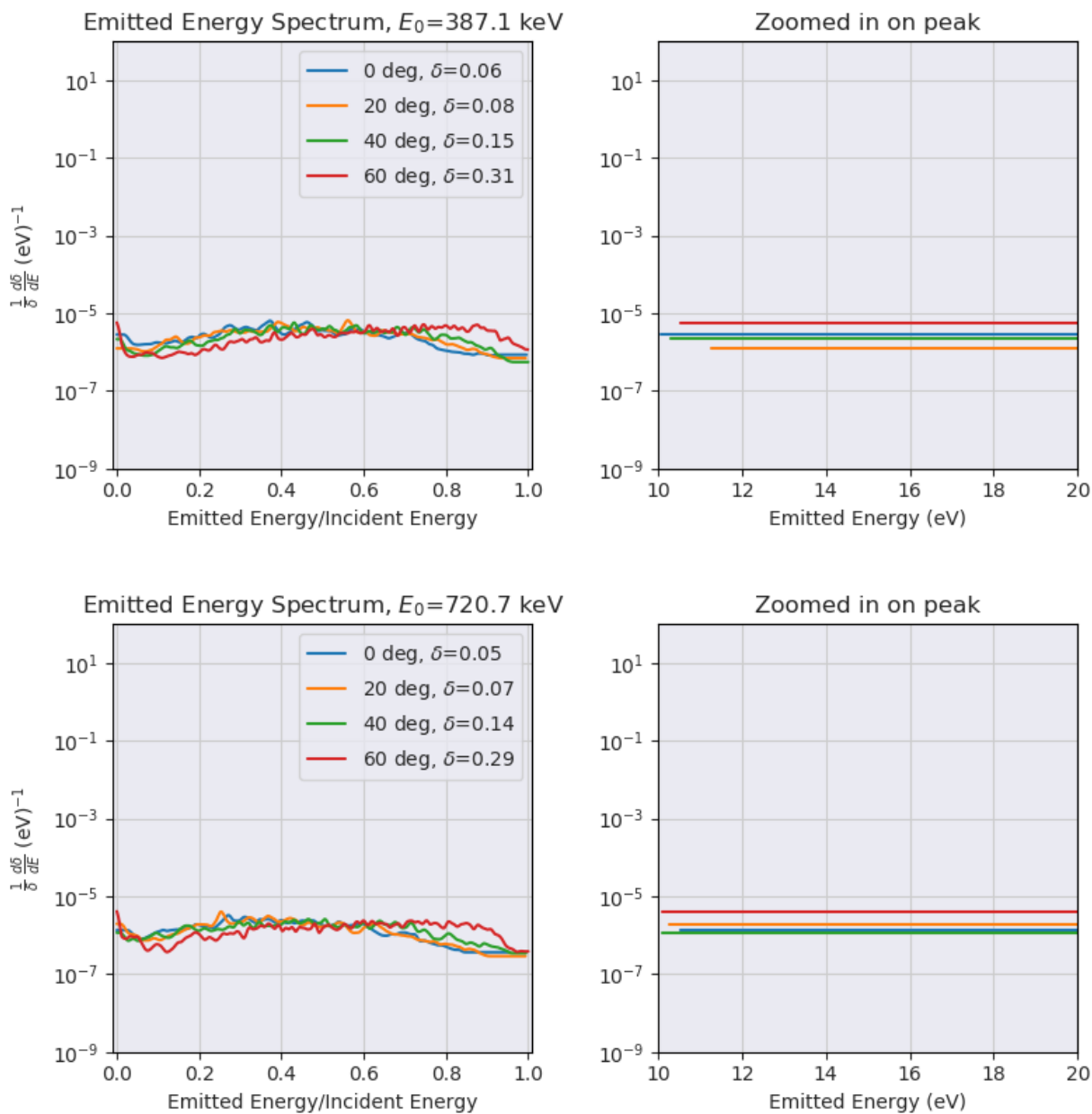


Figure B- 58: EES from GEANT4's Livermore Models for Electrons Incident on Beryllium Oxide with Energies E_0 of 387.1 keV and 720.7 keV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

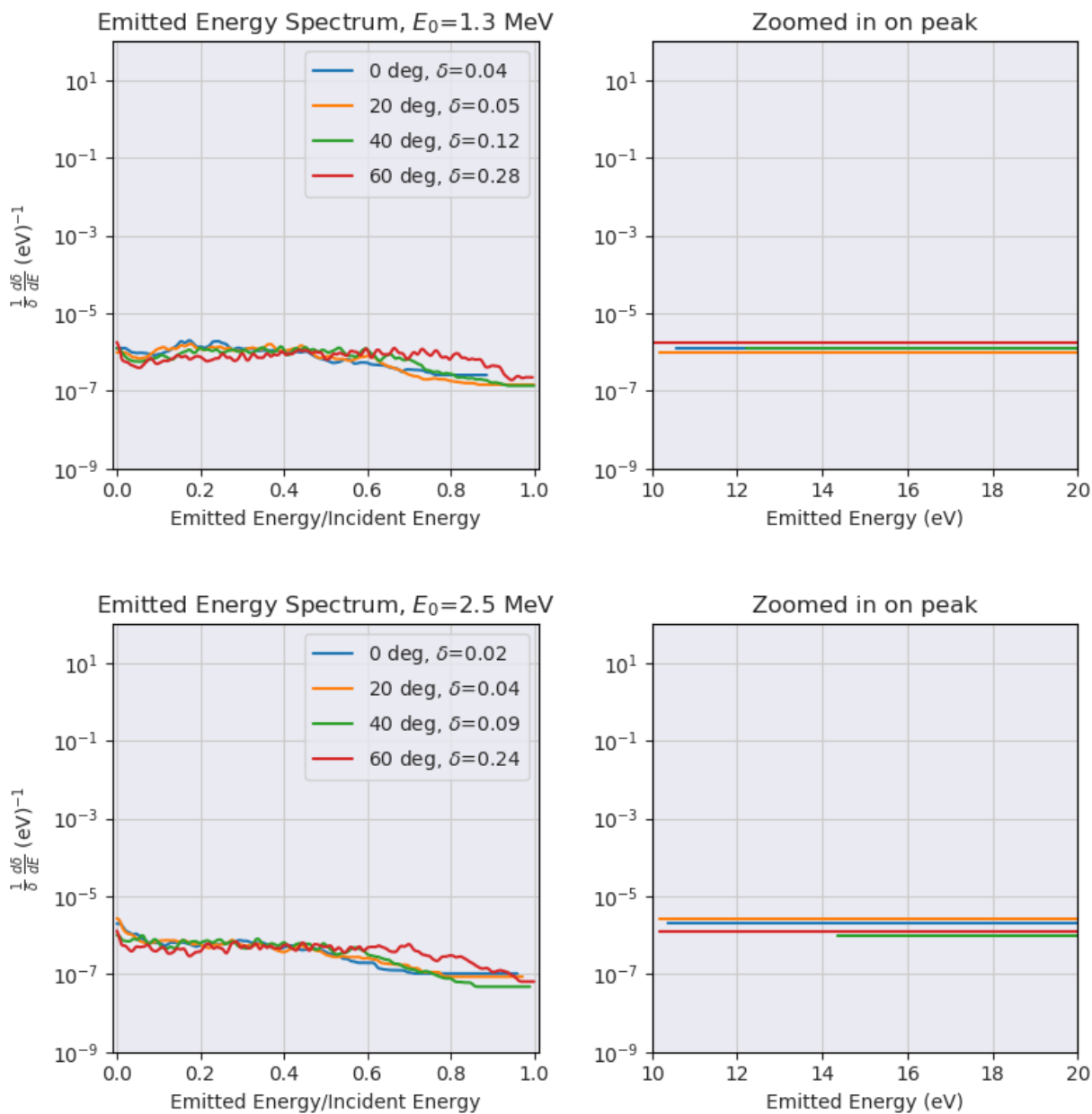


Figure B- 59: EES from GEANT4's Livermore Models for Electrons Incident on Beryllium Oxide with Energies E_0 of 1.3 MeV and 2.5 MeV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

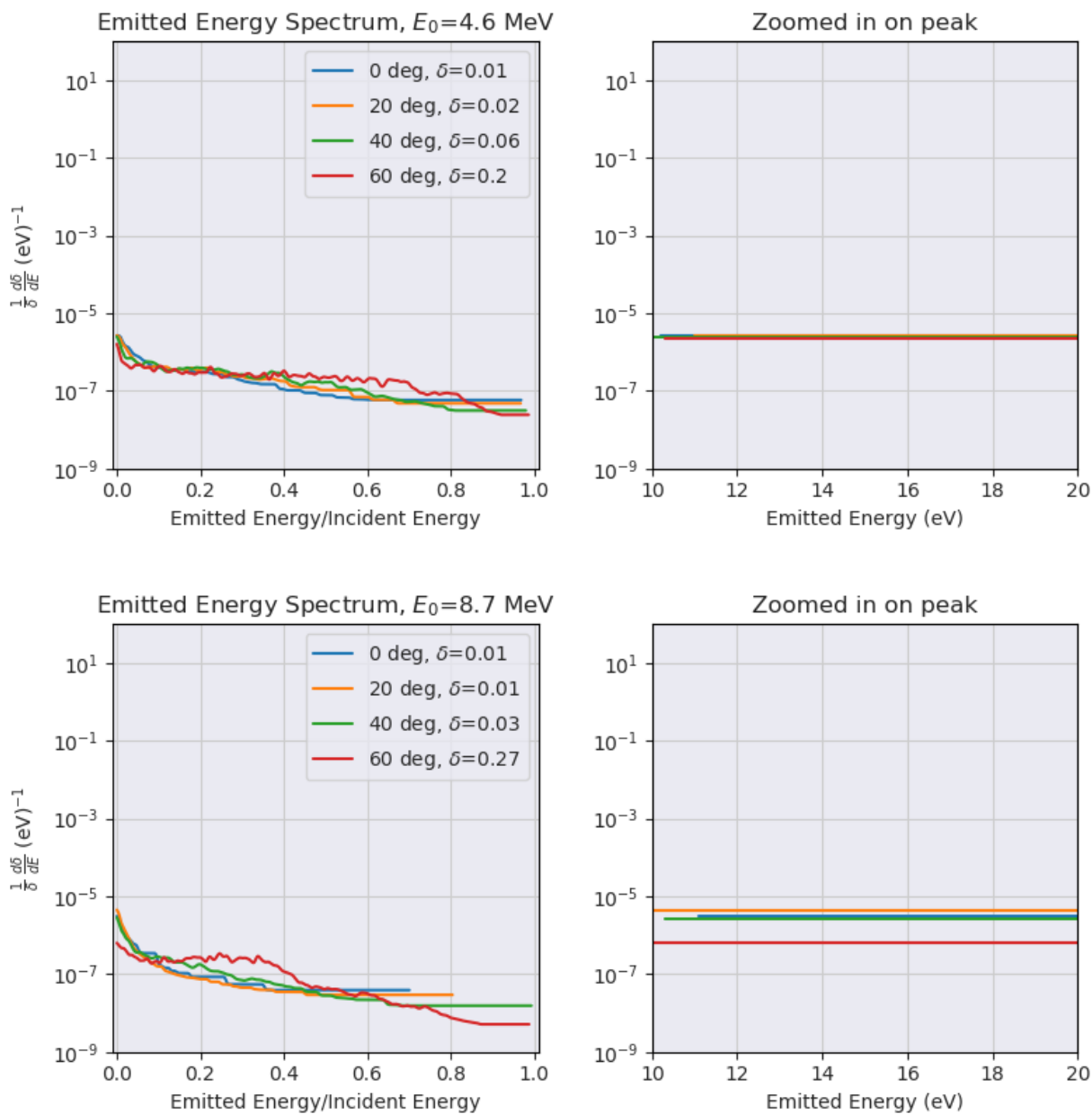


Figure B- 60: EES from GEANT4's Livermore Models for Electrons Incident on Beryllium Oxide with Energies E_0 of 4.6 MeV and 8.7 MeV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

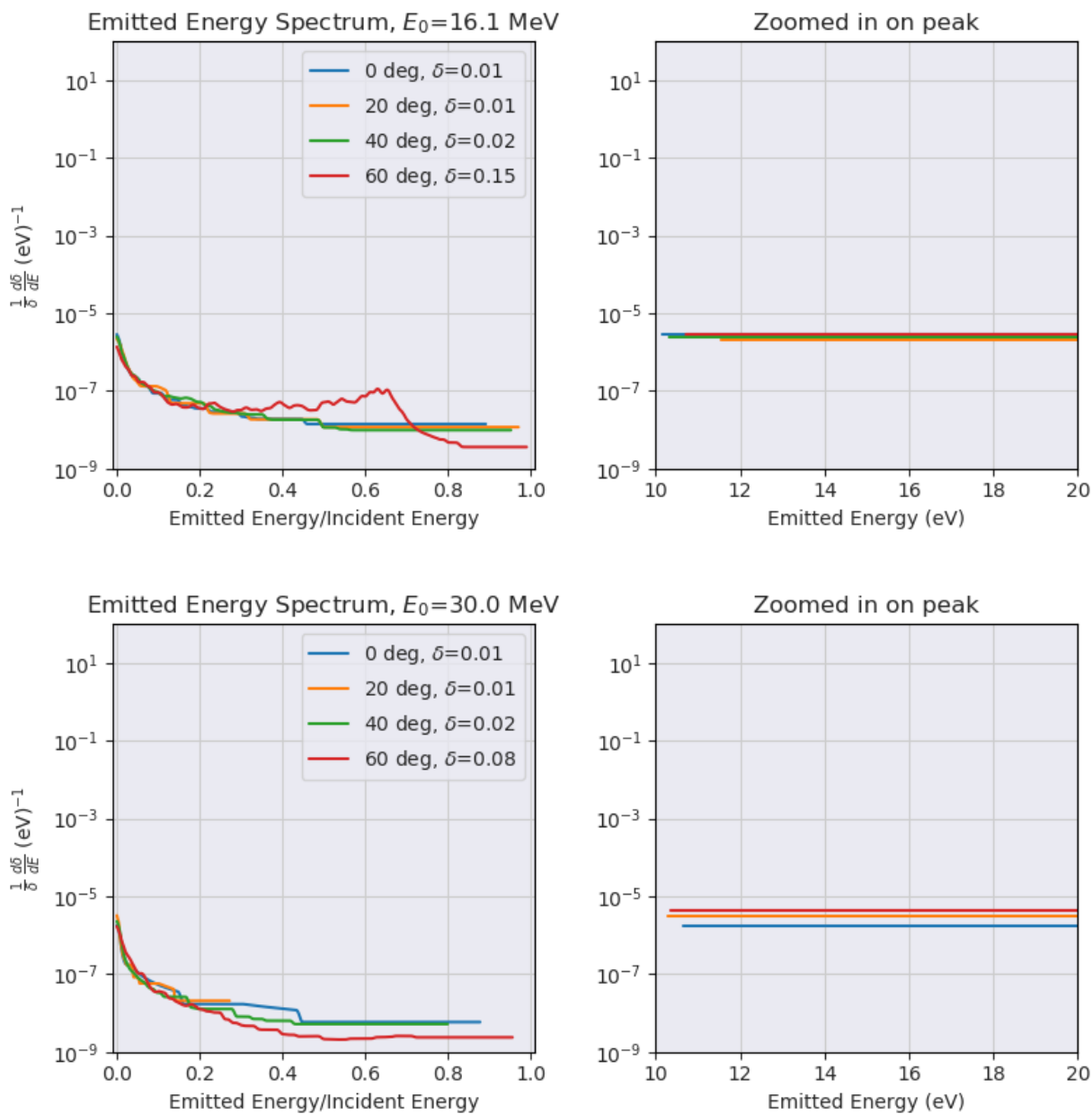


Figure B- 61: EES from GEANT4's Livermore Models for Electrons Incident on Beryllium Oxide with Energies E_0 of 16.1 MeV and 30.0 MeV (left), and Zoomed into the Emitted Energy Range 10-20 eV (right).

APPENDIX C: GEANT4 SEY Curves

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This appendix provides the SEY curves as generated using the GEANT4 Livermore models for the materials considered in Appendices A and B: copper, stainless steel, aluminum, niobium, graphite, aluminum oxide (alumina), and beryllium oxide. The incident energies and angles are the same as in Sections 3.2.7 and 3.2.8. The GEANT4 SEY curves for copper are shown in Figure C-1, stainless steel in Figure C-2, aluminum in Figure C-3, niobium in Figure C-4, graphite in Figure C-5, aluminum oxide in Figure C-6, and beryllium oxide in Figure C-8.

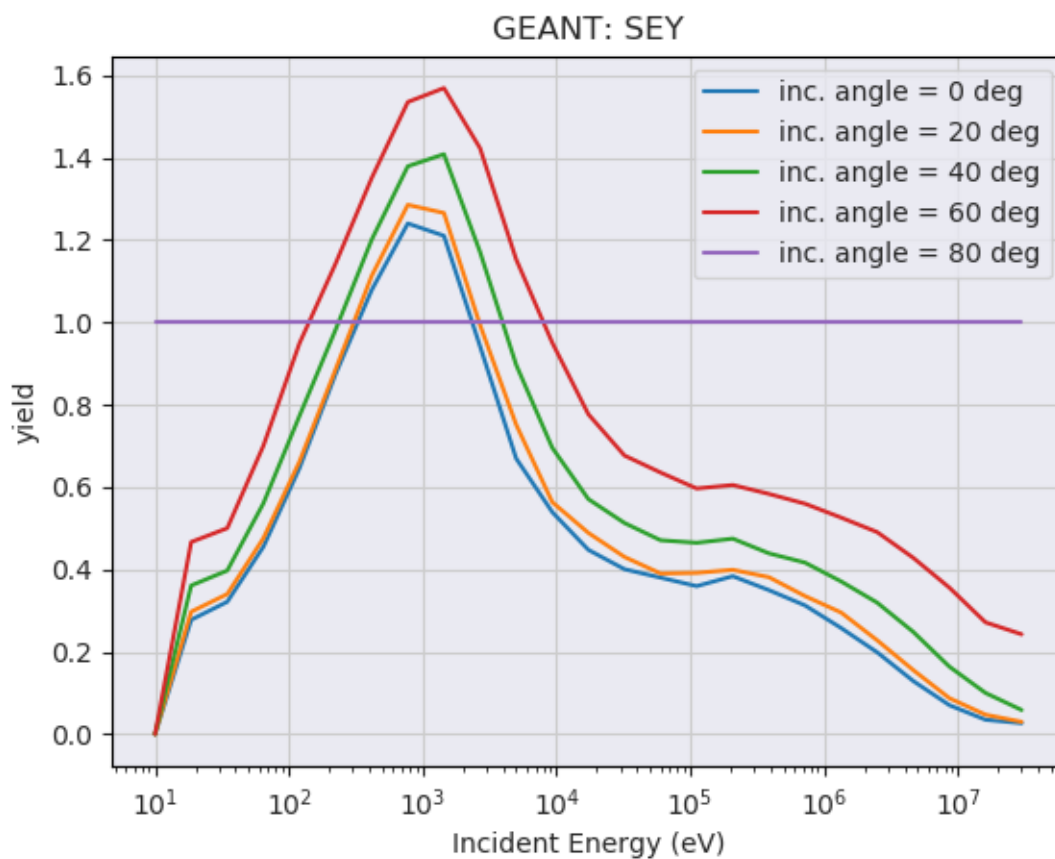


Figure C- 1: SEY Curves for Copper at Incident angles of 0, 20, 40, 60, and 80 Degrees.

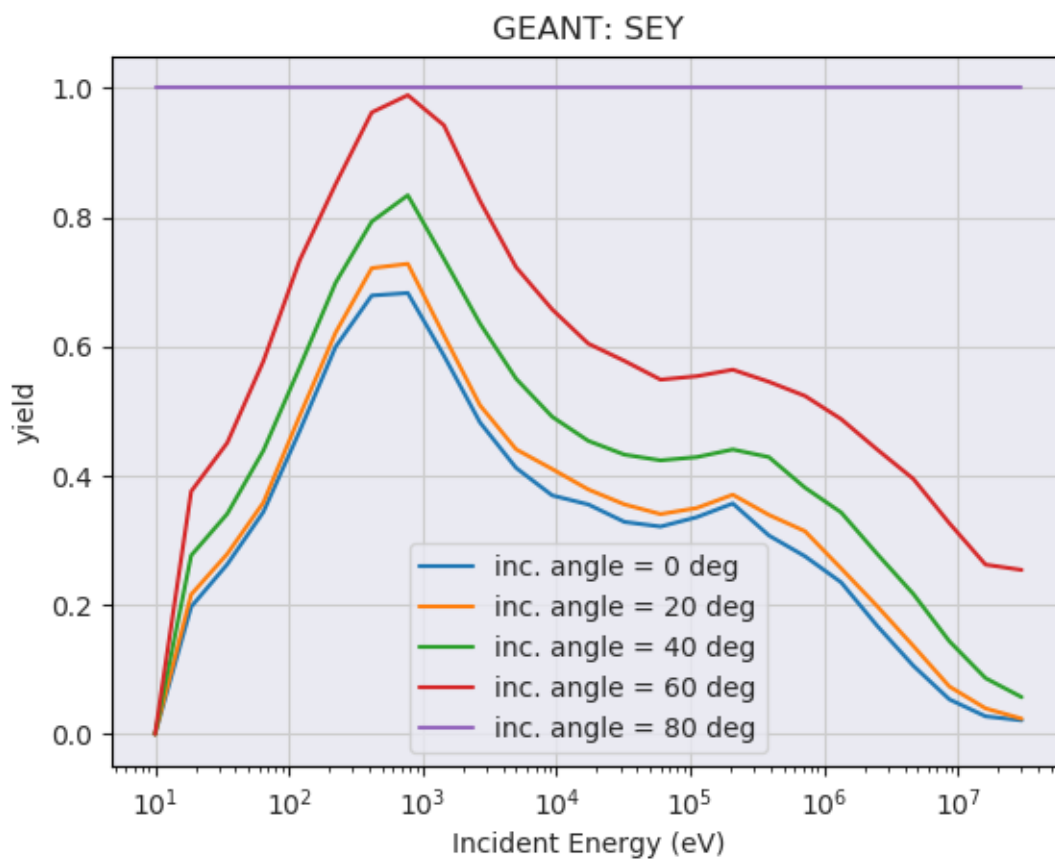


Figure C- 2: SEY Curves for Stainless Steel at Incident Angles of 0, 20, 40, 60, and 80 Degrees.

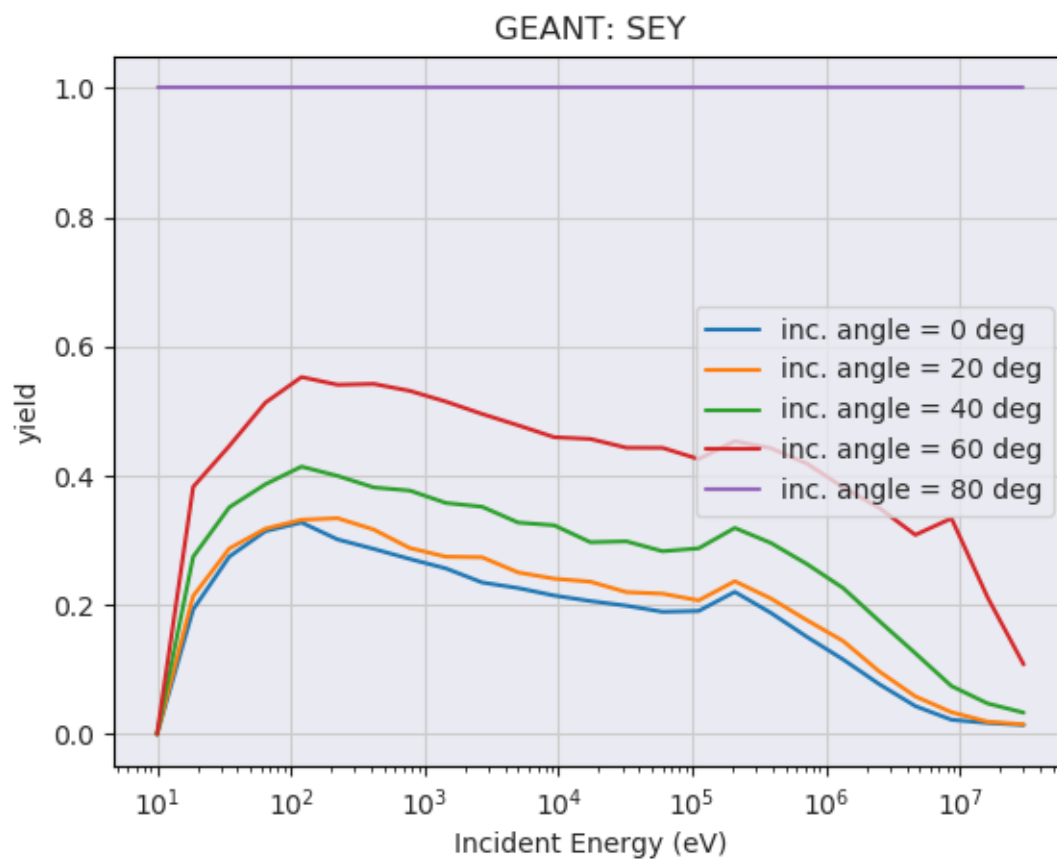


Figure C- 3: SEY Curves for Aluminum at Incident Angles of 0, 20, 40, 60, and 80 Degrees.

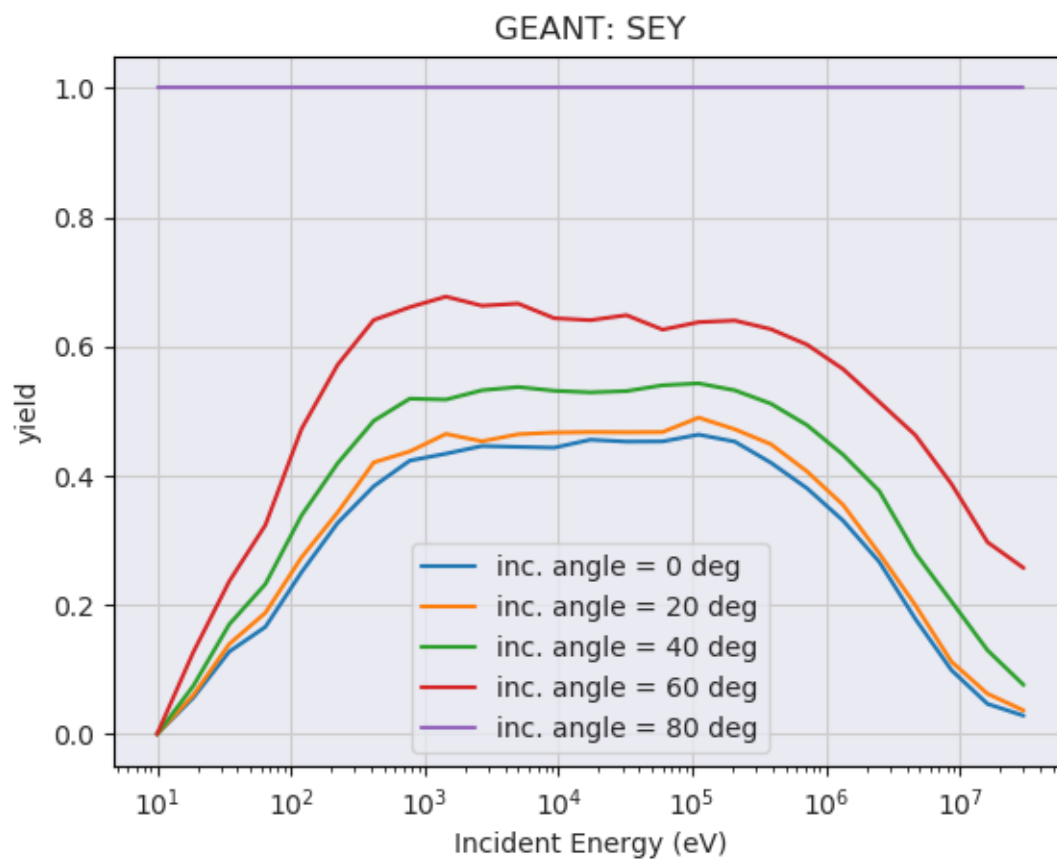


Figure C- 4: SEY Curves for Niobium at Incident Angles of 0, 20, 40, 60, and 80 Degrees.

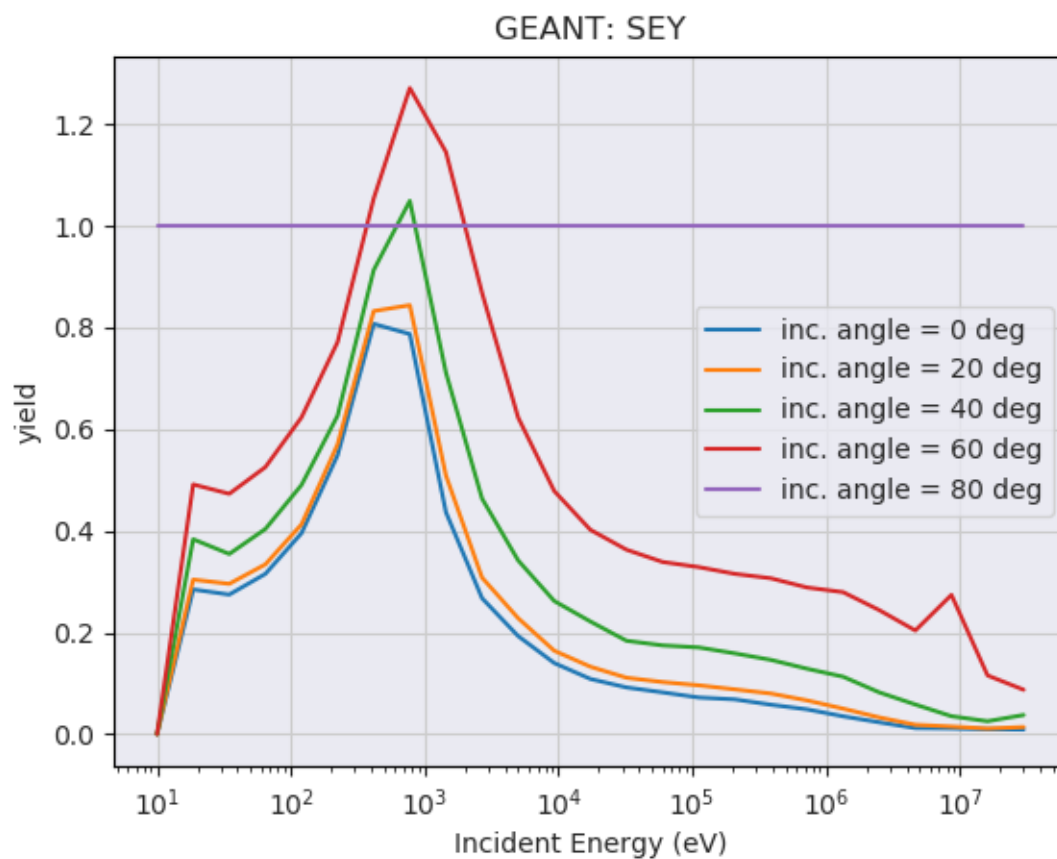


Figure C- 5: SEY Curves for Graphite at Incident Angles of 0, 20, 40, 60, and 80 Degrees.

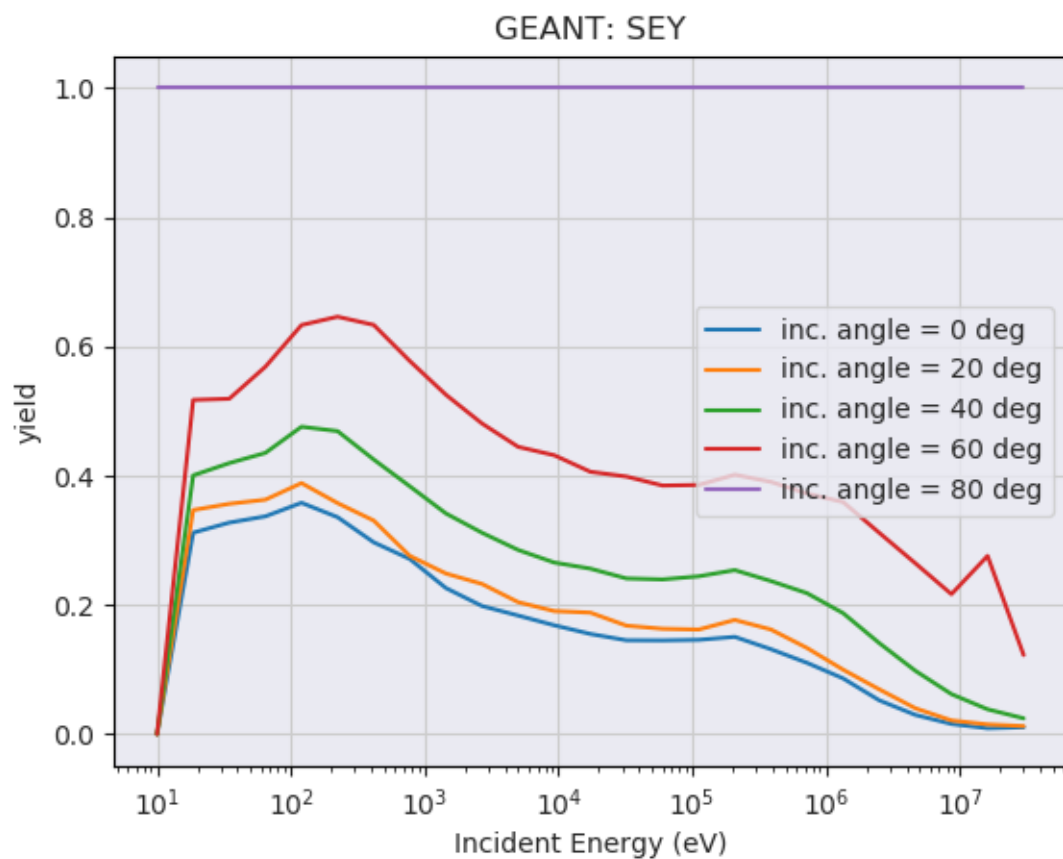


Figure C- 6: SEY Curves for Aluminum Oxide (Alumina) at Incident Angles of 0, 20, 40, 60, and 80 Degrees.

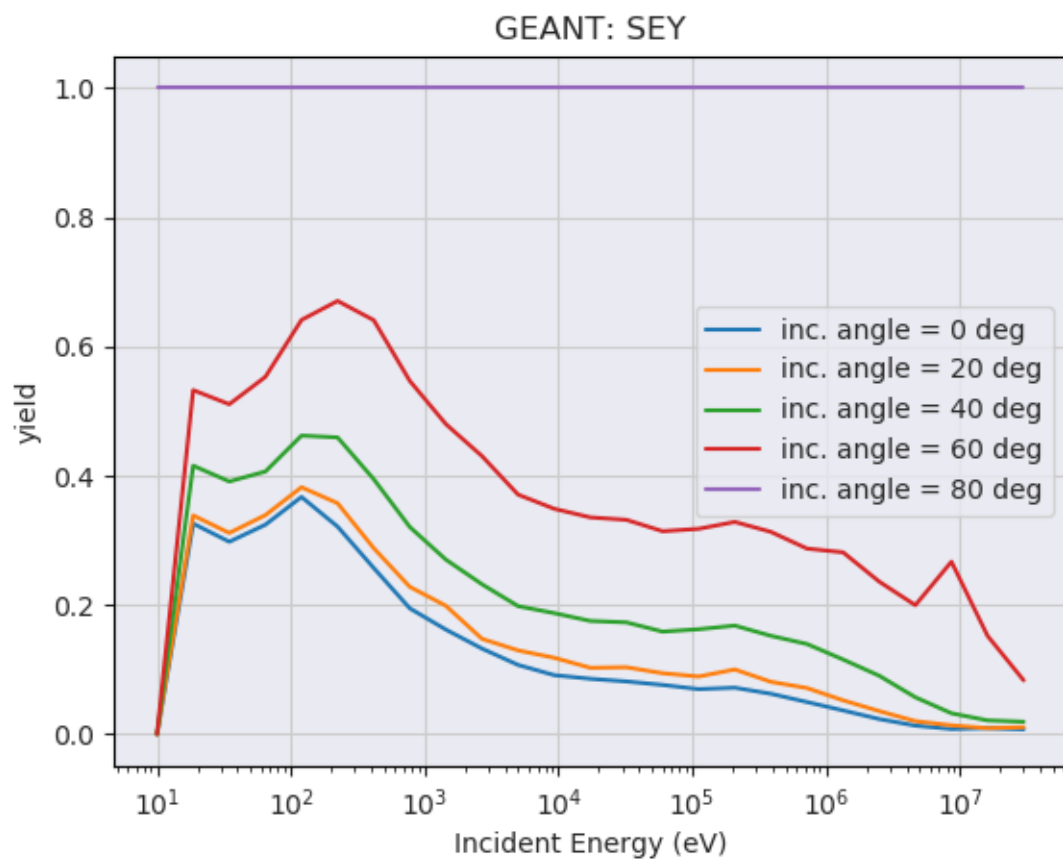


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APPENDIX D: Assessment of GEANT4 SEY Deficiency

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Section 4.1 presented the results of a simple additive correction to the Vaughan SEY curve, and evaluated how well the resulting model can represent simulated GEANT4 SEY data. This presents a more fundamental question about how valid is the GEANT4 data that we are trying to match. One of the key limitations of GEANT4 is the presence of a low energy threshold of 10 eV, below which no secondary electrons can be generated. Unfortunately, true secondary electrons tend to follow a Maxwell-Boltzmann flux distribution with temperatures on the order of a few eV, resulting in the majority of true secondary electrons occurring below 10 eV. However, the tail end of this distribution will extend above 10 eV, so in this Appendix we examine the GEANT4 data in this tail, in the hopes of gaining some insight into the true secondary electron contributions to the overall SEY.

Within the GEANT4 data, let us somewhat arbitrarily define scattered electrons between 10 eV and 15 eV to be true secondary electrons. Likewise, let us define any scattered electrons greater than 99% of the incidence energy to be reflected electrons, and the remainder of electrons to be scattered electrons. We can then plot the relative contributions of these components to the overall SEY reported by GEANT4. Furthermore, we can display histograms of the scattered electrons that occur within the energy range of 10 eV to 20 eV, and determine if the behavior qualitatively looks like the tail end of a Maxwell-Boltzmann energy distribution.

Figure D-1 shows the relative SEY components for copper as generated by applying the above heuristics to the GEANT4 data. We note that for high energies, the true secondary component tends to zero, and becomes negligible somewhere between 10 keV and 100 keV; the reflected electron component also tends to be low for these energies and greater. Figure D-2 shows the histograms of the scattered electron energies between 10 eV and 20 eV, for four different incidence energies between 100 eV and 1000 eV. We note that these histograms are not suggestive of the tail end of an underlying Maxwell-Boltzmann energy distribution, which does potentially raise some questions about the validity of the GEANT4 data.

Similar plots are shown respectively for stainless steel in Figure D-3 and Figure D-4, aluminum in Figure D-5 and Figure D-6, niobium in Figure D-7 and Figure D-8, graphite in Figure D-9 and Figure D-10, aluminum oxide in Figure D-11 and Figure D-12, and finally beryllium oxide in Figure D-13 and Figure D-14. For all the cases, we note that the true secondary component tends to zero, and becomes negligible somewhere between 1 keV and 100 keV, and the reflected electron component is likewise small above these energies; these observations gave rise to the statement in Section 4.1.6 that above a certain energy around 10 keV, only scattered electrons contribute to the SEY.

Some of the low emission energy (10 eV to 20 eV) histogram plots may be somewhat consistent with an underlying Maxwell-Boltzmann distribution since the histograms decrease on average from lower-to-higher energies, but most of the histograms appear to have an unexpected dip near

the 10 eV boundary, which is not explained with a Maxwell-Boltzmann distribution. The graphite emission energy histograms (Figure D-10) look qualitatively similar to the copper histograms, and are not suggestive of the tail end of a Maxwell-Boltzmann distribution.

The authors believe that caution is warranted with the GEANT4 data, but that the SEY curves provide qualitative results against which we can test proposed corrections to Vaughan's SEY curve.

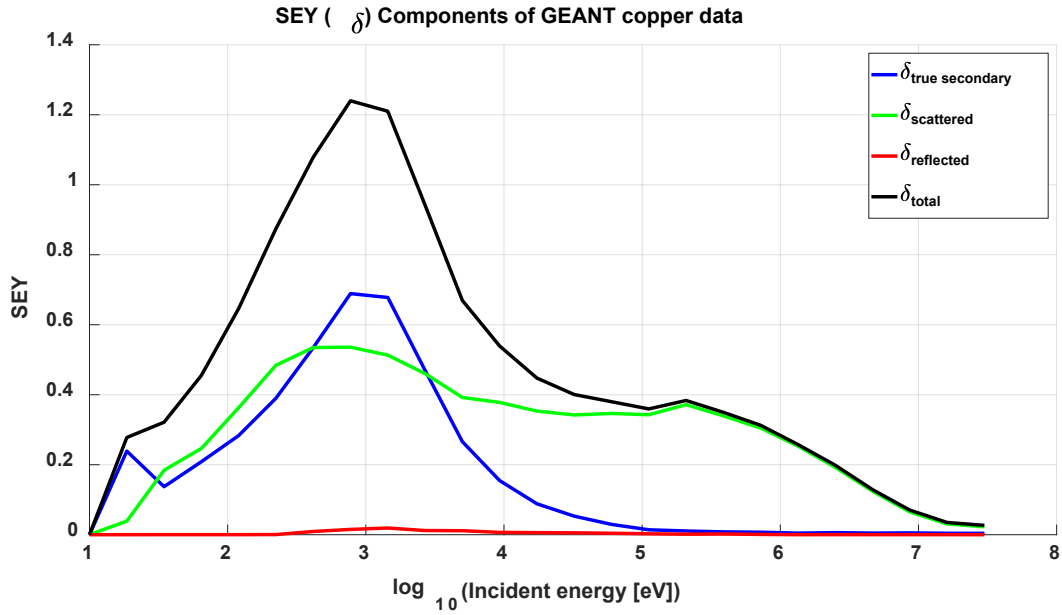


Figure D- 1: Copper SEY Components Generated by GEANT4; True Secondary Electrons Are Defined to Have Energies Between 10 eV (low energy limit) and 15 eV.

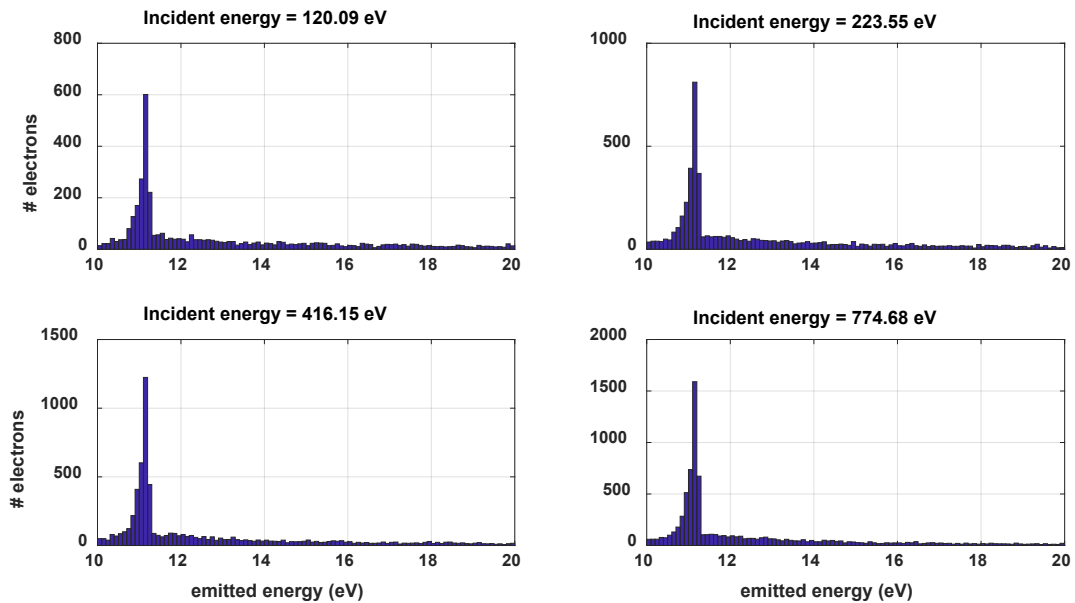


Figure D- 2: Copper Scattering Energy Histogram Between 10 eV (GEANT4 Low Energy Limit) and 20 eV at Four Incident Energies Between 100 eV and 1000 eV.

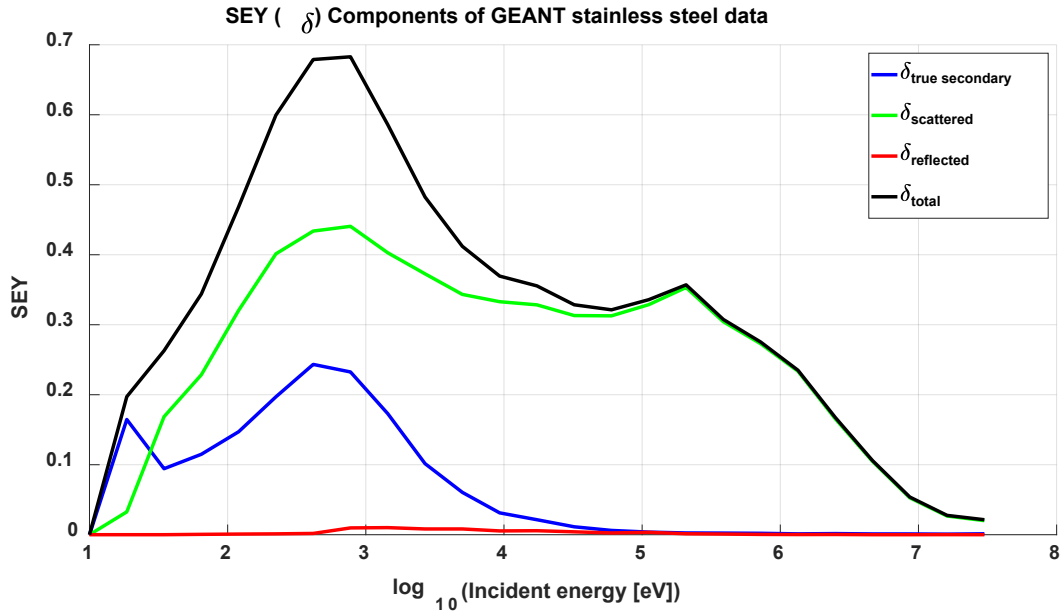


Figure D- 3: Stainless Steel SEY Components Generated by GEANT4; True Secondary Electrons are Defined to Have Energies Between 10 eV (low energy limit) and 15 eV.

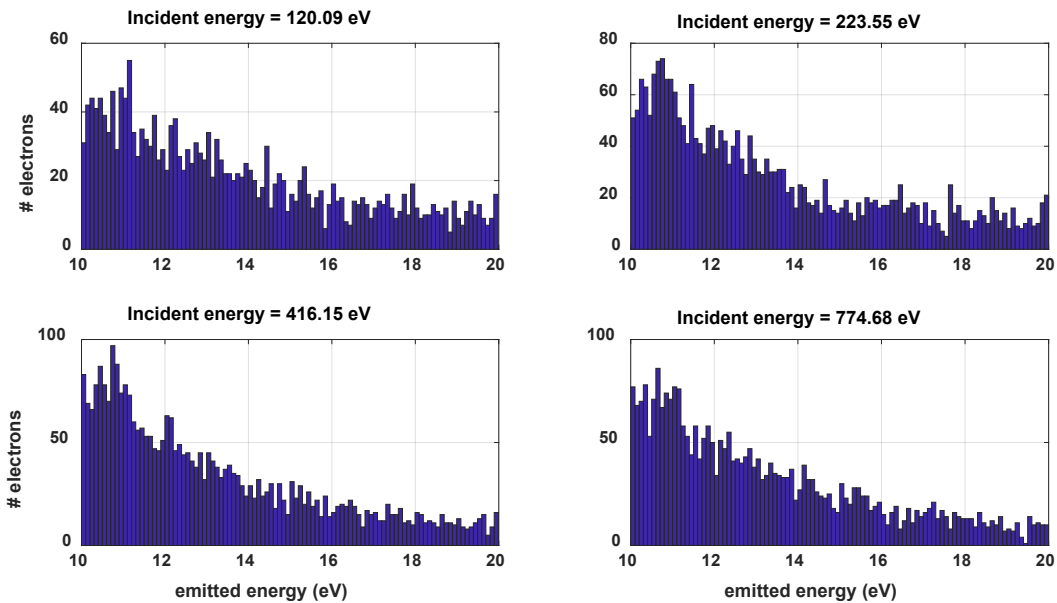


Figure D- 4: Stainless Steel Scattering Energy Histogram Between 10 eV (GEANT4 Low Energy Limit) and 20 eV at Four Incident Energies Between 100 eV and 1000 eV.

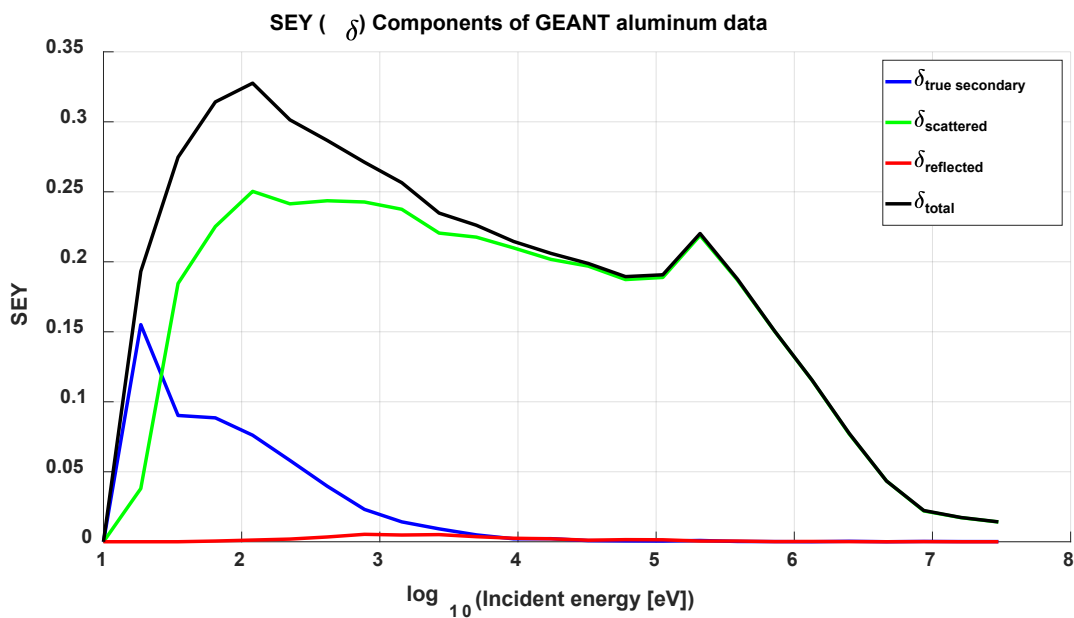


Figure D- 5: Aluminum SEY Components Generated by GEANT4; True Secondary Electrons are Defined to Have Energies Between 10 eV (low energy limit) and 15 eV.

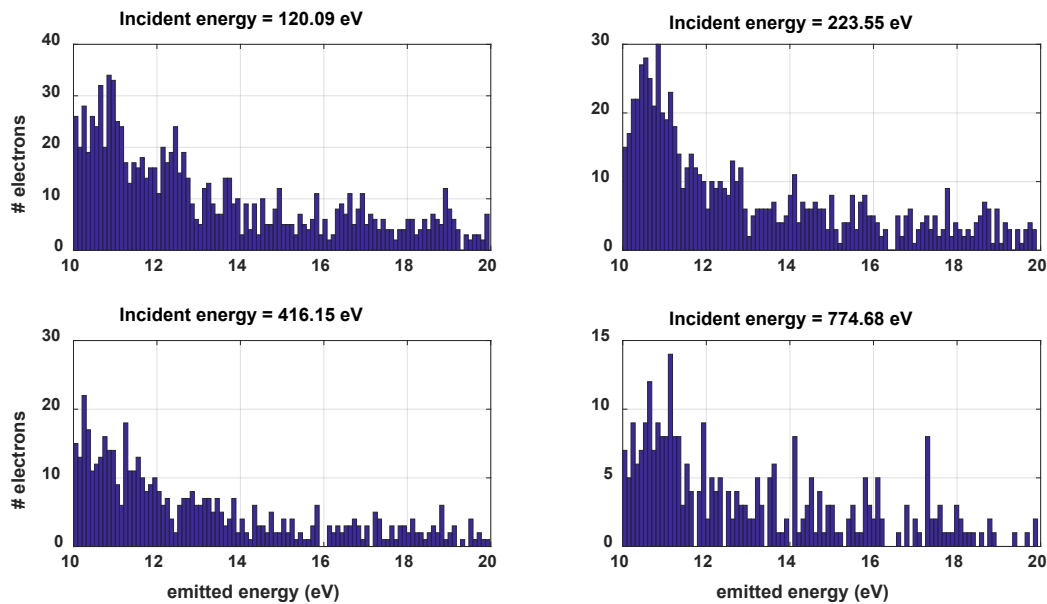


Figure D- 6: Aluminum Scattering Energy Histogram Between 10 eV (GEANT4 Low Energy Limit) and 20 eV at Four Incident Energies Between 100 eV and 1000 eV.

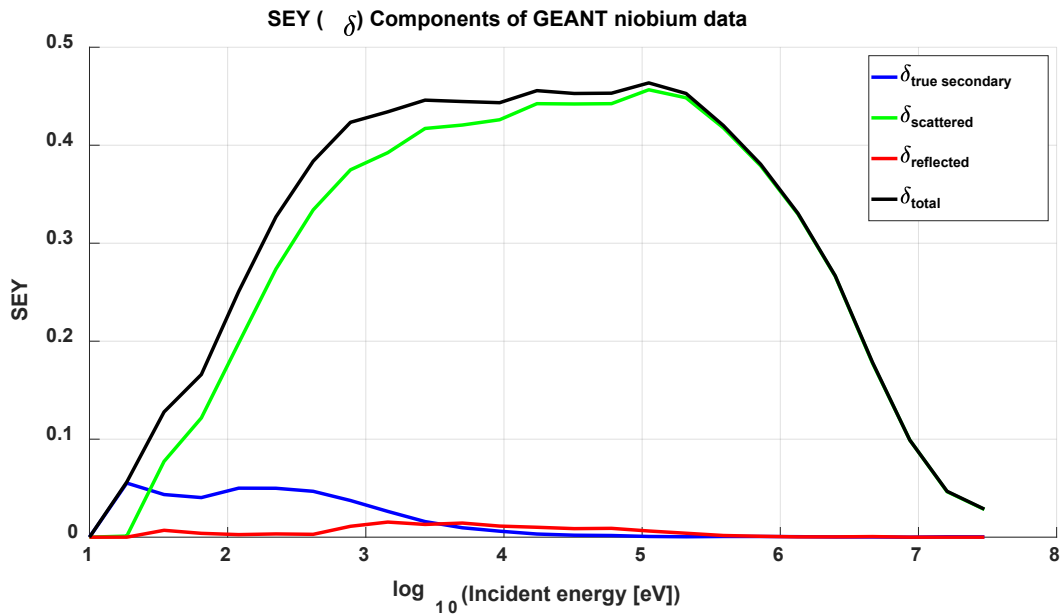


Figure D- 7: Niobium SEY Components Generated by GEANT4; True Secondary Electrons are Defined to Have Energies Between 10 eV (low energy limit) and 15 eV.

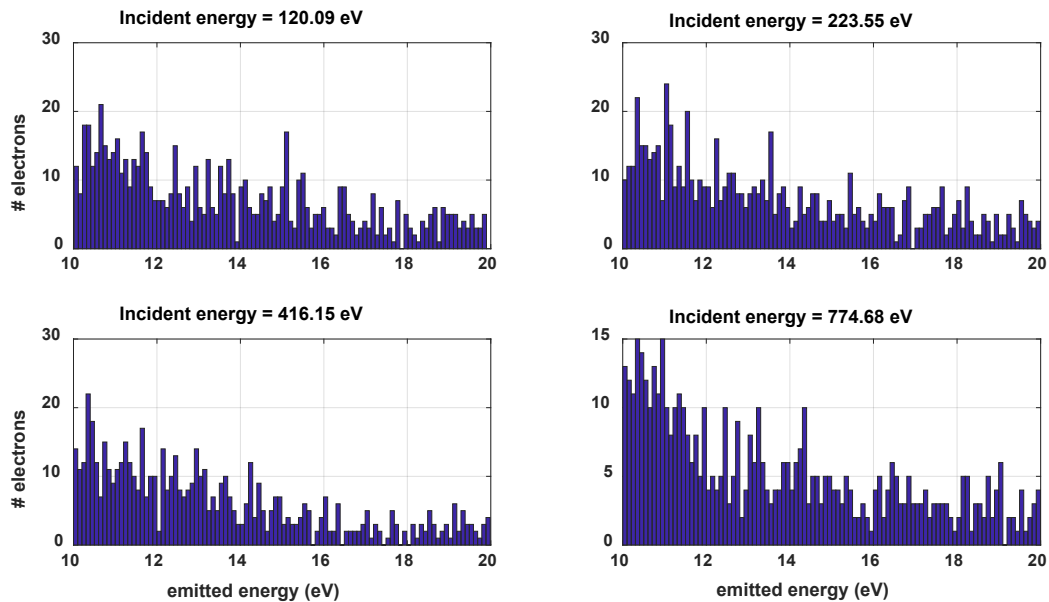


Figure D- 8: Niobium Scattering Energy Histogram Between 10 eV (GEANT4 Low Energy Limit) and 20 eV at Four Incident Energies Between 100 eV and 1000 eV.

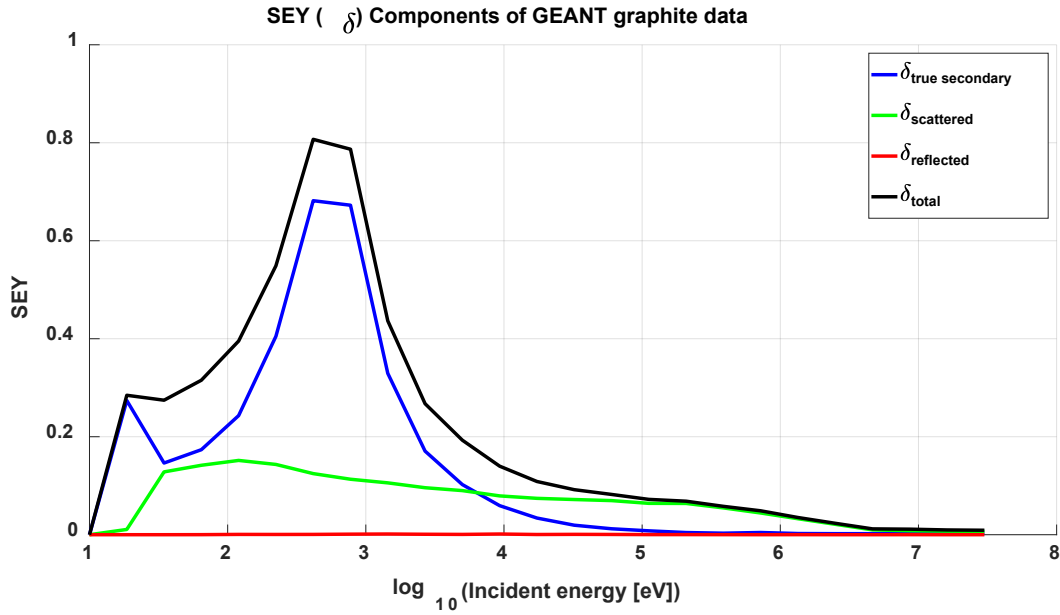


Figure D- 9: Graphite SEY Components Generated by GEANT4; True Secondary Electrons are Defined to Have Energies Between 10 eV (low energy limit) and 15 eV.

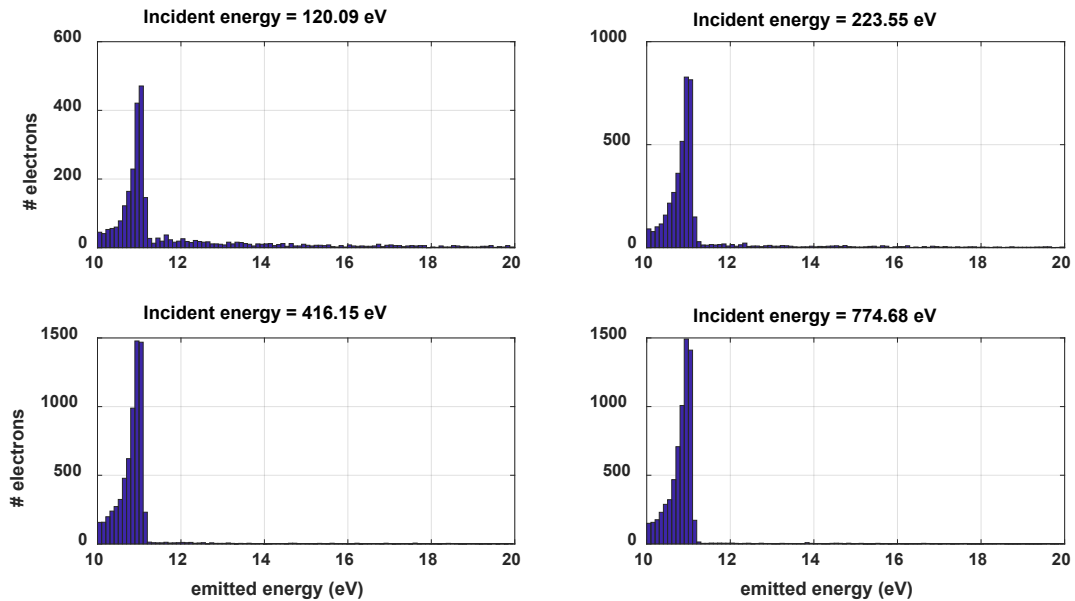


Figure D- 10: Graphite Scattering Energy Histogram Between 10 eV (GEANT4 Low Energy Limit) and 20 eV at Four Incident Energies Between 100 eV and 1000 eV.

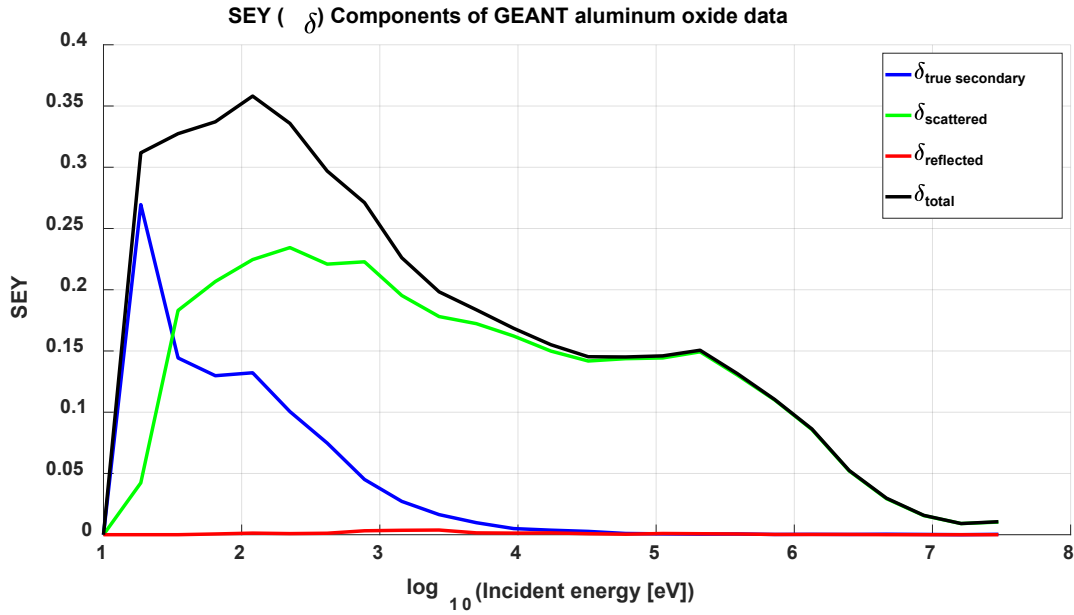


Figure D- 11: Aluminum Oxide SEY Components Generated by GEANT4; True Secondary Electrons are Defined to Have Energies Between 10 eV (low energy limit) and 15 eV.

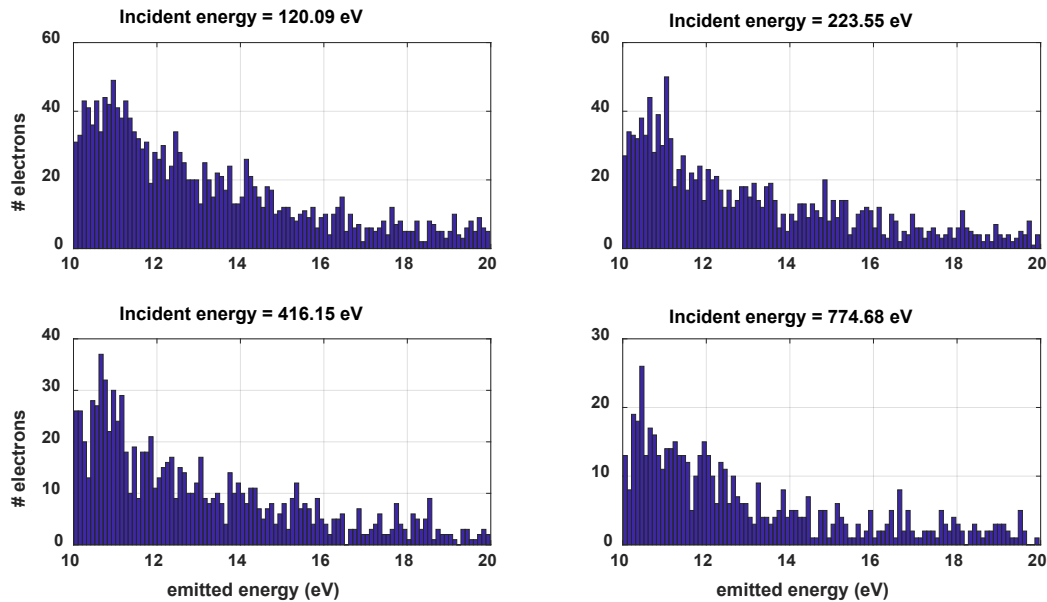


Figure D- 12: Aluminum Oxide Scattering Energy Histogram Between 10 eV (GEANT4 Low Energy Limit) and 20 eV at Four Incident Energies Between 100 eV and 1000 eV.

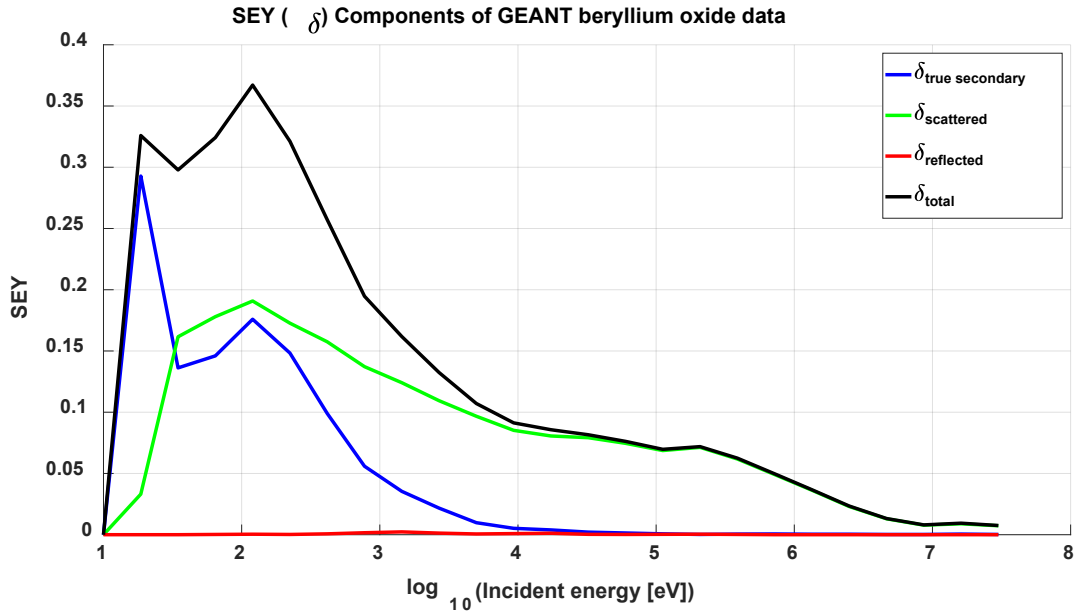


Figure D- 13: Beryllium Oxide SEY Components Generated by GEANT4; True Secondary Electrons are Defined to Have Energies Between 10 eV (low energy limit) and 15 eV.

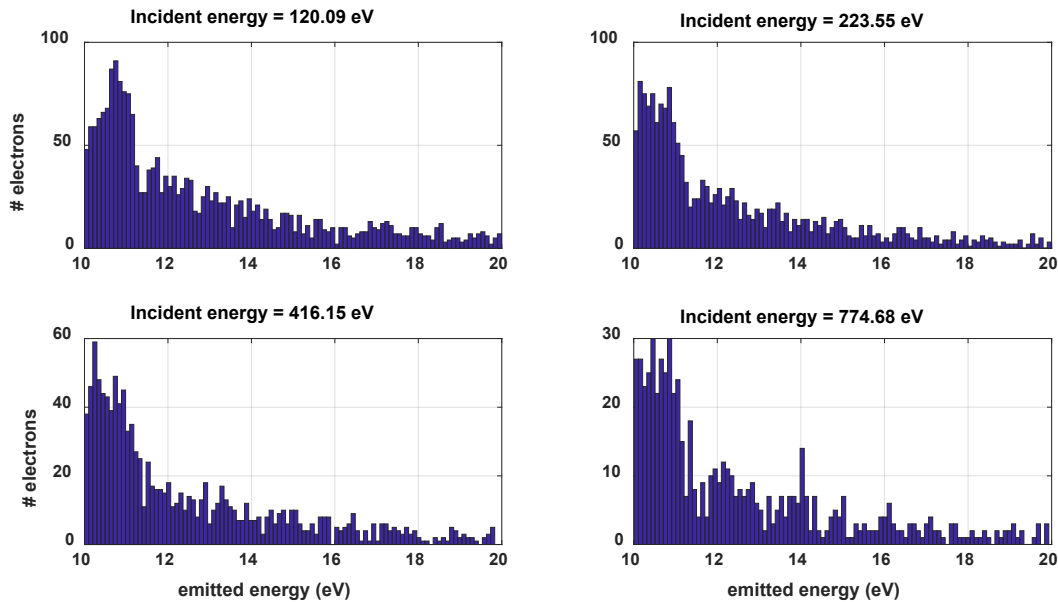


Figure D- 14: Beryllium Oxide Scattering Energy Histogram Between 10 eV (GEANT4 Low Energy Limit) and 20 eV at Four Incident Energies Between 100 eV and 1000 eV.

LIST OF SYMBOLS ABBREVIATIONS, AND ACRONYMS

$A(0)$	Normal-incidence peak magnitude for correction SEY curve, see section 4.1.4
$\delta_{\max 0}$	Maximum SEY at normal incidence in Vaughan model, see section 4.1.2
$E_c(0)$	Normal-incidence energy parameter for correction SEY curve, see section 4.1.4
E_0	Threshold energy in Vaughan model, see section 4.1.2
EES	Energy emission spectrum/spectra
$E_{\max 0}$	Incident energy at peak of Vaughan curve at normal incidence, see section 4.1.2
FWHM	Full width half max
HEP	High energy physics
HPM	High power microwave
$k(0)$	Normal-incidence width parameter for correction SEY curve, see section 4.1.4
k_s	General angle-dependence parameter for SEY, see sections 4.1.2 and 4.1.4
k_{sd}	Angle-dependence parameter for Vaughan SEY curve, see section 4.1.2
k_{se}	Angle-dependence parameter for Vaughan SEY curve, see section 4.1.2
k_{sd2}	Angle-dependence parameter for correction SEY curve, see section 4.1.4
k_{se2}	Angle-dependence parameter for correction SEY curve, see section 4.1.4
n	Shape parameter for correction SEY curve, see section 4.1.4
SEE	Secondary electron emission
SEY	Secondary electron yield
SM	Standard Model
θ	Incidence angle measured from surface normal

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