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Monte Carlo based corrections for the dosimetry of x-ray microbeams with diamond detectors

Richard P. Hugtenburg^{1,2} and Dimitri D. H. Reynard^{1,3}

¹Swansea University Medical School, Singleton Park, Swansea, SA2 8PP, UK

²Department of Medical Physics and Clinical Engineering, Singleton Park, Swansea Bay University Health Board, Swansea, SA2 8QA, UK

³Université Grenoble Alpes, 15 rue des Universités, St Martin D'Herès, Grenoble, 38400, France

E-mail: r.p.hugtenburg@swansea.ac.uk

Abstract. X-ray microbeams are a potential, novel mode of radiation therapy and dosimetry methods are under development that require micrometric spatial precision. The microDiamond detector has the requisite resolution and is composed of diamond which is closely tissue-equivalent. The high density of diamond however perturbs of secondary electrons and Monte Carlo methods are needed to determine corrections to accurately measure clinical parameters. The PENELOPE Monte Carlo code has been used to calculate corrections for the output factor (OF) and peak-to-valley dose ratio (PVDR). A high-performance computing (HPC) system was found to be necessary and the calculation took 72 hours when performed on a cluster of 100 CPUs. The correction for the output factor was found to be 1.009 ± 0.016 (2 s.d.). The correction factor for the peak-to-valley ratio was found to be 1.144 ± 0.013 (2 s.d.) and was larger due to Compton scattering of the microbeam in the extracameram components of the detector, in particular the 300 micron bulk diamond crystal. It was found that considerable improvements in efficiency could be achieved without loss of precision by switching off electron transport for electrons that are generated far from the sensitive element of the detector.

1. Introduction

Radiation therapy with X-ray microbeams is a promising avenue for the treatment of radioresistant tumours. X-rays from a 3rd generation synchrotron light-source has been proposed as method of achieving sufficient dose-rate for the microbeam delivery to be unaffected by patient motion (see recent reviews by Bräuer-Krisch *et al* 2015 [1] and Bartzsch *et al* 2020 [2]). Clinical aspects are discussed in the review of Grotsky *et al* 2015 [3]. Microbeam treatment fields are characterised by a large variation between high dose regions, due to the primary radiation (the peaks), and low dose regions, due to scattered radiation (the valleys). The difference in X-ray spectral quality and distribution of these dose components presents a considerable challenge to treatment planning and verification; in particular requiring that dosimeters have high orders of tissue-equivalence in addition to achieving the resolution necessary to resolve microbeams.

In this work we consider the use of the microDiamond (PTW, Freiburg, DE) detector, a dosimeter that has been shown to have good dose-rate linearity [4] as well as being able to accurately resolving microbeams [5]. The microDiamond detector is expected to have excellent tissue-equivalence due to its construction from chemical vapour deposition (CVD) diamond ($Z = 6$), however



the presence of the diamond bulk, with a density of 3.51 g cm^{-3} , generates perturbations in the secondary electron fluence, affecting the determination of shape of the microbeam as well as its response to photon radiation. Several other detectors have been considered for their use in microbeam dosimetry, with most achieving sufficiently high precision, but few achieving comparable tissue-equivalence. Of note is recent success in improving the precision of the readout from radiochromic film, which is closely tissue-equivalent in terms of effective atomic number, $Z_{\text{eff}} = 6.73$ [6], and density ($\rho \sim 1.4 \text{ g/cm}^3$), with a confocal microscopy [7].

The effects of departure from tissue equivalence can be accounted for with Monte Carlo modelling and a formalism that has been proposed by Bouchard *et al* 2015 [8], that offers a general approach to determining detector correction factors that accounts for the contribution from both the detector sensitive element and the extra-cameral components surrounding the sensitive volume, has been used here. Monte Carlo can be used in this way to predict the response of the detector due to variation in the photon spectrum with position and electron transport in the vicinity of the sensitive volume, however due to the complex structure of the diamond detector and the small sensitive volume, the approach requires the use of parallel Monte Carlo methods via a high-performance computer (HPC) system.

Two clinically important parameters are the output factor (OF) and the peak-to-valley dose ratio (PVDR). The output factor enables the dose to be calculated in the microbeam (the peak dose) from measurements of a broad-beam of similar quality, where an ionisation chamber measurement can be used in combination with a traceable dose-standard. The peak-to-valley dose ratio is used to calculate the dose between microbeams. As the valley-dose is due to scattered radiation it is diffuse and is expected to have similar clinical effect to a broad-beam. While the precision required for the microbeam dose is not currently known, it is reasonable to assume that the valley dose would need to be determined with comparable precision to conventional (broad-beam) radiation therapy, i.e. of order of 3%. Interestingly the scattering process that generates the valley dose is strongly influenced by the high degree of polarisation of the X-ray synchrotron beam source, which creates a distinct asymmetry in the shape of the valley dose distribution [10]. Polarisation has not been included in the modelling as the contribution from the square fields considered here to a central point of measurement of the OF and PVDR is independent of the polarisation. Calculations of the correction factors that need to be employed for measurements of the OF and PVDR with the microDiamond detector are presented and level of uncertainties in both cases will be discussed.

2. Methods

A model of the microDiamond has been built using the Monte Carlo code PENELOPE, consisting of a layer of $1 \text{ }\mu\text{m}$ thick aluminium that forms the Schottky diode on the surface of the sensitive layer of diamond of dimension $1.4 \text{ }\mu\text{m}$ thick, 2.2 mm diameter positioned on a diamond bulk of thickness $300 \text{ }\mu\text{m}$ and encased in epoxy resin and polyether ketone polymer (PEEK) and contained within an aluminium and RW3 water-equivalent plastic housing (figure 1). Apart from the aluminium layer, no attempt has been made to model the electrical contacts or stem.

The microbeam field has been modelled with an overall dimension of $2 \times 2 \text{ cm}^2$, with $50 \text{ }\mu\text{m}$ microbeams repeated every $400 \text{ }\mu\text{m}$. The $50 \text{ }\mu\text{m}$ microbeams were assumed to be parallel and incident perpendicular to the water phantom. This approximation is expected to be reasonable given the large distance from the synchrotron wiggler insertion device to the phantom. A photon spectrum derived for the ID17 beamline at ESRF in a previous study [11] has been used. The X-ray energy ranges from 50 keV to 300 keV with a peak intensity at 90 keV . The assumption of negligible primary beam between microbeams may be unreasonable if the collimator system forming the microbeam is not sufficiently thick and in practice it may be necessary to determine a contribution to the valley dose due to leakage.

Calculations were performed for the detector placed in central peak and valley positions at a depth of 2 cm in a water phantom. Use was made of splitting in order to lend importance to photon and electron trajectories traversing the small sensitive volume of the diamond, with the calculation taking 72 hours of real-time with 200 processors, achieving a statistical precision of 2% (2 s.d). The

calculation is repeated with all of the components of the detector replaced with water and one further calculation of the detector placed in an open 2×2 cm² field was required to compute the output factor.

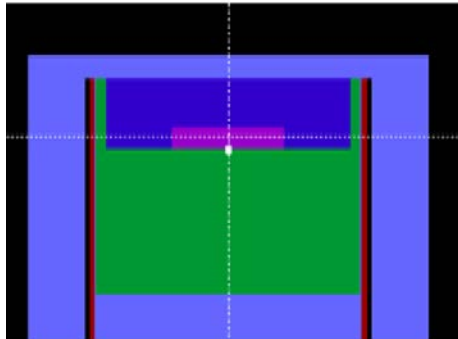


Figure 1. Scale model used with the PENELOPE Monte Carlo code. The diamond bulk (magenta) is surrounded by epoxy resin (blue) and PEEK plastic (green), contained in an aluminium lined (red) RW3 (black) housing of overall diameter 6.9 mm. The detector is surround by water (blue) and positioned at a depth of 2 cm. The sensitive diamond layer above the diamond bulk and the aluminium surface are not visible in the diagram.

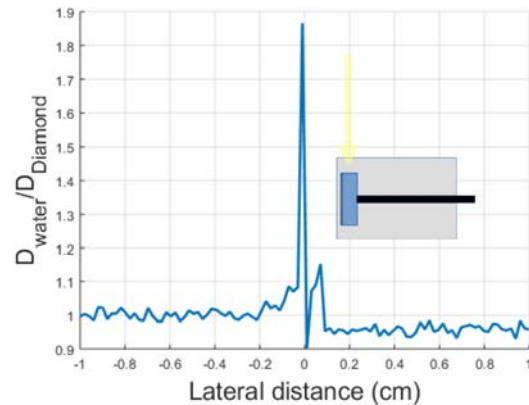


Figure 2. Relative response of the microDiamond as a function of distance from the center of a single microbeam. The response depends on the direction of secondary electrons entering the sensitive volume of the diamond. The inset shows the arrangement of the beam and the orientation of the detector relatively to the x-axis, where the beam in the example given is at a position -0.02 cm from the sensitive volume.

3. Results

The relative response of the microDiamond to a water-equivalent medium was calculated in 200 μ m steps for a range of distances from -1 to 1 cm from a single 50 μ m wide microbeam (figure 2). The contribution for each microbeam to the peak and to the valley is determined by summing the energy deposition from all 50 microbeams. The correction factor determined for the measurement of the central peak was found to be 1.103 ± 0.007 , due predominantly to the microbeam that straddles the sensitive volume. The lower cross-section of carbon versus water at these energies reduces the response of the diamond detector while the higher density of the diamond bulk on the range of Compton electrons increases it slightly. The correction factor for the open 2×2 cm² field was found to be 1.089 ± 0.010 , therefore the overall correction to the output factor is 1.009 ± 0.016 . The correction factor for the center-most valley is 0.964 ± 0.007 and the overall correction factor for the peak-to-valley ratio was 1.144 ± 0.013 .

Although the overall correction factors for the valley dose measurements is small, large variations in the response to microbeams in the vicinity of the sensitive volume are evident, and balance to an extent. These variations are shown to be due to extracamerall components of the detector which have a particularly strong influence on the response of the detector when measuring immediately adjacent valleys. It is found that Compton scattering of a microbeam traversing the diamond bulk leads to enhancement factor of 1.9, while Compton scattering in the PEEK plastic (density = 1.32 g cm^{-3}) and RW3 (density = 1.045 g cm^{-3}) components leads to a smaller, but non-negligible enhancement of the response of approximately 1.1, where it is noted that RW3 has a small (0.2%) but non-negligible titanium ($Z=22$) content. Asymmetry in the response at distances further from the sensitive volume is due to two effects, the difference in scattering conditions for the diamond detector which increases the response and the reduced response to those photons when they interact in the vicinity the diamond sensitive layer, which decreases the response.

Although the calculation time was expected to be large, as the sensitive volume presents a cross-section that is 3.5 million times smaller than the open field, it has been shown that control of the range of secondary electrons can additionally boost the speed of the calculation substantially. For example it is reasonable to assume that electron transport is only important in the vicinity of the microbeam and that electrons generated by the Compton scatter of the primary microbeams will not reach the sensitive volume for all microbeams, apart from the central microbeam. The speed-up associated with these additional approximations is a factor of 20, which would reduce the overall calculation time to 720 hours, easily accessible on modern HPC systems.

4. Conclusions

Despite the excellent tissue-equivalence of the diamond detector a significant correction is shown to be required due to the perturbation of electron fluence in the vicinity of the diamond crystal. Monte Carlo calculations on a HPC system have shown that the corrections are, in the case of the clinically important peak-to-valley ratio, significant and as expected time-consuming. The analysis points to potential improvements in the efficiency of the calculation and confidence in the use of diamond detectors as a convenient on-line dosimetry method.

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