Modelling single shot damage thresholds of multilayer optics for high-intensity short-wavelength radiation sources

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Abstract: The single shot damage thresholds of multilayer optics for high-intensity short-wavelength radiation sources are theoretically investigated, using a model developed on the basis of experimental data obtained at the FLASH and LCLS free electron lasers. We compare the radiation hardness of commonly used multilayer optics and propose new material combinations selected for a high damage threshold. Our study demonstrates that the damage thresholds of multilayer optics can vary over a large range of incidence fluences and can be as high as several hundreds of mJ/cm². This strongly suggests that multilayer mirrors are serious candidates for damage resistant optics. Especially, multilayer optics based on Li₂O spacers are very promising for use in current and future short-wavelength radiation sources.

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1. Introduction

Multilayer coated optics [1] are used in many experiments at the new generation of extreme ultraviolet (XUV) and soft X-ray (SXR) radiation sources. These short-wavelength Free Electron Lasers (FELs) [2], High Harmonic Generation [3,4] and plasma-based X-ray lasers [5,6] instruments provide ultra-short (from atto- to nanoseconds) pulses of very high intensity that may induce radiation damage in optical coatings. To take full advantage of these high-intensity short-wavelength radiation sources, optics are required that can withstand high powers. Studies on the radiation hardness of optics are, therefore, of high importance. Previously, single shot damage to multilayer optics has been studied to understand the underlying physical mechanisms [7–10]. A model that explains the damage induced by femtosecond XUV pulses, in Mo/Si and MoN/SiN multilayer optics, was developed [7,8]. Recent results on Mo/Si, irradiated with the higher photon energies available at the LCLS source (Stanford, USA) support the model [11]. Experiments and modelling reveal that the onset of damage occurs when the temperature in one of the material layers reaches its melting temperature.

Systematic experimental studies on damage by high-intensity sources, however, are scarce due to the limited access to such sources. For that reason, we performed a theoretical investigation to predict and compare the single shot damage thresholds of several multilayer material combinations. For our studies, we selected commonly used materials for multilayer optics, as well as new material combinations that are appropriate for short wavelengths in the XUV and SXR ranges. In this work, our selection criteria placed priority on increasing the damage threshold rather than on optimizing the reflectance. The results are important for optimizing the design of optics for current and future short-wavelength radiation sources.
2. Modelling and material selection criteria

2.1. Modelling parameters

The model developed to estimate the multilayer damage threshold of multilayer optics under irradiation with femtosecond XUV/SXR pulses is described in detail in [7,8]. In summary: the incident radiation is primarily absorbed by electrons in the multilayer structure. The locally deposited energy density is proportional to the product of the local field intensity, the real part of the refractive index, and the absorption coefficient. It is worth mentioning that the maximum absorbed energy density at the sample surface corresponds to the resonant irradiation conditions with maximum reflectance. In a typical situation, the depth profile of the absorbed energy density is non-uniform with local maxima in the reflector layers.

Photoelectrons, with kinetic energies in the order of hundreds eV, have a mean free path that is in the order of a few Angstroms [12] and ballistic transport of energy occurs on a length scale equal to the thickness of up to a few bilayers. Secondary electrons are excited by photoelectrons, due to Auger electron emission and impact ionisation. Their energy is smaller than that of the primary electrons and their mean free path is also smaller, which results in a smaller energy dissipation range. Due to the energy exchange between excited electrons, the electron population thermalizes at elevated temperatures. This happens on a time scale of 100 fs. Further energy transport can be described by thermal diffusion in the electron gas. The large temperature difference between the spacer and reflector layers on a very short length scale (single layer thickness) creates very large temperature gradients, which makes the diffusive energy transport very fast.

In contrast, the mean temperature gradient over the full multilayer structure and substrate is much lower and corresponds to the exponential decay of the absorbed energy density. The energy transfer on this length scale is much slower (orders of magnitude). One can assume that it is not significant on a time shorter than the time scale of the heat exchange between the electron population and the lattice. This happens on a time scale of picoseconds and leads to the increase of the lattice temperature and decrease of electron temperatures, until they (locally) equalize. Such a state is considered as the initial state for calculation in the model. It is characterized by a smooth temperature profile, which is the same for the electrons and the lattice over the full multilayer and substrate structure. Since the thickness of the bilayers is much smaller than the length scale of the exponential decay of the absorbed energy density, each bilayer is assumed to have a flat temperature profile that can be estimated from the deposited energy density (averaged over each bilayer) and the temperature dependent enthalpy of the materials.

The process of energy dissipation into the substrate cools down the sample to room temperature on a microsecond time scale [7,8]. In a solid material this is too fast for the atoms to move significantly and to influence the interfaces or the layer structure. However, in a melted material, the atomic diffusivity is enhanced by many orders of magnitude as compared to a solid - 13 orders of magnitude in liquid silicon (10^{10} nm^2/s in liquid silicon compared to 10^{-3} nm^2/s in solid silicon, just below the melting temperature), for example [7]. In the case of melted material, atomic interdiffusion can occur on a nanosecond time scale, before the melted layers solidify. As a result the structure of the multilayer coating is disturbed, either due to decreased interface sharpness, or to complete destruction of the layer structure. This leads to the loss of reflectance (partially or completely, respectively). Both situations are considered as damage of the multilayer structure. It was shown by Khorsand et al. [7] and Sobierajski et al. [8] that permanent damage occurs when the average bilayer temperature reaches the melting temperature of one of the materials. Thus, the model-predicted damage threshold is the radiation fluence for which the average temperature in the top bilayer equals the melting temperature of one of the bilayer materials.

Using this model, the calculated damage thresholds of Mo/Si and MoN/SiN were found to correspond to the damage thresholds obtained experimentally for irradiations with
femtosecond pulses at 13.5 nm wavelength \[7,8\]. Moreover, similar damage mechanisms (induced by melting of layers) were observed for the case of irradiation with nanosecond pulses \[9\]. However, the damage thresholds obtained experimentally with nanosecond pulses were much higher (an order of magnitude) than those obtained with femtosecond pulses and our model. This is because the pulses were much longer and significant heat dissipation occurs during irradiation. Nevertheless, the results indicate that our model is still able to estimate the lower limit of the damage threshold in the case of nanosecond pulses.

We now apply the model to other material combinations. We have calculated the damage thresholds of multilayer optics, deposited on a crystalline Si substrate, based on the optical constants, material constants (molar mass, density and melting temperature) and the temperature dependent enthalpy of Li, Li\(_2\)O, B, B\(_4\)C, a-C (amorphous carbon), a-Si (amorphous silicon), Si, SiC, Si\(_3\)N\(_4\), Sc, Ti, V, Cr, Fe, Co, CoO, Ni, NiO, Cu, Mo, Mo\(_2\)B\(_5\), Mo\(_3\)C, Ru, Sb, La, W and Pt \[13,14\]. With the exception of a-C and a-Si, all materials are assumed to be crystalline, since no enthalpy values of amorphous materials are available. In addition, we assume that the melting temperature of bulk materials apply to the very thin layers in the multilayers.

To give an illustration of the difference in damage threshold values for multilayers containing crystalline or amorphous layers, we compared Mo/Si multilayers having different properties of the silicon layers. In the calculations, we checked the influence on the damage threshold of individual parameters: the melting temperature, the temperature dependent enthalpy, and the optical constants. Substituting the optical constants of crystalline Si to that if amorphous Si has no effect on the damage threshold. Substituting the enthalpy of crystalline Si to that of amorphous Si, the damage threshold is increased by approximately 6%. Finally, when changing the melting temperature from 1687 K (crystalline Si) to 1250 K (amorphous Si), the damage threshold is decreased by approximately 34%. Within this temperature range, the damage threshold depends linearly on the melting temperature. We presume that the difference between the melting temperatures of crystalline and amorphous materials has the largest influence on the damage thresholds for all multilayer systems. Therefore, it is preferred to make multilayer optics with crystalline layers in order to increase the radiation hardness.

In our model, it has been assumed that there was no interface diffusion or roughness (\(\sigma = 0\) nm) hence, no compound formation is taken into account. This simplifies the modelling and comparison between different systems, while also providing the most accurate damage threshold predictions. The latter is often true because damage is caused by melting, so compound formation can only reduce the damage threshold if the compound has a lower melting temperature than its components.

We consider coatings consisting of 600 bilayers because deposition of such stacks has been demonstrated to be experimentally achievable by energy-modulated ion-assisted deposition to reduce the interface roughness and interdiffusion \[15\]. It has been shown that the reflectance of a 600 Cr/Sc bilayer mirror can reach 20.7% at near-normal incidence. In our model, the maximum reflectance and damage thresholds as a function of photon energy in the range of 60-620 eV (20 to 2 nm wavelengths) are calculated. We consider the light to be incident at normal incidence, while the multilayer optic is considered to have an optimized period, \(d\), so that the well-known modified Bragg’s law is satisfied \[16\]:

\[
\lambda = 2d \cos \theta \sqrt{1 + \frac{n^2 - 1}{\cos^2 \theta}},
\]

where \(\theta\) is the angle from normal incidence and \(n = 1 - \delta + i\beta\) is the mean of the refractive index of the multilayer, with \(\delta = (d_a \delta_a + d_b \delta_b) / (d_a + d_b) = \Gamma \delta_a + (1 - \Gamma) \delta_b\), and \(\beta = \Gamma \beta_a + (1 - \Gamma) \beta_b\). Material A corresponds to the reflector layer and B to the spacer layer.
where \( d_A \) and \( d_B \) are the layer thicknesses (with \( d_A + d_B = d \)) and \( \Gamma \) is the material thickness ratio. Due to the restrictions mentioned above, the present study of the multilayer optical damage thresholds should be, in the first instance considered as qualitative. Nevertheless, it represents the first investigation of this kind and provides new candidate multilayer systems that offer promise for optics suitable for high-intensity short-wavelength radiation sources.

2.2. Material selection criteria

To obtain the highest reflectance, the best pair of reflecting and spacer materials will have a high optical contrast, minimal absorption and form smooth and compositionally abrupt interfaces [17]. The general selection criteria are given by (1) high refractive index contrast between the reflector and spacer, (2) low extinction coefficients, (3) low miscibility between the material pairs, i.e., low interdiffusivity and low chemical reactivity, (4) smooth and continuous growth properties, and (5) ease of use. Ease of use is determined by availability, and health and safety concerns [17]. Besides the highest achievable reflectance also bandwidth, stress and lifetime (long term thermal stability) are considered important for most applications.

For normal incidence reflection of wavelengths in the range 2.3 – 4.4 nm, low miscibility and smooth growth properties become increasingly important, due to the very small multilayer period. This is because the Debye-Waller factor and the ratio \( \sigma/d \) plays an increasingly dominant role in determining the reflectance of the multilayer. Though, here we note that that \( \sigma \) relates to a combination of the interface roughness \( \sigma_i \) and interdiffusion \( \sigma_d \) \(( \sigma^2 = \sigma_i^2 + \sigma_d^2 ) \) [16,18]. The influence of \( \sigma \) becomes apparent when one compares the experimental maximum reflectance with the theoretical maximum reflectance of multilayer systems [19]. For these short wavelengths the experimental values are much smaller (less than half) than the theoretical maxima. In most cases, this is related to the fact that the combinations of materials with high optical contrast have a large negative formation enthalpy \( \Delta H_f \) and, hence, there is a high probability of forming compounds at the interfaces, which decreases the optical contrast inside the multilayer. It has been found that, in practice, the highest reflectance is obtained using material pairs that have positive (or slightly negative) \( \Delta H_f \) [17]. We propose to use alternative materials for multilayer systems in the SXR region, based on the criteria of positive \( \Delta H_f \) [20], which will be discussed in section 3.

In addition, since, for the intense short-wavelength radiation sources, one of the most important selection criterion is the damage threshold, instead of the maximum (theoretical) reflectance. Hence, we also consider material pairs that have a mutually positive \( \Delta H_f \) and not necessarily the highest possible optical contrast. Moreover, since such systems are more likely to have sharper interfaces (\( \sigma \) approaches 0), they could have a comparable or even higher experimentally realizable reflectance than multilayers with the highest optical contrast and negative \( \Delta H_f \). Furthermore, the positive \( \Delta H_f \) holds promise for improving interface sharpness via controlled annealing [21–23].

The multilayer material combinations investigated here can be categorised in four groups, optimized for photon energies below (1) the boron absorption K-edge (188 eV; 6.6 nm); (2) the carbon edge (284 eV; 4.4 nm); (3) the scandium edge (420 eV; 3.1 nm), and (4) in the complete water window (284 – 532 eV; 4.4 – 2.3 nm).

3. Results and discussion

3.1 Boron edge

W/B_4C, Ru/B_2C, Mo/B_4C, Mo/B, La/B_4C and La/B are widely used in multilayer systems for photon energies below the boron absorption K-edge. The theoretically calculated maximum reflectance and damage thresholds as a function of photon energy of the first 5 material combinations above are shown in Fig. 1. These calculations as based on ideal (\( \sigma = 0 \)) multilayer structures (600 bilayers) of these material combinations using a reflectance-

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optimized $\Gamma$ value of 0.4. La/B was found to be comparable to La/B$_4$C and is omitted in the graph for sake of clarity. Also plotted in Fig. 1 are the curves for Mo$_2$B$_5$/B$_4$C, for reasons that will be explained below.

From Fig. 1 it can be seen that below the boron absorption edge multilayers with La as the reflecting layer show the highest reflectance while lowest reflectance is obtained from W. In practice, the highest reflectance has been obtained with La/B$_4$C with a reflectance of 49% near-normal incidence [24]. From Fig. 1 it can also be seen that both La- and W-based multilayers have the lowest damage thresholds, but for different reasons. For La, the low damage threshold can be ascribed to the low melting temperature of La. For W, however, the low damage threshold is due to the high absorption of W, which results in a high average bilayer temperature and subsequent melting of B$_4$C or B. Because Mo has a lower absorption coefficient than W, Mo-based multilayers have a much higher damage threshold than W-based multilayers. Mo/B$_4$C has a higher damage threshold compared to Mo/B, which has a higher reflectance. This is due to the higher melting temperature of B$_4$C (2740 K) compared to B (2350 K). Ru/B$_4$C shows a higher reflectance than Mo/B$_4$C, but has a lower damage threshold, due to the lower melting temperature of Ru (2607 K).

The Mo/B and Mo/B$_4$C multilayers, however, form thick interfaces of molybdenum borides during deposition, due to the large negative $\Delta H_f$ between Mo and B (larger than between Mo and C), which reduces the contrast and, hence, the maximum reflectance [25]. Substituting the Mo layer with a layer of molybdenum boride to create a Mo$_2$B$_5$/B$_4$C multilayer, leads to a reduced chemical driving force for interdiffusion and, hence, results in a thermally more stable multilayer [23,26]. In addition, this system shows smoothening of the interfaces by controlled annealing, which results in a reflectance (of 24%) comparable to that of an as-deposited Mo/B$_4$C multilayer system, despite the lower theoretical maximum reflectance of Mo$_2$B$_5$/B$_4$C [25]. From Fig. 1 it is evident that the Mo$_2$B$_5$/B$_4$C multilayer system has the highest damage threshold with a maximum of 463 mJ/cm$^2$ in the vicinity of the absorption edge. Therefore, Mo$_2$B$_5$/B$_4$C fulfils our selection criteria and is a very promising candidate for use in intense short-wavelength radiation sources.

As mentioned above, La-based multilayers have the highest reflectance but, due to the very low melting temperature of La (1193 K), these multilayers are not suitable for use in intense radiation sources. In contrast, LaN has a much higher melting temperature (2723 K), and the reflectance curve is almost unchanged compared to La-based multilayers. Unfortunately, no temperature dependent enthalpy values are known for LaN, so we could not calculate the damage threshold. To obtain an approximate damage threshold, we used the material and optical constants of LaN and the enthalpy values of La to calculate the damage threshold of LaN/B$_4$C. In the likely situation that the enthalpy values of LaN are higher than those of pure La, the calculated damage thresholds are likely to be underestimated. Under this assumption, the calculated damage threshold of LaN/B$_4$C is indeed much higher than that of La/B$_4$C. Our calculations show that LaN/B$_4$C has a maximum damage threshold of 342 mJ/cm$^2$ around the absorption edge, which is even higher than that of Mo/B$_4$C.
Fig. 1. Reflectance and damage threshold for multilayers optimized for photon energies below the boron absorption K-edge, using $\Gamma = 0.4$. Mo$_2$B$_5$/B$_4$C exhibits the highest damage threshold.

3.2. Carbon edge

Theoretically, high reflectance optics for photon energies below the carbon absorption K-edge can be obtained with C as the spacer layer and V, Cr, Co, Fe or Ni as the reflector layer displaying large optical contrast. These systems have been extensively studied [19], however, they show much lower experimental reflectance because of roughness and intermixing at the interfaces. W/C is often used despite its lower theoretical maximum reflectance. The best performances in practice have been achieved in optics designed to operate at large angles of incidence, allowing larger multilayer periods. In these cases, Co/C and Ni/C, which form the sharpest interfaces, are the materials of choice [27]. The best performance at near-normal
incidence has been achieved with Co/C multilayer optics showing a reflectance of 15% [28]. It should be noted that Co and Ni are the only materials that have a positive $\Delta H^\circ$ when combined with C.

Figure 2 shows the maximum theoretical reflectance and damage thresholds of the above-mentioned systems for 600 bi-layer optics and near-optimum $\Gamma = 0.3$. Curves for CoO/C and LaN/C are also plotted, and will be discussed below. Despite the highest experimental reflectance, the calculated damage thresholds for Co/C and Ni/C are the lowest among all the
investigated systems. For the pure metallic reflector layers, the highest damage threshold is obtained from V/C. The damage threshold is the highest for V and decreases for Cr, Fe, Co and Ni, respectively, which can be directly related to the decreasing melting temperature of these materials. W/C has a low damage threshold due to the large absorption in W and the resulting high average bilayer temperature.

With the aim of overcoming the low damage threshold of Co/C, we investigated CoO/C because CoO has a much higher melting temperature (2206 K) than Co (1768 K). Indeed, from Fig. 2 it can be seen that the damage threshold is increased by a factor of 2 with respect to pure Co, and the peak reflectance is also slightly higher. Furthermore, passivation with oxygen or nitrogen could result in better separation between the layers and, hence, multilayers with sharper interfaces and reflectance values that are higher in practice [29].

In analogy to the discussion on the boron edge, LaN could also be an interesting reflector material, despite its low optical contrast with C. Indeed, the maximum reflectance of LaN/C is comparable to that of the other multilayer systems, except that the peak of maximum reflectance below the C edge is very narrow. Most interestingly, the calculated damage threshold of LaN/C (where the La enthalpy have been used in calculations) below the C edge is dramatically higher than that of all the other multilayer structures, which makes it a very promising candidate for optics subjected to intense radiation sources.

It should be noted that damage to multilayers containing amorphous carbon could start at lower radiation fluences than calculated above. Recently, it was shown that a 40 nm thick amorphous carbon layer will crystallize when irradiated by femtosecond 830 eV x-ray FEL pulses [30]. This graphitization was observed to occur at 1050 K, much below the melting temperature (3900 K) of carbon. If we assume that, at photon energies below the carbon absorption edge, this phase transition occurs also at 1050 K, then the values of the calculated damage threshold, as plotted in Fig. 2, are drastically lowered, as illustrated in Fig. 3. To avoid damage by graphitization, one could induce this phase transition in the entire multilayer by controlled annealing.

![Graph showing damage thresholds for carbon based multilayers optimized for photon energies below the carbon absorption K-edge. Here it is assumed that graphitization at 1050 K is the primary cause of damage.](image-url)
3.3. Scandium edge

The scandium absorption edge is one of the few edges located in the biologically important water window. This wavelength regime requires multilayers having very small periods. Due to an increased influence of interface imperfections on the reflectance for smaller periods (related to the Debye-Waller factor) [18], there exist only a few known high-reflecting multilayer systems. Theoretically, Fe, Co and Ni have high optical contrast with spacer materials like Sc, Ti, V, and Cr. However, none of these multilayer material combinations have shown high reflectance at near-normal incidence (where the smallest periods are required), because of the large intermixing, which is itself related to the negative formation enthalpies of compounds [18]. The best performance in the water window regime has been achieved using Cr/Sc with a reflectance up to 20.7% [15,31], despite the lower optical contrast between Cr and Sc. This can be attributed to the formation of sharper interfaces, which is related to the slightly positive formation enthalpy for the combination of Cr and Sc. An even higher reflectance (32%) was achieved using B₄C as a barrier layer between Cr and Sc [32].

Since Cr/Sc has the highest experimental reflectance in the water window, we studied the damage threshold of Cr/Sc and other multilayers optimized for the scandium absorption L-edge.

In Fig. 4, the reflectance and damage threshold of the commonly used Cr/Sc, Fe/Sc, and W/Sc multilayers are plotted. As before, Γ is optimized for reflectance at the Sc edge. The curves for newly proposed V/Sc, La/Sc, and LaN/Sc multilayers are also plotted. V and La have a smaller optical contrast with Sc, but the large positive enthalpy of formation could result in a higher reflectance after deposition. Despite having lower optical contrast, V/Sc shows the highest theoretical peak reflectance for a multilayer with 600 bilayers, though the width of the main reflectance peak is narrower. In addition, V/Sc has the highest damage threshold, followed by Cr/Sc. Again, the W-based multilayer has a low damage threshold, due to absorption, while La/Sc has the lowest damage threshold, due to the low melting temperature of La. Using LaN instead of La results in a similar reflection curve and an increase of the damage threshold value by a factor of almost 2, which is still much lower than that of V/Sc and Cr/Sc below the Sc edge itself.

The widely used Cr/Sc system seems to be a good multilayer, based on the damage threshold below the Sc edge. Nonetheless, V/Sc may be better, because it has a slightly higher damage threshold and the possibility of higher experimental reflectance, due to the formation of sharper interfaces, which could be improved by controlled annealing. An additional advantage of V/Sc is that it has a second reflectance peak inside the water window at the V absorption edge, situated at 513 eV (the Cr edge is beyond the water window at 575 eV). By adjusting the Γ value of V/Sc to around 0.65, the theoretical maximum reflectance below the V edge reaches 40%.
3.4. Water window

As an alternative for currently used multilayer systems with limited performance in the water window, we propose new material combinations that use Li$_2$O as a spacer material. Pure Li has optimum optical constants throughout the full water window region [33] and a positive ΔH$^\circ$ with most materials, but has a very low melting temperature (454 K) and is, therefore, not suitable for making a damage resistant multilayer. Li$_2$O and LiF, in contrast, have much higher melting temperatures (1843 K and 1118 K respectively), while still possessing optical properties that are very good for spacer materials. Because Li$_2$O has the highest melting
temperature, we chose this material as spacer and calculated the damage thresholds of Li$_2$O-based multilayers with different reflector materials. To the best of our knowledge, Li$_2$O spacers have never been investigated for optical multilayers, with only a single mention as a possible spacer material [34].

The materials with highest optical contrast and reasonably low absorption are Fe, Co, Ni and Cu, which have melting temperatures of 1811 K, 1768 K, 1728 K, and 1357.6 K, respectively. The oxides of these materials have lower extinction coefficients but less optical contrast with Li$_2$O. However, of all oxides, CoO and NiO have the highest melting...
temperatures of 2206 K and 2228 K, respectively, and could, therefore, still be interesting as high damage threshold multilayers. Furthermore, the highly negative formation enthalpy of the pure metals with oxygen could lead to the extraction of oxygen from Li$_2$O, leading to less sharply defined layers. This problem could be diminished by using CoO and NiO as reflecting layers. The reduced intermixing could then result in better defined layers and, hence, in an experimentally achievable reflectance closer to the theoretical maximum.

Figure 5 shows the calculated reflectance and damage thresholds for these multilayer systems for $\Gamma = 0.3$. All the systems we propose exhibit reflectance of more than 20% across the full water window. This is in contrast to the narrow reflectance peaks of the currently used multilayer optics, which are optimized below the (few) absorption edges. Co/Li$_2$O has the highest reflectance. Pure metal reflectors show a peak in reflectance at the oxygen K-edge (532 eV), while CoO and NiO lose some reflectance near the O edge, because of reduced optical contrast. The damage thresholds of a Li$_2$O spacer, paired with Fe, Co, Ni, and Cu decrease with decreasing melting temperature of the metal layers, which are the first to melt and, therefore, the layer where damage is initiated. The highest damage threshold is obtained from NiO and CoO, where Li$_2$O is the layer that melts. The drop in the damage threshold for multilayers containing CoO for energies above 440 eV is due to damage to the Si substrate, because 600 bilayers are not sufficient to saturate the reflectance near the O edge.

Taking into account the damage threshold, the theoretical and expected reflectance after growth, the best multilayer candidate for the full water window region is NiO/Li$_2$O. For applications where high reflectance is more important, Co/Li$_2$O is the best multilayer choice, while still possessing a very high damage threshold.

The large reflectance bandwidth of Li$_2$O-based multilayers makes them especially interesting for applications where wavelength scanning is required. Although this can be implemented in the usual way by changing the angle of incidence using a fixed multilayer period, we propose another method: by using laterally-graded multilayers (normally used for angle compensation) the mirror position can be scanned to select the desired wavelength in the full water window range, while maintaining operation at near-normal incidence angles. Furthermore, Li$_2$O-based multilayers have the potential to significantly advance the development of compact SXR microscopes to support a broader use in the research community and industry [35–39].

4. Summary and conclusions

The success of high-intensity short-wavelength radiation sources depends, to a large extent, on the availability of optics that can withstand high power loads. Damage studies on optics are, therefore, of high importance for good design choices of optics in beamlines and end-stations at current and future radiation sources. Experimental studies on damage by high-intensity sources, however, are scarce, due to the limited access to such sources. For that reason, we performed a theoretical investigation on many material combinations for multilayer optics for XUV and SXR radiation.

Single shot damage thresholds were calculated for several commonly used, and newly proposed material combinations for multilayer optics. We used a model that was developed to investigate the damage mechanisms in Mo/Si and MoN/SiN multilayers, to study multilayers suitable for wavelengths down to 2 nm. The current study represents the first investigation of this kind on the multilayer damage thresholds.

We consider multilayers usable below different absorption edges and in the water window, and propose several new multilayer systems. For the boron edge the most promising multilayer with high damage threshold is Mo$_2$B$_5$/B$_4$C, however, LaN/B$_4$C is also expected to have a high damage threshold. For the carbon edge, CoO/C appears to be a good alternative to Co/C and V/C, while LaN/C is also promising. For the scandium (and vanadium) absorption edge we propose to use V/Sc instead of the commonly used Cr/Sc. The multilayer that shows the most potential is NiO/Li$_2$O, with a calculated damage threshold of more than 500 mJ/cm$^2$.
near the oxygen absorption edge. This multilayer system could simplify experiments designed for applications in the water window regime. As an overview, the most interesting multilayer combinations are displayed in Fig. 6, which shows the theoretical maximum reflectance and the calculated damage thresholds as a function of the photon energy in the range of 60 to 620 eV.

Our investigation demonstrates that the damage threshold of multilayers can vary over a large range, from a few tens to hundreds of mJ/cm². This finding also allows us to conclude that multilayer mirrors are serious candidates for damage resistant optics.

Fig. 6. Reflectance and damage threshold for several multilayers optimized for photon energies below different absorption edges and the water window.
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