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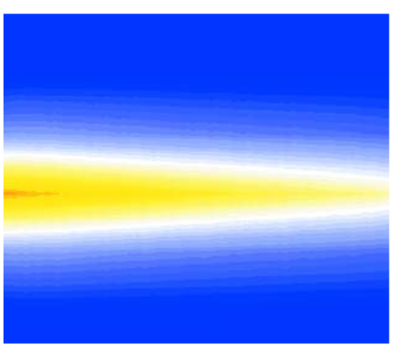

Time and space resolved modelling of the heating induced by synchrotron X-ray nanobeams

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X-ray synchrotron sources, possessing high power density, nanometric spot size and short pulse duration, are extending their application frontiers up to the exploration of direct matter modification. In this field, the use of atomistic and continuum models is now becoming fundamental in the simulation of the photoinduced excitation states and eventually in the phase transition triggered by intense X-rays. In this work, the X-ray heating phenomenon is studied by coupling the Monte Carlo method (MC) with the Fourier heat equation, to first calculate the distribution of the energy absorbed by the systems and finally to predict the heating distribution and evolution. The results of the proposed model are also compared with those obtained removing the explicit definition of the energy distribution, as calculated by the MC. A good approximation of experimental thermal measurements produced irradiating a millimetric glass bead is found for both of the proposed models. A further step towards more complex systems is carried out, including in the models the different time patterns of the source, as determined by the filling modes of the synchrotron storage ring. The two models are applied in three prediction cases, in which the heating produced in $Bi_2Sr_2CaCu_2O_{8+\delta}$ microcrystals by means of nanopatterning experiments with intense hard X-ray nanobeams is calculated. It is demonstrated that the temperature evolution is strictly connected to the filling mode of the storage ring. By coupling the MC with the heat equation, X-ray pulses that are 48 ps long, possessing an instantaneous photon flux of $\sim 44 \times 10^{13}$ photons s^{-1}, were found to be able to induce a maximum temperature increase of 42 K, after a time of 350 ps. Inversely, by ignoring the energy redistribution calculated with the MC, peaks temperatures up to hundreds of degrees higher were found. These results highlight the importance of the energy redistribution operated by primary and secondary electrons in the theoretical simulation of the X-ray heating effects.

1. Introduction

Since the first-generation synchrotrons, X-ray source characteristics have evolved under the strong demand for higher and higher spatial and temporal resolution. Today, peak brilliances up to 10^{26} photons s^{-1} mm^{-2} $mrad^{-2}$ (0.1% bandwidth)$^{-1}$ are achieved with third-generation synchrotron sources, and X-ray beams with nanometric spot sizes of ~50–100 nm and pulses of hundreds of photons s^{-1} with energies in the pJ range are routinely achieved (Mino *et al.*, 2018; Martínez-Criado *et al.*, 2016). However, the downside of this ongoing evolution of X-ray sources is that such beam characteristics can exceed the threshold where photon-flux density can affect the organization of matter (Bras & Stanley, 2016).