Applying DFTB approach to study X-ray-induced phase transitions in solids

Vladimir Lipp[1*], Victor Tkachenko[2,3,1], Michal Stransky[3,4], Bálint Aradi[5], Thomas Frauenheim[5,6] and Beata Ziaja[1,2**]

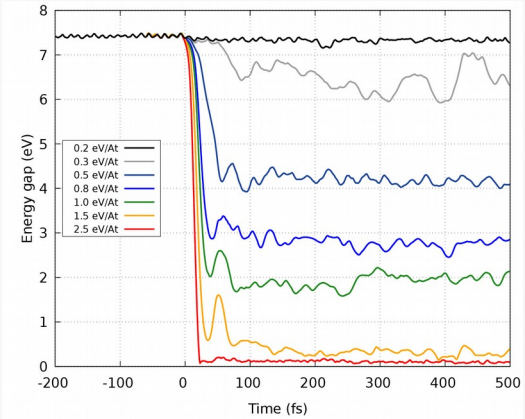
[1] Center for Free-Electron Laser Science CFEL, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany; [2] Institute of Nuclear Physics, Polish Academy of Sciences, Kraków, Poland; [3] European XFEL, Schenefeld, Germany; [4] Institute of Physics of the Czech academy of Sciences, Prague, Czech Republic; [5] Bremen Center for Computational Materials Science, Universität Bremen, Bremen, Germany; [6] Computational Science Research Center (CSRC) Beijing and Computational Science Applied Research (CSAR) Institute Shenzhen, Shenzhen, China

*vladimir.lipp@desy.de, **ziaja@mail.desy.de

Abstract

We present a dedicated computational approach, XTANT+, developed to study X-ray induced phase transitions in a broad range of solid materials, including those of high chemical complexity. The latter becomes possible due to the implementation of the versatile density functional tight binding code DFTB+ to follow band structure evolution in various materials. The outstanding performance of the implementation is demonstrated with a comparative study of XUV induced graphitization in diamond.

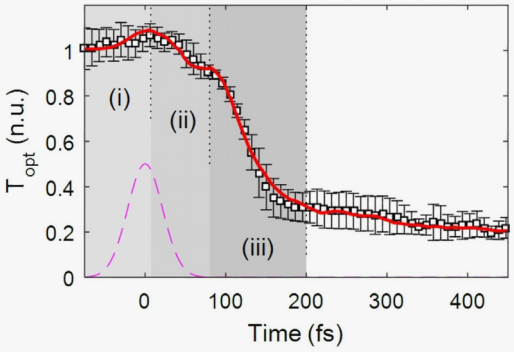
Predicted energy gap in diamond [3]



Earlier results: Diamond graphitization with TTB [1,2]

Absorbed dose: 1 eV/atom
Pulse duration: 52.5 fs
FEL photon energy: 47.4 eV

Probe photon energy: 2 eV
Probe pulse duration: 32.8 fs
Angle of pulse incidence: 20°



Conclusion

1. We developed and implemented a new hybrid MC/DFTB/MD model describing X-ray-excited solids.

2. We applied the model to study X-ray damage in diamond and obtained good agreement with the earlier work.

3. The new model can be applied to more targets, has more robust underlying theory, and opens up the possibility to use all features of the well established DFTB+ code [4].

References: [1] Medvedev et al., *4open* 1, 3 (2018). [2] Tavella et al., *High energy density physics* 24, 22 (2017). [3] Lipp et al., *Scientific Reports*, accepted (10.1038/s41598-022-04775-1). [4] https://dftbplus.org.