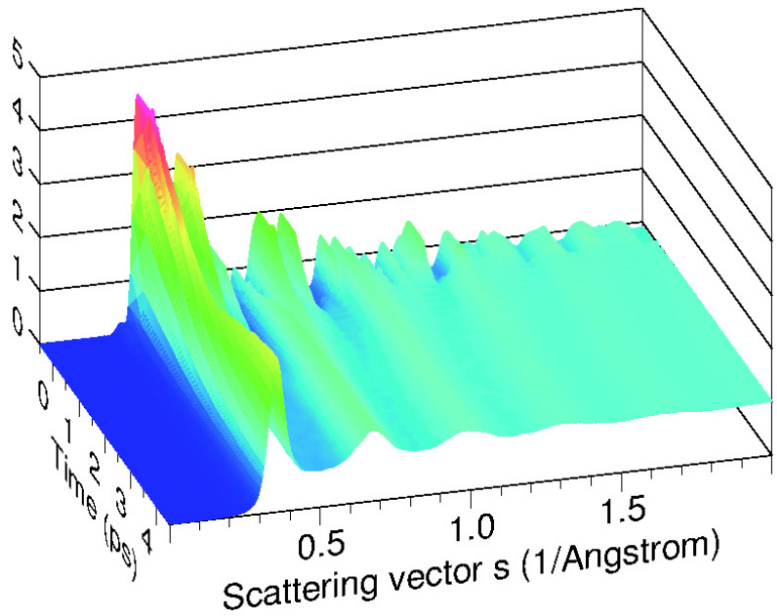
# *Highly-Excited Valence Electron Systems*




Structure function of Sb as a function of the scattering vector s and the time after ultrashort laser excitation. The structure function before excitation (time = 0 ps) is characterized by peaks which disappear after the excitation.

## Introduction

The application of ultrashort laser pulses in the field of materials processing is promising, because it provides a novel way to manipulate matter: Atomic bonds can be softened or hardened faster than the timescale of the motions of the atoms. The atomic movements are generally not affected directly by the laser light, but only indirectly by the induced bond strength changes. The thus induced atomic pathways cannot be reached by conventional thermodynamic means. Ultrafast laser-induced structural changes can be measured optically, by means of time-resolved electron diffraction, and using new x-ray sources, like, XFEL in Hamburg. Our research provides the relevant theory that is necessary to understand these ultrafast processes on an atomic scale and that can be used to predict new phenomena.

## Methods

We explained the electronic origin of ultrashort laserinduced bond strength changes.[1] Atomic pathways were reproduced by combining experimental data with optical properties that we computed under highly excited conditions.[2] A Code for Highly-excIted Valence Electron Systems (CHIVES) was programmed and found to be 200 times faster than state-of-the-art methods at the same level of accuracy.[3] Using CHIVES, in laserexcited

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Project Term
2015 - 2015

Project Areas
Optics, Quantum Optics and Physics of Atoms, Molecules and Plasmas, Particles, Nuclei and Fields

Clusters
Lichtenberg Cluster Darmstadt, Linux Cluster Kassel

University
University Kassel



JUSTUS-LIEBIG-UNIVERSITÄT GIESSEN
TECHNISCHE UNIVERSITÄT DARMSTADT
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Si we predicted thermal phonon squeezing at low excitation densities[4]  and fractional diffusion at high excitation levels.[3] We also studied laser-excited TiO2, BN-nanotubes, diamond, and germanium. CHIVES makes use of two levels of parallelization: MPI-parallel distribution of k points over different nodes and OPENMP-parallel computation of all properties related to a single k point. Huge parallel clusters, like, LichtenbergCluster in Darmstadt and the Linux-Cluster in Kassel are essential to achieve the above-mentioned results at the forefront of science.

## Outlook

Future planned research includes (1) extension of CHIVES to insulators and to the semimetal Sb, (2) implementation of schemes to efficiently treat surfaces, (3) simulation of coherent phonons, and (4) a study of the role of electron-phonon coupling. Apart from these scientific goals we are committed to continually improve CHIVES, among other things, for the hardware provided by HPC Hessen. In Sb, preliminary results show a decay of diffraction peaks within a few picoseconds after intense ultrashort excitation (Figure 1).

## Reference

[1] N. S. Grigoryan, E.S. Zijlstra, and M.E. Garcia (2014), Electronic origin of bond softening and hardening in femtosecond-laser-excited magnesium, New Journal of Physics 16, 013002. http://doi.org/10.1088/1367-2630/16/1/013002

[2] H. Katsuki, J. C. Delagnes, K. Hosaka, K. Ishioka, H. Chiba, E. S. Zijlstra, M.E. Garcia, H.Takahashi, K. Watanabe, M. Kitajima, Y. Matsumoto, K. G. Nakamura, and K. Ohmori (2013), All optical control and visualization of ultrafast 2D atomic motions in a single crystal of bismuth, Nature Communications 4, 2801. http://doi.org/10.1038/ncomms3801

[3] E. S. Zijlstra, A. Kalitsov, T. Zier, and M.E. Garcia (2013), Fractional diffusion in silicon, Advanced Materials 25, 5605. https://doi.org/10.1002/adma201302559

[4] E .S. Zijlstra, A. Kalitsov, T. Zier, and M.E. Garcia (2013), Squeezed thermal phonons precurse nonthermal melting of silicon, Physical Review X 3, 011005. https://doi.org/10.1103/PhysRevX.3.011005

## *Last Update:* 2022-07-08 00:38