Parallel GPU computing in light scattering metrology of ultrafast surface dynamics

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Abstract: Phase-retrieval algorithms are developed for parallel computing of surface autocorrelation function (ACF) and for solving the inverse problem of light scattering. A real-time visualization of ACF was achieved for transient spectroscopy of materials.

The time- and angle-resolved hemispherical elastic light scattering (TARHELS) measurements were performed to study surface dynamics of VO_2 upon photoinduced insulator-metal phase transition. The imaging of ultrafast optical diffraction by TARHELS technique provides statistical information about the evolution of surface irregularities of different sizes. We collected the images of light scattering by the sample surface and these data were used to calculate the bidirectional scatter distribution function (BSDF) of the surface [1]. The BSDF can be calculated directly from the angle-resolved light scattering data as

$$BSDF(\theta,\varphi) = \frac{1}{I_0}\left(\frac{dI_s(\theta,\varphi)}{d\Omega}\right)\frac{1}{cos\theta}, \qquad (1)$$

where I_0 is the intensity of incident light, dI_s is the intensity of light scatter into solid angle $d\Omega$, and φ is the azimuthal angle. The statistical distribution of the surface roughness versus spatial frequency is given by the power spectral density (PSD) function. The relation between BSDF and PSD is given by

$$PSD(f) = \frac{\lambda^4 BSDF(f)}{16\pi^2 Q cos\theta}, \qquad (2)$$

where Q is an optical factor that depends on light polarization, scattering angle, and dielectric constants. The information on the correlation of the surface irregularities can be obtained from autocorrelation function (ACF). Using the Wiener-Khinchin theorem the ACF can be defined as the Fourier transform of PSD

$$ACF(r) = \int_{-\infty}^{\infty} PSD(f) e^{i2\pi f r} df. \qquad (3)$$

The absence of experimental data for BSDF or PSD introduces significant artifacts in the calculation of ACF. Therefore, in most of the cases, the correct calculation of ACF requires partial reconstruction of PSD data. The rigorous solution of the inverse scattering problem is very difficult task. Nevertheless, it is possible to reconstruct the PSD function by using iterative algorithms [2]. In this work we applied Gerchberg-Saxton error reduction (ER) algorithm [3], which produces a robust and precise reconstruction of the ACF and PSD pair [4].

The TARHELS measurements were performed for thin films of VO_2 deposited on single crystal sapphire substrates. The insulator-to-metal phase transition of VO_2 was induced by femtosecond light pulses delivered from Spectra-Physics Ti:Sapphire laser system. This system generates optical pulses with central wavelength $\lambda = 800\, nm$, and 130 fs duration. Using the beta barium borate (BBO) crystal, the probe pulse was frequency doubled.

The correct calculation of ACF from PSD can be affected in practice by bandwidth limits with the absence of PSD data at low spatial frequencies blocked by the sample holder. To solve this problem, we developed the parallel computing procedure based on Gerchberg-Saxton algorithm for the phase retrieval problem. The algorithm was written for graphics processing unit (GPU, NVIDIA Tesla K80) by using parallel computing platform CUDA.

For the analysis of scattering data, we use the scientific data analysis software "Igor Pro". By applying the data transfer operation, the scattering data were linked with external computational procedures written in C++. The important feature of the current implementation is the high-performance GPU CUDA computing which increases the calculation speed in about 15 times. Here the "Igor Pro" software was used only for data visualization, while the main computations were performed in external procedures. As it is shown in Fig. 1, the synchronization of GPU CUDA computing with “Igor Pro” software was performed via XOP toolkit and dynamic-link library DLL.

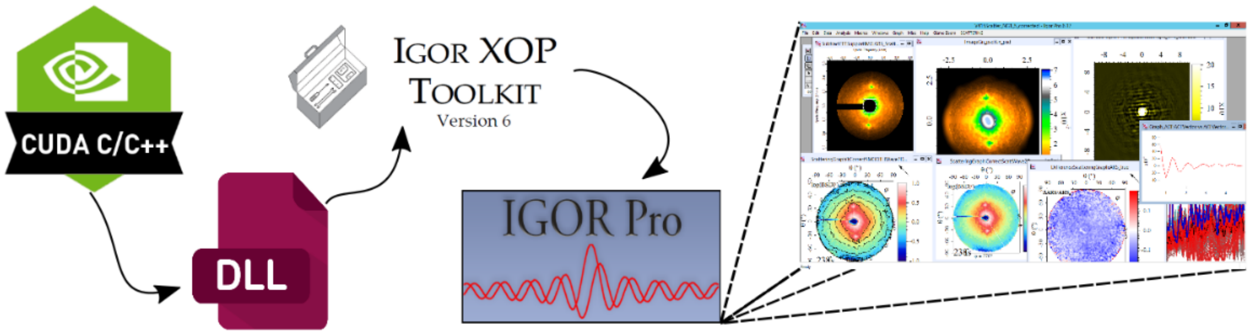

Fig. 1. Interaction of GPU CUDA procedures with “Igor Pro” data analysis software.

Figure 2 shows the main procedure for rigorous computation of ACF along with the reconstruction of PSD within regions where the experimental data are absent. The scattering BSDF indicatrix obtained for photoexcited VO_2 was recalculated into PSD function by using Elson’s scattering theory [5] and Eq. (2). The region blocked by the sample holder was cut, and the obtained PSD* data were scaled and reoriented to PSD** indicatrix suitable for the Gerchberg-Saxton ER procedure. The ACF was calculated by using Eq. (3) and ER iterative algorithm. This algorithm implements the CUDA Fast Fourier Transform library (cuFFT) for the parallel computing inside of NVIDIA Tesla K80 card. Similar procedure was applied also to solve inverse scattering problem for the reconstruction of VO_2 surface shape and phase of scattered light.

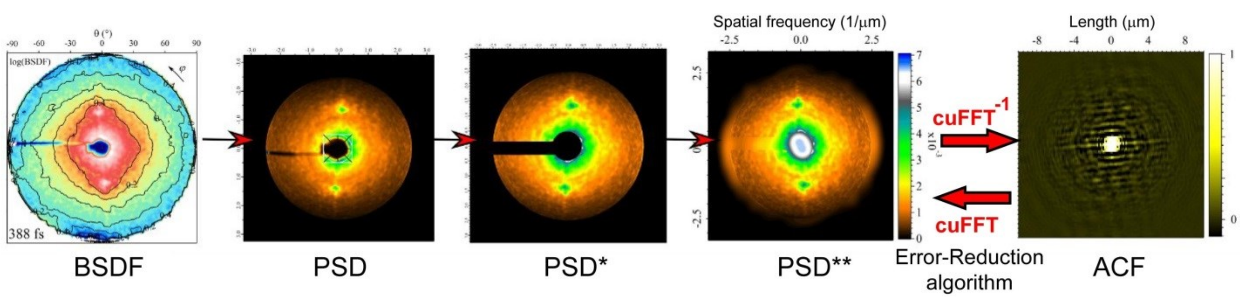

Fig. 2. Computations of ACF along with partial reconstruction of PSD function for photoexcited VO_2 surface.

In summary, the TARHELS experimental technique provides unique opportunity to investigate the ultrafast surface dynamics and light-induced phase transition phenomena in phase-change materials. The multiprocessing programing of GPU significantly speeds-up the reconstruction of PSD function and provides accurate calculations of ACF, allowing the real-time numerical analysis of diffraction data.

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