NUMERICAL SIMULATION OF ENERGY TRANSFER FROM ULTRASHORT PULSE WAVE TO ELECTRON AND LATTICE

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Sophisticated structures with optically designed structures enable optimal response of materials to light irradiation, and have a profound impact on the development of everything such as high-resolution sensing and photothermal catalysis [1, 2]. In such instances, the transient processes of electron and lattice motion are significant. However, they are not well understood due to their complex and fast progression. The objective of this study is to clarify the dynamics of the behavior of materials when irradiated by electromagnetic waves. To evaluate this, the electrons and lattices were modeled by the time-dependent density functional theory (TDDFT) and classical molecular dynamics (MD), and followed the time evolution of the system during the irradiation of electromagnetic waves.

The time waveform of the incident electric field in the simulation is shown in Figure 1. The light intensity is $10^{13}$ W/cm\textsuperscript{2} and the central frequency is 3.10 eV. Figure 2 shows the total energy excluding the kinetic energy of the lattice and the kinetic energy of the lattice in the TDDFT-MD simulation results for the silicon crystal. During the application of an electric field, the energy of the system increases rapidly, while the kinetic energy of the lattice remains almost unchanged. In other words, the energy increase of the system is dominated by the interaction between the electromagnetic waves and the electrons. The kinetic energy of the lattice then begins to fluctuate after 300 fs due to electron-lattice interactions. The numerical analysis therefore shows that the lattice system is hardly displaced directly by the applied electric field but receives energy through the interaction with the electron system.

References

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