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Semiclassical approach for laser-metal interaction

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The comprehensive modeling of laser material machining [1-3] is complex, with multi-scale time and space, multi-phase, and possibly chemical reactions. For laser processing of metals, a two-temperature model (TTM) has been proposed as the simplest continuum model [4]. In the TTM, empirical parameters are employed for all material properties, and the penetration depth models the dynamics of the electromagnetic field. The most critical assumption of the TTM is the quasi-equilibrium of the electron temperature and the electron-lattice interaction term.

Recently, the first-principles approach employing time-dependent density functional theory (TDDFT) [5] has been applied to laser-matter interactions [6]. Although TDDFT offers a compromise between accuracy and computational feasibility, its computational cost remains high. Electron-electron collisions (which are not included in TDDFT) play an important role in the laser-metal interactions.

The Vlasov equation has been employed in nuclear physics and electron dynamics in metal clusters to describe the collision process of fermi particles [7]. Because the Vlasov Eq. treats the distribution function of space, momentum, and time, it requires tremendous computational resources. In general, the computational cost is reduced by assuming that the distribution function is the summary quasi-particles. In this work we employ the quasi-particle approach for the Vlasov Eq. in the periodic system with LDA exchange-correlation potential which is used in TDDFT.

As the first step, we calculate the linear response of bulk Al. Figure 1 shows the complex conductivity and the refractive index. Our Vlasov approach agrees with the TDDFT and experimental results, although the computational cost is much lower than TDDFT. As the next step, we also calculate the energy absorption under an intense laser field. We found that the Vlasov approach shows reasonable agreement with TDDFT in various laser parameters.

The dynamics of the light field is also important point to understand the laser-matter interaction. We have combined the Vlasov Eq. with Maxwell Eqs to study the energy absorption and flow at the surface. We found that above approach describes the exponential decay of absorbed energy and transport at the surface of the thin Al film.

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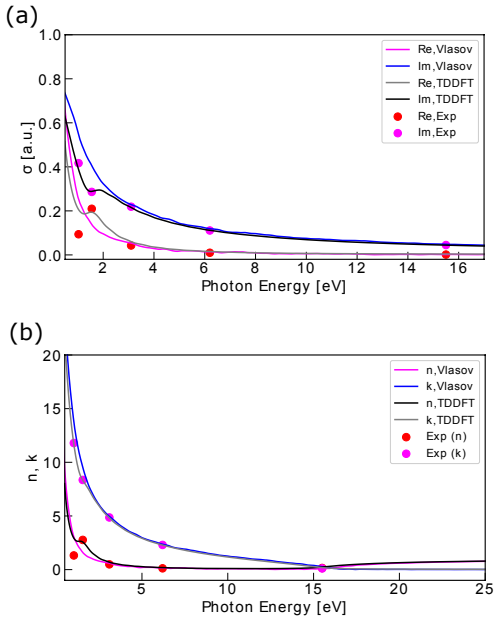

Figure 1 (a) Conductivity and (b) refractive indexes of bulk-Al with the Vlasov equation and TDDFT [9]. The filled circles indicate the experimental results [8].

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