Heat Transport Analysis of Femtosecond Laser Ablation with Full Lagrangian Modified Molecular Dynamics

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The purpose of this study is to analyze the heat transport mechanism of femtosecond laser ablation. Under the condition that laser pulse duration is on the order of femtoseconds, a thermal nonequilibrium state exists and must be taken into account. In order to describe physical phenomena such as heat transport under a nonequilibrium state, a new method, modified molecular dynamics in which molecular dynamics (MD) couples with the two-temperature model (TTM) in a particle-based method, is proposed. In this method, MD simulates the motion of an atom and TTM simulates both electron heat conduction and thermal exchange through electron-atom interactions. This approach yields the use of laser intensity as a parameter. For nonequilibrium heat transport, electron heat conduction transports most of the absorbed laser energy and becomes the dominant heat transport mechanism. At thermal equilibrium, above the ablation threshold fluence, electron heat conduction and thermal waves are dominant, while below the ablation threshold fluence, only electron heat conduction is dominant.

KEY WORDS: heat transport mechanism; laser ablation; modified molecular dynamics; two-temperature model.

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1. INTRODUCTION

Since its invention, the laser has played an important role in many industrial processes. In recent years, ultra-short pulse lasers have been rapidly developed and employed in material micro-processing. Especially, low fluence femtosecond laser ablation has advantages in precision material processing, that is, there exists neither a liquid phase in the irradiated target nor a corona on the circumference of the ablated hole. On the contrary, for long laser pulses (>10 ps), a considerable part of the absorbed laser energy rapidly propagates deeply into the target and the liquid phase appears to produce a corona on the circumference of the ablated hole. In precision processing with fs laser ablation, it is difficult to determine the optimal parameters such as laser intensity and pulse duration because physical phenomena, such as heat transport which is the main factor of fs laser ablation, are not well understood.

In order to elucidate the details of heat transport with femtosecond laser irradiation and to determine the optimal parameters, many fundamental studies have been conducted through well-established experiments [1–5] and numerical simulations [6–10]. Experimentally, Momma et al. [3] investigated the dependence of ablation depth on laser pulse energy and pulse duration and demonstrated theoretically and experimentally the existence of optimal parameters, which make precision material processing with fs laser ablation possible. By means of a simple scaling law, they derived the condition to be satisfied by the optimal combination of parameters, e.g., laser intensity and pulse duration. According to that condition, the thermal diffusion length must be shorter than the laser optical penetration depth. The above condition implies that almost all the electron thermal energy is quickly transferred to the lattice through the interaction between electrons and the lattice and the remainder, which is negligibly small, is transferred beyond the optical penetration depth by electron heat conduction.

Furthermore, numerical simulations have been developed through two independent approaches, namely, the two temperature model (TTM) and molecular dynamics (MD). In Ref. 6, Anisimov and Khokhlov proposed a phenomenological TTM to describe the electron and lattice temperatures during short-pulse laser heating of metals. This model, however, is not based on a rigorous derivation. Qiu and Tien [7] succeeded in deriving TTM rigorously from the Boltzmann equation and gave physical meaning to the TTM of Anisimov and Khokhlov. The TTM governing equations consist of electron and lattice energy balance equations. The net energy is exchanged through an electron-lattice interaction term which appears in each equation. The advantage of TTM is the ability to describe the