A Numerical Method for Studying Thermal Deformation in 3D Double-Layered Thin Films with Imperfect Interfacial Thermal Contact Exposed to Ultrashort-Pulsed Lasers

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Introduction

Ultrashort-pulsed lasers have been attracting worldwide interest in science and engineering, because their pulse durations are of the order of sub-picoseconds to femtoseconds and they possess exclusive capabilities of limiting the undesirable spread of the thermal process zone in the heated sample [1]. Up to date, many models that focus on heat transfer in the context of ultrashort-pulsed lasers have been developed. However, there are only a few mathematical models for studying thermal deformation induced by ultrashort-pulsed lasers. In particular, Dai and his colleagues [2,3] used a fourth-order compact finite difference scheme for solving the dynamic equations of motion so that the non-physical oscillations in 3D cases can be prevented. In this article, we consider a 3D double-layered metal thin film with imperfect thermal contact between layers and study thermal deformation in the 3D thin film exposed to ultrashort-pulsed lasers. It should be pointed out that layered metal thin films are considered because they are widely used in engineering applications due to the fact that a single metal layer often cannot satisfy all mechanical, thermal and electronic requirements. Because of multilayers, the imperfect thermal contact between layers may occur sometimes and hence the stress and displacement caused by the hot-electron-blast effect across the interface between layers may change sharply or discontinue, resulting in possible thermal damage. As we know, the temperature change across an imperfect thermal contact interface can be expressed by the fourth-power law for radiation, which gives a nonlinear temperature distribution around the interface. However, finding a mathematical model governing stress and displacement changes across such an interface can be challenging. Most existing models for stress change across the interface are complicated when applied for the 3D metal thin metal film exposed to ultrashort-pulsed lasers. In this study, we avoid seeking a mathematical model for stress change across the interface and obtain successfully the stress change across the interface based on only the fourth-power law for radiation and using an iterative numerical method.

Model and Numerical Results

Consider a 3D double-layered metal thin film with imperfect interfacial thermal contact between layers in Cartesian coordinates, which is exposed to an ultrashort pulsed laser, as shown in Fig. 1. The governing equations for studying thermal deformation in the metal thin film are dynamic equations of motion and energy equations (parabolic two-step equations) [1-3] where the heat source is given by an ultrashort-pulsed laser. The boundary conditions are assumed to be stress free and no heat losses from the surface in the short time response. The interfacial thermal condition is assumed to be imperfectly thermal contact. Thus, the nonlinear interfacial condition for electron temperature can be expressed by the fourth-power law for radiation. Following the approach used in [2,3], we introduce three velocity components into the model and re-write the dynamic equations of motion. We then construct a staggered grid as shown in Fig. 2. To avoid non-physical oscillations in the solution, we further follow the approach used in [2,3] and employ a fourth-order accurate compact finite difference scheme for calculating stress derivatives. As such, the governing equations are solved using the implicit finite difference schemes, which iteratively obtain electron and lattice temperatures, stresses, strains, velocities, and displacements.

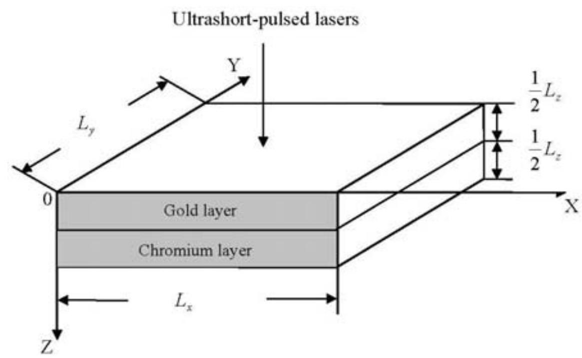

Fig. 1. A 3D thin film irradiated by ultrashort-pulsed lasers.

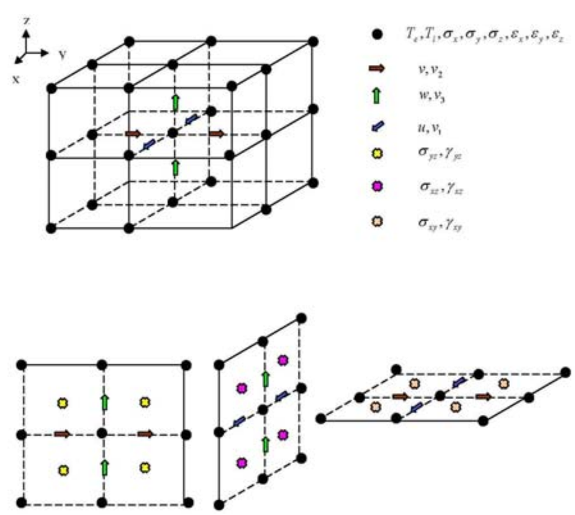

Fig. 2. A 3D staggered mesh and locations of variables.

To test the applicability of the developed numerical scheme, we investigated the temperature rises and thermal deformations in a 3D double-layered thin film consisting of a gold layer on a chromium padding layer with the dimensions 100μm x 100μm x 0.1μm. We assumed that the laser was focused on the center of the top surface of the thin film. The time increment was chosen to be 0.005 ps and initial temperature was set to be 300 K.

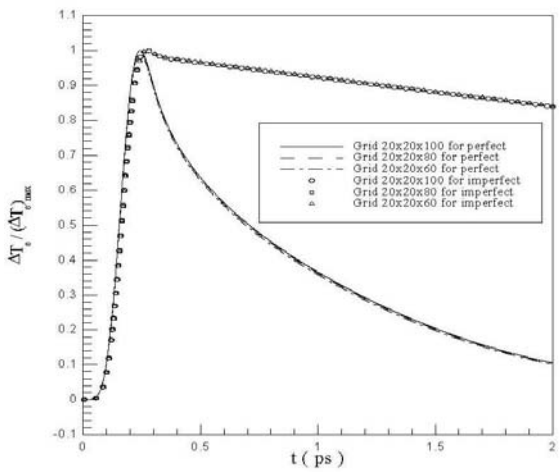

Fig. 3. Change in electron temperature at the center of top surface of thin films versus time with a laser fluence J=500 J/m^2.

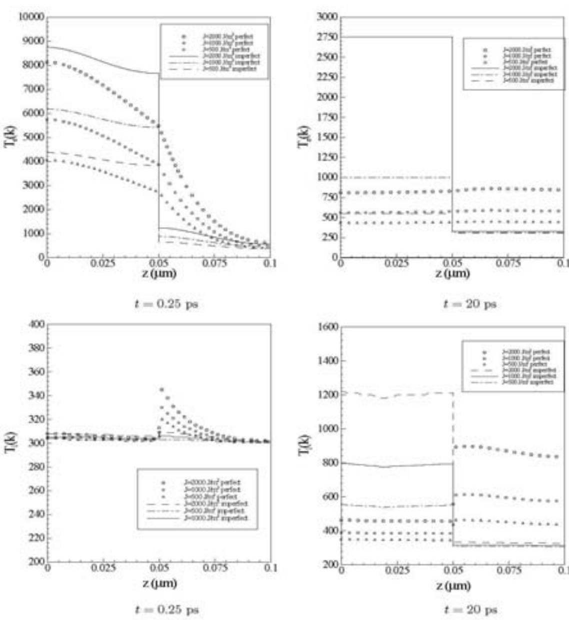

Fig. 4. Electron and lattice temperature profiles along z at center at different times with a mesh of 20x20x80.

Fig. 3 shows comparisons of changes in electron temperature at the center of the gold surface with a laser fluence J=500 J/m^2 between the perfect thermal contact [3] and the imperfect thermal contact at the interface. Furthermore, it can be seen that the mesh size had no significant effect on the solution and hence the solution is considered to be convergent.

Fig. 4 shows comparisons of electron temperature and lattice temperature along z at center between the perfect thermal contact [3] and the imperfect thermal contact at the interface at different times. It shows clearly that there is a sharp discontinuity of electron temperature at the interface when the imperfect thermal contact exists between two bonded thin layers. In particular, we see that the lattice temperature profiles between these two cases are completely different.

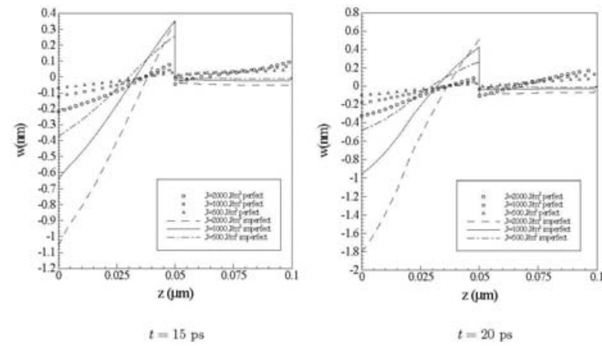

Fig. 5. Displacement (w) profiles along z at center at different times with a mesh of 20x20x80.

Fig. 5 shows comparisons of displacement (w) along z at center between the perfect thermal contact [3] and the imperfect thermal contact at the interface at different times. The negative value indicates that the displacement moves in the negative z-direction, while the positive value implies that it moves in the positive z-direction. It can be seen from this figure that for the imperfect thermal contact case sharp discontinuity of displacement exists at the interface, and the gold layer undergoes severe displacement alteration from negative to positive while the displace alteration in the chromium layer is almost absent.

References

1. D. Y. Tzou, J. K. Chen, and J. E. Beraun, Hot-electron blast induced by ultrashort-pulsed lasers in layered media, Int. J. Heat Mass Transfer, 2002, 45, 3369-3382.
2. S. Zhang, W. Dai, H. Wang, and R. V. N. Melnik, A finite difference method for studying thermal deformation in a 3D thin film exposed to ultrashort-pulsed lasers, Int. J. Heat Mass Transfer, 2007, 53, 457-484.
3. S. Zhang, P. Wang, and W. Dai, A finite difference method for studying thermal deformation in 3D double-layered micro-structures exposed to ultrashort-pulsed lasers, The Open Applied Mathematics Journal, 2008, 2, 104-125