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Editor's Choice

Phase filed simulation of dendritic growth of copper films irradiated by ultrashort laser pulses

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ABSTRACT

A phase field model (PFM) is combined with a two-dimensional two-temperature model (TTM) to simulate the evolution of dendritic growth during re-solidification of ultrafast laser-material interaction. The dynamic solidification conditions at different locations of the melting pool obtained from TTM are fed into the quantitative PFM based on the macro-micro coupled method. A series of simulations are executed to investigate the influence of laser parameters, such as laser influence and pulse duration, on melting pool characteristics and local dendrite morphology. Besides, dendrite structures calculated at different areas of the melting pool were discussed based on local solidification conditions, and the simulated dendrite arm spacing (DAS) for various cooling rates was made comparison with previously published experimental data. The simulated results reveal that the maximum temperature gradient has significant influence on the local dendritic competitive growth, while the laser parameters effect the local microstructure distinctly due to the changes of solidification conditions. This work demonstrates the potential application of PFM to predict the microstructure morphology presented in ultrashort laser-material interaction and other industrially relevant conditions with complex solidification conditions.

1. Introduction

With rapid development of laser manufacturing during the past few decades, researches on ultrafast laser-material interaction have attracted significant attentions. Compared with long-pulsed laser processing, ultrashort-pulsed laser material processing which has been widely regarded as an effective means for precise micro/-nano machining has minimal heat affected zone (HAZ) and collateral damage, less debris contamination, and good reproducibility [1,2]. According to the ultrashort duration time and the extremely small irradiation radius (a few microns), it is difficult to observe the melting pool characteristics and dendritic growth process in the experiment. Due to these limitations, numerical simulation has been commonly employed to study the ultrafast energy transmission and phase changes during the processing. In the micro-scale regime, traditional phenomenological laws, such as Fourier's law of heat conduction are not applicable [3]. Over the last two decades, two-temperature model (TTM) proposed by Anisimov [4] was widely employed as the classical physical model to simulate the non-equilibrium thermal transport and temperature distributions during the ultrafast processing. Considering interfacial energy balance and nucleation dynamics during rapid melting and resolidification in ultrafast laser-material interaction, an implicit interfacial tracking method using temperature dependent thermal properties [5] was proposed by Zhang and Chen [3] and then derived into a two dimensional axisymmetric model by Baheti et al. [6] A critical point model was proposed by Ren [7] to calculate dynamic reflectivity and absorption coefficient and was incorporated into a TTM to study ultrafast laser-material interaction. Ren also used a comprehensive model [8] to study the thermal ablation of metal films irradiated by a single femtosecond laser pulse and laser bursts. Besides, Huang [9] simulated ultrafast phase change processes of metal films irradiated by femtosecond laser pulse trains and discussed the effect of film thickness [10].

During ultrafast laser-material interaction, the thermal effect will be relatively obvious with high frequency. Although some interfacial properties of resolidification have been calculated among previous works [3,5–10], the characteristics of melting pool and the development of microstructures during ultrafast laser-material interaction has not been studied. Over the past few decades, numerical methods have been employed as powerful tools to study the morphology and calculate the size of dendrites during solidification. Originally, morphological parameters such as the primary dendrite spacing and tip undercooling were simulated using analytical models [11,12]. Recently, phase field model

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(PFM) [13–16] and cellular automaton (CA) method [17,18] have been employed as two of the most effective numerical methods for dendrite growth of pure metals and alloys. Comparing the two methods, CA method is limited to the grid orientation and simulation precision, while PFM is able to simulate arbitrarily-oriented dendritic growth quantitatively in spite of a higher computational cost. It is notable that the computation efficiency of PFM has been improved a lot as the asymptotic analysis [19] under the thin interface was carried out which makes it possible to resolve a smaller capillary length to interface thickness ratio.

In most previous studies, the PFM was commonly used to simulate dendritic growth of pure metals [13–15] and alloys [16,20] under the static condition, i.e., constant temperature and cooling rate. Nevertheless, the variation in solidification conditions in melting pool plays an important role in the morphology evolution and size of the microstructure. In this paper, the solutions of a two-dimensional TTM in different areas of the melting pool are fed into a quantitative PFM to study the microstructure evolution during ultrafast laser-material interaction. In analogy with the macro-micro coupled method, different small parts of the thermal model are set as the computational domains for local dendritic growth, the temporal temperature distribution in the melting pool is delivered to PFM, and the local solidification conditions vary with the thermal model during microstructure evolution. The influence of laser parameters on microstructure evolution during the interaction is investigated. In addition, temperature distribution and dendritic growth in different domains of melting pool is also discussed.

2. Modeling method

A copper film with thickness L, width M and initial temperature T_0 is subjected to ultrashort laser pulses which are Gaussian in time with a FWHM (Full Width at Half Maximum) pulse duration t_p. The simulation model is shown in Fig. 1(a). The center ($x = y = 0$) of the front surface of the copper film is coincident with the center of the Gaussian beam in order to describe the longitudinal section of the copper film. A two dimensional PFM is incorporated into a two dimensional TTM in order to model the whole process of the laser-material interaction. The temperature distribution of different parts of melting pool offered by TTM is regarded as the input of the PFM. By doing this, the local dendritic structures can be simulated under relatively realistic solidification conditions.

2.1. Thermal analysis

According to the distinct nature of ultrashort laser pulse compared to long-pulsed laser, a two dimensional two-temperature model [6] is established for thermal analysis as follows:

$$C_e \frac{\partial T_e}{\partial t} = \nabla(k_e \nabla T_e) - G(T_e - T_l) + S(x, y, t) \tag{1}$$

$$C_l \frac{\partial T_l}{\partial t} = \nabla(k_l \nabla T_l) + G(T_e - T_l) \tag{2}$$

where C and k are volumetric heat capacity and thermal conductivity, G is electron-phonon coupling factor. S represents laser heat source, e and l indicate electron and lattice, while x and y are horizontal and ordinate coordinate, respectively. Eq. (1) is valid in the entire process, while Eq. (2) is fitted for both solid and liquid phases except the solid-liquid interface.

The heat capacity of electron is considered to be in direct proportional to T_e when $T_e < 0.1T_F$ (Fermi temperature) based on the previous researches [6,21], while this condition is not valid in the situation when the electron temperature is comparable to Fermi temperature which is attainable in this process [21]. According to the data obtained by first principles [22] of the electron heat capacity and electron-phonon coupling factor for copper, two explicit functions were established by Ren et al. [7]:

$$C_e(T_e) = \begin{cases} 117.47T_e,\ T_e < 2 \times 10^3 K \\ -2.049 \times 10^4 - 26.64T_e + 0.0996T_e^2 - 1.122 \times 10^{-5} T_e^2 \\ +5.735 \times 10^{-10} T_4^{-4} - 1.524 \times 10^{-14} T_e^5 + 2.044 \times 10^{-19} T_e^6 \\ -1.094 \times 10^{-24} T_e^7, 2 \times 10^3 K \leqslant T_e \leqslant 50 \times 10^3 K \end{cases} \tag{3}$$

in unit of $\mathrm{Jm^{-3}\,K^{-1}}$, and

$$G(T_e) = \begin{cases} 0.56 \times 10^{17},\ T_e < 2,750K \\ 1.341 \times 10^{17} - 1.407 \times 10^{14} T_e + 5.988 \times 10^{10} T_e^2 - 7.93 \times 10^6 T_e^3 \\ +555.2T_e^4 - 0.023272T_e^5 + 6.041 \times 10^{-7} T_e^6 - 9.529 \times 10^{-12} T_e^7 \\ +8.377 \times 10^{-17} T_e^8 - 3.15 \times 10^{-22} T_e^9, 2,750K \leqslant T_e \leqslant 50 \times 10^3 K \end{cases} \tag{4}$$

in unit of $\mathrm{Wm^{-3}\,K^{-1}}$. In this way, the data can be more accurate rather than using a single formula over the whole process.

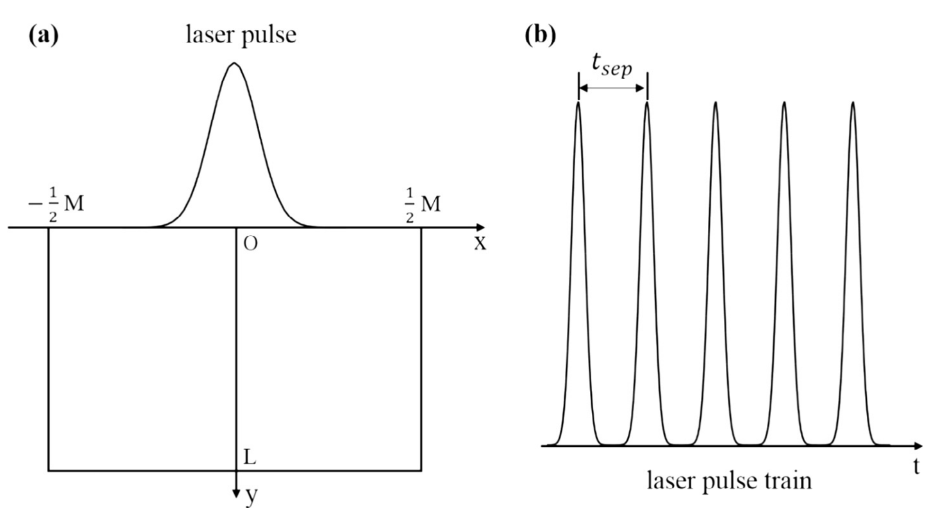

Fig. 1. Simulation model (a) and laser pulse train (b).