APEM journal

Advances in Production Engineering & Management
Volume 16 | Number 4 | December 2021 | pp 457–472
https://doi.org/10.14743/apem2021.4.413

ISSN 1854-6250
Journal home: apem-journal.org
Original scientific paper

Molecular-dynamics study of multi-pulsed ultrafast laser interaction with copper

Yin, C.P.[a], **Zhang, S.T.**[a], **Dong, Y.W.**[a,*], **Ye, Q.W.**[a], **Li, Q.**[b]

[a]School of Aerospace Engineering, Xiamen University, Xiamen, P.R. China
[b]ENN Energy Power Technology (Shanghai) Co., Ltd, Shanghai, P.R. China

ABSTRACT

Ultrafast laser has an undeniable advantage in laser processing due to its extremely small pulse width and high peak energy. While the interaction of ultrafast laser and solid materials is an extremely non-equilibrium process in which the material undergoes phase transformation and even ablation in an extremely short time range. This is the coupling of the thermos elastic effect caused by the pressure wave and the superheated melting of the material lattice. To further explore the mechanism of the action of ultrafast laser and metal materials, the two-temperature model coupling with molecular dynamics method was used to simulate the interaction of the copper and laser energy. Firstly, the interaction of single-pulsed laser and copper film was reproduced, and the calculated two-temperature curve and the visualized atomic snapshots were used to investigate the influence of laser parameters on the ablation result. Then, by changing the size of the atomic system, the curve of ablation depth as a function of laser fluence was obtained. In this paper, the interaction of multi-pulsed laser and copper was calculated. Two-temperature curve and temperature contour of copper film after the irradiation of double-pulsed and multi-pulsed laser were obtained. And the factors which can make a difference to the incubation effect were analyzed. By calculating the ablation depth under the action of multi-pulsed laser, the influence of the incubation effect on ablation results was further explored. Finally, a more accurate numerical model of laser machining metal is established and verified by an ultra-short laser processing experiment, which provides a new calculation method and theoretical basis for ultra-fast laser machining of air film holes in aviation turbine blades, and has certain practical guiding significance for laser machining.

ARTICLE INFO

Keywords:
Ultrafast laser,
Multi-pulsed laser;
Ablation;
Copper;
Modelling and simulation;
Two-temperature model;
Molecular dynamics;
Laser machining

**Corresponding author:*
yiweidong@xmu.edu.cn
(Dong, Y.W.)

Article history:
Received 22 September 2021
Revised 22 November 2021
Accepted 3 December 2021

References

[1] Mills, B., Heath, D.J., Grant-Jacob, J.A., Eason, R.W. (2018). Predictive capabilities for laser machining via a neural network, *Optics Express*, Vol. 26, No. 13, 17245-17253, doi: 10.1364/OE.26.017245.
[2] Rethfeld, B., Ivanov, D.S., Garcia, M.E., Anisimov, S.I. (2017). Modelling ultrafast laser ablation, *Journal of Physics D: Applied Physics*, Vol. 50, No. 19, Article No. 193001, doi: 10.1088/1361-6463/50/19/193001.
[3] Templeton, J.A., Jones, R.E., Wagner, G.J. (2010). Application of a field-based method to spatially varying thermal transport problems in molecular dynamics, *Modelling and Simulation in Materials Science and Engineering*, Vol. 18, No. 8, Article No. 085007, doi: 10.1088/0965-0393/18/8/085007.
[4] Bogaerts, A., Aghaei, M., Autrique, D., Lindner, H., Chen, Z.Y., Wendelen, W. (2011). Computer simulations of laser ablation, plume expansion and plasma formation, *Advanced Materials Research,* Vol 227, 1-10, doi: 10.4028/www.scientific.net/AMR.227.1.
[5] Ivanov, D.S., Zhigilei, L.V. (2003). Combined atomistic-continuum modeling of short-pulse laser melting and disintegration of metal films, *Physical Review B*, Vol. 68, No. 6, Article No. 064114, doi: 10.1103/PhysRevB.68.064114.

[6] Amouye Foumani, A., Niknam, A.R. (2018). Atomistic simulation of femtosecond laser pulse interactions with a copper film: Effect of dependency of penetration depth and reflectivity on electron temperature, *Journal of Applied Physics*, Vol. 123, No. 4, 043106, doi: 10.1063/1.5009501.
[7] Povarnitsyn, M.E., Fokin, V.B., Levashov, P.R. (2015). Microscopic and macroscopic modeling of femtosecond laser ablation of metals, *Applied Surface Science*, Vol. 357, Part A, 1150-1156, doi: 10.1016/j.apsusc.2015.09.131.
[8] Liang, J.-G., Ni, X.-C., Yang, L., Wang, Q.-Y. (2005). Numerical simulation of the ablation on copper with ultrashort laser pulses, *China Laser*, Vol. 32, No. 9, 1291-1294, doi: 10.3321/j.issn:0258-7025.2005.09.029.
[9] Winter, J., Rapp, S., Schmidt, M., Huber, H.P. (2017). Ultrafast laser processing of copper: A comparative study of experimental and simulated transient optical properties, *Applied Surface Science*, Vol. 417, 2-15, doi: 10.1016/j.apsusc.2017.02.070.
[10] Wang, Q., Luo, S., Chen, Z., Qi, H., Deng, J., Hu, Z. (2016). Drilling of aluminum and copper films with femtosecond double-pulse laser, *Optics & Laser Technology*, Vol. 80, 116-124, doi: 10.1016/j.optlastec.2016.01.001.
[11] Karim, E.T., Shugaev, M.V., Wu, C., Lin, Z., Matsumoto, H., Conneran, M., Kleinert, J., Hainsey, R.F., Zhigilei, L.V. (2016). Experimental characterization and atomistic modeling of interfacial void formation and detachment in short pulse laser processing of metal surfaces covered by solid transparent overlayers, *Applied Physics A*, Vol. 122, Article No. 407, doi: 10.1007/s00339-016-9944-7.
[12] Fokin, V.B., Povarnitsyn, M.E., Levashov, P.R. (2017). Simulation of ablation and plume dynamics under femtosecond double-pulse laser irradiation of aluminum: Comparison of atomistic and continual approaches, *Applied Surface Science*, Vol. 396, 1802-1807, doi: 10.1016/j.apsusc.2016.11.208.
[13] Wu, Z., Dong, Y., Zhang, S., Liao, T., Yan, W., You, Y. (2021). Discussion on effect of laser parameters and trajectory in combined pulse laser drilling, *International Journal of Hydromechatronics*, Vol. 4, No. 1, 43-54, doi: 10.1504/IJHM.2021.114175.
[14] Anisimov, S.I., Kapeliovich, B.L., Perelman, T.L. (1974). Electron emission from metal surfaces exposed to ultrashort laser pulses, *Soviet Journal of Experimental and Theoretical Physics*, Vol. 66, No. 2, 375-377.
[15] Zhang, Z., Xu, Z., Wang, C., Liu, S., Yang, Z., Zhang, Q., Xu, W. (2021). Molecular dynamics-guided quality improvement in the femtosecond laser percussion drilling of microholes using a two-stage pulse energy process, *Optics & Laser Technology*, Vol. 139, Article No. 106968, doi: 10.1016/j.optlastec.2021.106968.
[16] Qui-lin, X., Li, Z., Xiao-geng, T. (2015). Ultrafast thermomechanical responses of a copper film under femtosecond laser trains: A molecular dynamics study, *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, Vol. 471, Article No. 20150614, doi: 10.1098/rspa.2015.0614.
[17] Rethfeld, B., Ivanov, D.S., Garcia, M.E., Anisimov, S.I. (2017). Modelling ultrafast laser ablation, *Journal of Physics D: Applied Physics*, Vol. 50, No. 19, Article No. 193001, doi: 10.1088/1361-6463/50/19/193001.
[18] Momma, C., Nolte, S., Chichkov, B.N., Alvensleben, F.v., Tünnermann, A. (1997). Precise laser ablation with ultrashort pulses, *Applied Surface Science*, Vol. 109-110, 15-19, doi: 10.1016/S0169-4332(96)00613-7.
[19] Zhang**,** Y.-F., Wang**,** L.-L., Gong**,** J.-L. (2016). Numerical simulation of femtosecond laser multi-pulse ablation of Ni-Ti alloy, *Journal of Photonics*, Vol. 45, No. 5, Article No. 0514002, doi: 10.3788/gzxb20164505.0514002.
[20] Lasemi, N., Pacher, U., Zhigilei, L.V., Bomati-Miguel, O., Lahoz, R., Kautek, W. (2018). Pulsed laser ablation and incubation of nickel, iron and tungsten in liquids and air, *Applied Surface Science*, Vol. 433, 772-779, doi: 10.1016/j.apsusc.2017.10.082.

APEM journal

Advances in Production Engineering & Management
Letnik 16 | Številka 4 | December 2021 | Strani 457–472
https://doi.org/10.14743/apem2021.4.413

ISSN 1854-6250
Spletna stran: apem-journal.org
Izvirni znanstveni članek

Študija molekularne dinamike ob interakciji večpulznega ultrahitrega laserja z bakrom

Yin, C.P.[a], **Zhang, S.T.**[a], **Dong, Y.W.**[a,*], **Ye, Q.W.**[a], **Li, Q.**[b]

[a]School of Aerospace Engineering, Xiamen University, Xiamen, P.R. China
[b]ENN Energy Power Technology (Shanghai) Co., Ltd, Shanghai, P.R. China

POVZETEK

Ultrahitri laser ima pri laserski obdelavi nesporno prednost zaradi izjemno majhne širine impulza in visoke vršne energije. Interakcija ultrahitrega laserja in trdnih materialov pa je izjemno neravnovesen proces, v katerem je material podvržen fazni spremembi in celo ablaciji. To je posledica povezave termo elastičnega učinka, ki ga povzroči tlačni val in taljenja mrežne strukture materiala. Za nadaljnje raziskovanje mehanizma delovanja ultrahitrih laserskih obdelav kovinskih materialov je bil uporabljen dvotemperaturni model povezan z metodo molekularne dinamike za simulacijo interakcije bakra in laserske energije. Najprej je bila ustvarjena interakcija laserja z enim impulzom in bakrenega filma, izračunana krivulja dveh temperatur in vizualizirani atomski posnetki pa so bili uporabljeni za raziskovanje vpliva laserskih parametrov na ablacijo. Nato smo s spreminjanjem velikosti atomskega sistema dobili krivuljo globine ablacije v odvisnosti od gostote moči laserja. V tem prispevku je bila izračunana interakcija laserja z več impulzi in bakra. Dobili smo dvotemperaturno krivuljo in temperaturni obris bakrenega filma po obsevanju z dvo- in večpulznim laserjem. Analizirani so bili dejavniki, ki lahko vplivajo na učinek inkubacije. Z izračunom globine ablacije med delovanjem večpulznega laserja smo dodatno raziskali vpliv inkubacijskega učinka na rezultate ablacije. Končno je na podlagi eksperimenta ultrakratke laserske obdelave vzpostavljen in preverjen numerični model laserske obdelave kovine, ki predstavlja novo metodo izračuna in teoretično osnovo za ultrahitro lasersko obdelavo lukenj za zračenje v lopaticah letalskih turbin in ima pomemben praktični pomen za lasersko obdelavo.

PODATKI O ČLANKU

Ključne besede:
Ultrahitri laser,
Večpulzni laser;
Ablacija;
Baker;
Modeliranje in simulacija;
Dvotemperaturni model;
Molekularna dinamika;
Laserska obdelava

**Kontaktna oseba:*
yiweidong@xmu.edu.cn
(Dong, Y.W.)

Zgodovina članka:
Prejet 22. septembra 2021
Popravljen 22. novembra 2021
Sprejet 3. decembra 2021