Atomistic simulations of nanoparticle generation by short pulse laser ablation of AgCu bilayers in liquid

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The ability of short pulse laser ablation in liquids (PLAL) to produce colloidal solutions of chemically clean nanoparticles has been employed in a broad range of practical applications. Large-scale atomistic simulations have yielded important insights into the fundamental mechanisms of PLAL [1,2] and provided a plausible explanation of the origin of the experimentally observed broad or bimodal nanoparticle size distributions [3]. In the computational effort reported in this presentation, we extend the atomistic simulations to investigation of the nanoparticle formation mechanisms in PLAL of Ag/Cu and Cu/Ag bilayer thin films. The nanoparticle compositions observed in the simulations exhibit an enhanced abundance of Ag-rich and Cu-rich nanoparticles and a strongly depressed population of well-mixed alloy nanoparticles. The computational predictions are verified in experiments performed at the University of Duisburg-Essen and Kiel University, Germany [4]. The surprising observation that the nanoscale spatial separation of the two components in the bilayer films manifests itself in the sharp departure from the complete quantitative mixing in the colloidal nanoparticles is explained by the complex dynamic interaction between the ablation plume and liquid environment revealed in the simulations.

[1] Shih C Y, Shugaev M V, Wu C and Zhigilei L V 2017 *J. Phys. Chem. C* **121** 16549–16567
[2] Shih C Y, Shugaev M V, Wu C and Zhigilei L V 2020 *Phys. Chem. Chem. Phys.* **22** 7077–7099
[3] Shih C Y *et al* 2018 *Nanoscale* **10** 6900–6910
[4] Shih C Y *et al* 2021 *J. Phys. Chem. C* in press, doi:10.1021/acs.jpcc.0c09970