Scilight

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Computational approach reveals mechanisms behind material modification through surface acoustic waves

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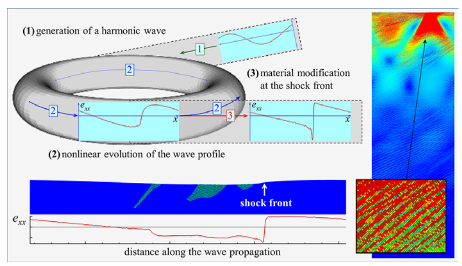
Model based on atomistic molecular dynamics describes unexplored nonlinear effects of surface acoustic waves and examines processes underlying acoustically induced surface modification.



In addition to a variety of active practical applications — including chemical sensing, signal processing, and nondestructive probing of materials' mechanical properties and microstructure — surface acoustic waves could be used to modify materials, but the poor understanding of the underlying mechanisms inhibits this specific application.

Shugaev et al. developed a computational approach capable of simulating the nonlinear effects of surface acoustic wave propagation and dissipation that current continuum approaches cannot. The computational model shows previously unexplored effects, such as the first snapshots of a new mechanism of energy dissipation at the surface acoustic wave shock front and observation of the emission of dislocations.

In addition to describing these new nonlinear effects, the model can investigate the acoustically induced processes that modify material surfaces as well as describe how the acoustic waves interact with surface defects.

The authors' new computational approach is based on the atomistic molecular dynamics simulation method, which has not been used to simulate the long-term nonlinear evolution of surface acoustic waves due to limitations on the time and length scales accessible to atomistic simulations. Simulating cyclic propagation of the wave, similar to a synchrotron used to accelerate particles, allowed the authors to sidestep these limitations.

"These results demonstrate the ability of the atomistic simulations to provide insights into the mechanisms of acoustically-induced localized plastic deformation and suggest future applications in the exploration of various acoustic effects involving material modification and damage," said author Leonid Zhigilei.

The computational approach speaks to the potential of using surface acoustic waves to process materials, and the authors hope it encourages the development of acoustic techniques for this purpose.

Source: "Molecular dynamics modeling of nonlinear propagation of surface acoustic waves," by Maxim V. Shugaev, Chengping Wu, Vladimir Yu. Zaitsev, and Leonid V. Zhigilei, *Journal of Applied Physics* (2020). The article can be accessed at https://doi.org/10.1063/5.0013302.