Molecular dynamics informed neural networks for predicting the nucleation of dislocations and modelling of shock waves in thin metal films

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Increase in strain rate up to 1 ns^{-1} in the femtosecond laser experiments [1] can lead to homogeneous nucleation of dislocations. There are two main problems in the description of this phenomenon: a complex dependence of nucleation threshold on the loading path and non-linear variation of stresses at elastic stage. Artificial neural networks (ANNs) are used to describe the complex behavior of stresses and nucleation threshold, while molecular dynamics (MD) simulations are used for generation of data sets for ANN training. We reconsider nucleation theory and apply ANNs for approximation of material characteristics at elastic stage, which provides quantitative correspondence with the direct MD simulation of nucleation event. The nucleation threshold weakly sensitive to strain rate; it makes relevant direct approximation of nucleation threshold by ANN. It is shown that in the dislocation nucleation mode the elastic precursor of plane shock wave in thin Al and Cu films has constant height in contrast to decaying precursor in the dislocation multiplication mode. This work is supported by the Russian Science Foundation (project No. 20-11-20153) in the part of description of dislocation nucleation and by the Ministry of Science and Higher Education of Russian Federation (state assignment No. 075-00250-20-03) in the part of construction of ANN-based tensoral equation of state.

[1] Kanel G I *et al* 2017 *Phys. Usp.* **60** 490–508