Atomistic simulation of shock compression of metal single crystals with preexisting dislocations

Bryukhanov I A

Institute of Mechanics, Lomonosov Moscow State University, Michurinskiy 1, Moscow 119192, Russia

ibryukhanov@imec.msu.ru

The molecular dynamics simulations of shock wave loading for metal single crystals are performed to understand the role of temperature and preexisting dislocations on the Hugoniot elastic limit (HEL) and spall fracture. It is shown that, in ideal crystals, the elastic precursor exhibits a form of plateau, and the HEL almost does not change with shock propagation distance. The HEL values tend to decrease with temperature for [110] perfect copper crystals, and to increase with temperature for [111] copper crystals [1]. The HEL increases with impact velocity and spreads over a range of 10 GPa between copper crystals of various orientations. Preexisting dislocations in single crystals allow the HEL to decay much faster than in ideal crystals. The HEL decay in Cu crystals slows down with increasing temperature, which leads to higher HEL values, while in Mo single crystals this does not occur, which is a consequence of the temperature dependence of dislocation mobility in fcc and bcc crystals. In most copper crystals, the presence of dislocations slows down the onset of spall fracture and reduces the rate of void growth [2]. An exception is [100] crystals, in which dislocations, on the contrary, reduce the spall strength and accelerate the spallation process. The comparison between spall fracture for the crystals with preexisting dislocations and the perfect ones provide a better understanding of which orientations are more brittle and which are more ductile.

The reported study is supported by the Russian Science Foundation (project No. 22-71-00088).

[1] Bryukhanov I 2023 *Int. J. Plast.* **165** 103599
[2] Bryukhanov I 2022 *Int. J. Plast.* **151** 103171