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Molecular-dynamics simulation of highly-symmetric grain boundary shock interaction VLADIMIR DREMOV, PHILIPP SAPOZHNIKOV, RFNC-VNIITF, EDUARDO BRINGA, LLNL — The defects present in a material (vacancies and interstitial atoms, dislocations, or grain boundaries) are of significant effect upon its properties including elastic-plastic ones. Here we present results of the molecular-dynamics simulations of the interaction of a shock wave with a highly-symmetric grain boundary in copper. The calculations were carried out for five slopes of the grain boundary (110) $\Sigma 5$ to the shock front and for two levels of loading: above the Hugoniot elastic limit but below the critical level at which the homogeneous dislocation production occurs and above that critical level. Shock-induced defects and their role in the shear stress relaxation have been analyzed. It has been shown that there are two competing shear stress relaxation mechanisms as a result of the grain boundary shock interaction. Calculations of the temperature evolution in the vicinity of the grain boundary make evidence for the possibility of local melting far below the intersection of the Hugoniot and the melting line.

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