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Modeling of Al crystal fracture under high-rate strain based on atomistic simulations[1] ALEXEY KUKSIN, GENRI NORMAN, VLADIMIR STEGAILOV, ALEXEY YANILKIN, Joint Institute for High Temperatures of RAS, Moscow, Russia — The work presents the kinetic model of fracture under high-rate strain based on the results of molecular dynamic (MD) simulations. Kinetic parameters for the model as functions of strain and temperature are obtained via statistical averaging over the multiple MD runs of (a) void nucleation in a crystal and (b) void growth under stretching. In the EAM model of monocrystal Al at temperatures close to the melting point the void formation is shown to be a process of crystal homogeneous melting and further cavitation in the melt formed. With the help of the model developed shock-wave loading is modeled and dynamic spall strength of the defectless Al crystal is calculated. The results obtained are compared with the experimental data [G.I. Kanel et al. // J. Phys.: Cond. Mat. 16 (2004) S1007]. While good agreement is observed in the high-temperature region, it becomes worse when temperature decreases. This fact could manifest the increasing role of defects. The dependence of the spall strength on loading duration and on strain rate is governed mostly by nucleation rate of voids and not by their growth rate.

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