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Molecular Dynamics and Hydrodynamics Simulations of Detonation Wave Refraction at the Boundary of TATB-like HE and Beryllium ILYA DERBENEV, VLADIMIR DREMOV, ALEXEY KARAVAEV, FILIPP SAPOZHNIKOV, Russian Federal Nuclear Centre - Institute of Technical Physics, LAURENT SOULARD, CEA/DAM Ile de France — Here we present results of investigations of the process of detonation wave refraction on the border with inert material. The effects of broad reaction zone in TATB-like HE and high sound speed in Be were of particular interest. Molecular Dynamics (MD) was chosen as an instrument of the investigation. An atomistic approach to the contrast of HydroDynamics (HD) does not use any phenomenological models for physical processes but intreatomic potentials. Therefore MD allows for the direct and explicit simulation of such phenomena as detonation kinetics, elastic-plastic transition mechanism and shear stress relaxation kinetics from the microscopic point of view. Nevertheless it was very interesting and important to compare results of MD and HD approaches to the same problem. To make possible hydrodynamics modeling the parameters of the models used in HD were determined from MD simulations. In the course, we used MD results to choose parameters for Be and TATB-like HE equations of state and to evaluate parameters of elastic- plastic transition models for these materials. HD and MD results have been compared and analyzed.

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