Abstract Submitted
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Molecular dynamics simulation of thermodynamic and mechanical properties and behavior of Be when shock loading VLADIMIR DREMOV, ALEXEY KARAVAEV, FILIPP SAPOZHNIKOV, MARINA VOROBYOVA, Russian Federal Nuclear Centre - Institute of Technical Physics, LAURENT SOULARD, CEA/DAM Ile de France — Classical MD approach has been applied to modeling Be properties and behavior when dynamic loading. Special attention has been paid to calculation of melting curve and physical properties when melting. Hugoniostat MD technique was applied to obtain Hugoniot of beryllium taking melting into account. The results of calculations were compared to experimental data and the results of ab initio and quantum MD calculations. The results of direct MD simulation of shock wave loading of nano-polycrystalline beryllium (hcp grains, average grain size ∼10nm) and the data on dynamic yield stress as depended on shock stress were obtained. So as the length of Be samples used was about 0.2 micron only ultra-fast stage (time-scale ∼20 ps) of the relaxation process behind shock front has been investigated. Results of the simulation have been discussed and analyzed along with experimental data

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