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Simple potentials of interatomic interaction for simulation of shock wave and quasistatic compression of metals with fcc, bcc and hcp crystal lattices VLADIMIR GOLUBEV, Russian Federal Nuclear Center - VNIIEF — Results on parametrization of the Morse and Buckingham potentials for simulation of conditions of not less than double compression of metals with various types of crystal lattices are presented. Practically all basic metals for which it is not marked obvious polymorphic transformations into the specified range of compression were examined. Zero isotherms of bulk compression of metals were used as the pivotal data, but not their physical properties. Fitting of parameters was carried out with the use of the GULP program. Conditions of one-and-a-half-fold and twofold compression were examined. Accuracy of fitting in the first case is approximately on the order higher, however and in the second case it is enough high. Quality and accuracy of the fitting of potential parameters were examined also depending on a number of atoms interacting with the chosen central atom. As a result it was offered to take into account interaction of the central atom with not less than 136 neighbor atoms located not less than on eight coordination spheres of considered lattices. As examples of use of the obtained potentials the results of molecular dynamic simulation of compression and loss of structural stability for fcc, bcc and hcp crystal lattices of metals in conditions of shock wave and quasistatic loading are quoted.

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