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Molecular Dynamics Simulation of Thermodynamic and Mechanical Properties of Be and Mg VLADIMIR DREMOV, ALEXEY KARAVAEV, ANDREY KUTEPOV, RFNC-VNIITF, LAURENT SOULARD, CEA/DAM — At ambient conditions Beryllium and Magnesium have HCP with the non-ideal c/a ration. This circumstance does not allow using the simple, spherically symmetric potential in MD simulations. The Modified Embedded Atom Model (MEAM) accounting for local environment and including angular forces has been applied to MD simulation of thermodynamic and mechanical properties of Be and Mg. Parameters of the MEAM have been fitted to available data on Be and Mg bulk and microscopic properties at ambient conditions using the theory of MEAM by M. Baskes. Bulk and shear moduli of monocrystalline materials have been calculated as functions of pressure and temperature. Ab-initio (DFT) calculations have also been carried out to obtain pressure dependence of elastic constants. Result of MD and ab-initio calculations have been averaged to obtain the corresponding values for polycrystalline materials and have been compared with available experimental data and phenomenological models.

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