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Shock Compression of Niobium Oxides from First-Principles[1]
PHILIPPE WECK, KYLE COCHRANE , NATHAN MOORE , Sandia National Laboratories — In order to assess the impact of oxidation on the properties of niobium subjected to shock loading, the equations of states (EOSs) of NbO and NbO_2 were studied within the framework of density functional theory (DFT), with Mermins generalization to finite temperatures. NbO typically forms during the initial rapid oxidation of Nb films and crystallizes in the cubic Pm3-m structure; NbO_2 adopts a tetragonal superstructure with a subcell of the rutile type, with space group I41/a. The shock Hugoniots for fully-dense and slightly porous NbO and NbO_2 were obtained from canonical ab initio molecular dynamics (AIMD) simulations with Erpenbecks approach based on the Rankine-Hugoniot jump conditions. Results suggest that the degree of oxidation markedly impacts the Hugoniot curves at high pressure, owing in part to the presence of multiple phase transitions above $\sim$ 60 and $\sim$ 30 GPa for NbO and NbO_2, respectively. At lower pressure, below $\sim$ 10 GPa, the effect of oxidation remains relatively limited according to the present AIMD simulations, although a study of Nb_2O_5 polymorphs subjected to shock loading would further rule out significant detrimental effect from higher oxidation.

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