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A molecular-dynamics study of shock-induced α-ω phase transformation of Ti BABAK SADIGH, LUIS ZEPEDA-RUIZ, Lawrence Livermore National Laboratory, THOMAS LENOSKY, Contractor, Lawrence Livermore National Laboratory, TOMAS OPPELSTRUP, JON BELOF, Lawrence Livermore National Laboratory — We present molecular-dynamics simulations of structural phase transformations in single-crystal hcp-Ti shocked along the (0001)-axis. The interatomic interaction potential is modeled within the Modified Embedded-Atom Method (MEAM) framework. Above a critical shock strength σ_{th}, a displacive structural transition is observed from the hcp phase into the ω-structure, whereupon a splitting of the shock-wave occurs and a two-wave shock structure is observed. We investigate the kinetics of this structural transition as a function of increasing shock strength beyond σ_{th}. We identify the atomistic mechanisms underlying the α-ω martensitic transformation and study the role of the pressure waves in driving the phase change by analyzing the evolution of local stress and temperature behind the shock fronts as well as in the interfacial regions between the two phases. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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