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Molecular dynamics study of tantalum spallation LAURENT SOULARD, JOELLE BONTAZ, CEA - DAM Ile-de-France, BP12, 91680 Bruyeres-le-Chatel — We present in this paper a molecular dynamics study of tantalum spallation. The spallation is the final stage of the damaging caused by a series of shock and rarefaction waves. This complex process is due to the nucleation, the growth and the coalescence of pores within a thin zone corresponding to the crossing of two rarefaction waves. Various experimental works allowed a partial description of this process. We present here a complementary analysis based on large classical molecular dynamics simulations in single and polycristal of tantalum. We use a rather sophisticated potential function (MEAM) associated with multi-million particle samples. The simulations were made on the TERA 10 computer of CEA-DAM, and needed several hundred processors. We examine at various times the apparition and the evolution of pores, and provide their spatio-temporal distribution. The one dimensional (in the hydrodynamics sense) and 3D cases are considered in order to understand the effects of lateral rarefaction waves in the spallation phenomenon. Comparisons with experimental data are shown.

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