Atomistic and continuum modeling of the fracture of refractory metals

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In this work, using molecular dynamics (MD), we studied the kinetics of pore formation in the following refractory metals: tantalum, tungsten, and titanium. Representative elements of the volume of metals, both with an initially ideal lattice and with pores, were subjected to uniform triaxial stretching. The MD simulation was carried out using the LAMMPS program [1] and interatomic potentials for Ta [2], W [3] and Ti [4]. At the initial stage of preparation, the pressure was relaxed to zero using the barostat; the temperature at the stage of preparation and stretching was maintained using the thermostat (from 300 to 3000 K). The system was held for 10 ps. Then the barostat was turned off, and tension was applied at the constant strain rate of 3/ns. The pore number and size distribution were determined using an algorithm from [5]. The MD results were used to verify the continuum fracture model [6] and identify its parameters. At the stage of nucleation, an exponential pore size distribution is established.

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