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Modelling the Shock Compression of Polycrystalline Metals SIMON CASE, Atomic Weapons Establishment, YASUYUKI HORIE, Air Force Materials Laboratory — A 2D mesh-free particle computational method is used to model the shock compression of polycrystalline metals. The code is evolved from the Discrete Element Method (DEM) code, DM2, developed by Horie et al. It is based on a Molecular Dynamics computational scheme, but with discrete particles representing mesoscale-sized portions of material rather than atoms. The model uses pair potentials to represent effective hydrostatic compression behaviour. However, in the new model the potential is a function of the representative area (volume in 3D) between particles, rather than their radial separation as in the original code. Complementary to the hydrostatic potential is an elastic perfectly plastic shear force, which facilitates the simulation of plastic deformation. A polycrystalline grain structure is computationally grown onto a regular 2D arrangement of particles, and a crystallographic orientation is assigned to each grain on a distributed basis. The heterogeneous deformation properties of the polycrystal are manifested through selection of spatially dependent particle interactions. For example particles adjacent across a grain boundary are given a reduced shear strength, whilst the longitudinal wave speed in each grain is dependent upon its crystallographic orientation with respect to the shock direction. Results of the shock compression reveal a non-planar shock front and a distribution of the shock induced particle velocity in a plane perpendicular to the shock direction, which are qualitatively in agreement with experiment.

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