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XRay Scattering in a Deformed Crystal by a Phase Field Method

ROBB THOMSON, retired, MARISOL KOSLOWSKI, Purdue Univ., RICHARD LESAR, LANL — We demonstrate the use of a phase field method for dislocated crystals, developed by one of us, for computing the scattering of Xrays. The model addresses deformation on a single slip plane by dislocations of a single burgers vector interacting with a set of point obstacles. The obstacles are introduced in two modes; one randomly on the slip plane, and the second in straight “walls.” The obstacles simulate blocking interactions by dislocations on different slip planes, and the “walls” represent the intersection of a secondary slip plane with the primary plane being simulated. In the small angle case, the scattering source is the local dilatation induced by the dislocations on the slip plane, and in the Bragg case, the scattering source is the change in local lattice constant. The small angle results show scattering with oscillations attributable to the width of the “walls.” In the Bragg case, the Laue spots are broadened by the dislocations, and the results directly confirm the picture of dipolar wall scattering introduced many years ago by H. Mughrabi.

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