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Molecular dynamics simulations of grain interactions in shock-compressed highly-textured columnar polycrystals PATRICK HEIGHWAY, DAVID MCGONEGLE, University of Oxford, UK, NIGEL PARK, AWE, UK, ANDREW HIGGINBOTHAM, University of York, UK, JUSTIN WARK, University of Oxford, UK — When a polycrystal is shock-compressed, the grains of which it is composed cannot deform as they would do in isolation, but must do so in such a way as to accommodate the presence of their neighbours. This is to say that every grain must interact with those adjacent to it. While experimental studies abound demonstrating the range of physical effects that can be attributed to grain interactions under quasi-static loading conditions, little consideration appears to have been given to the detection of such interactions under the conditions of shock-loading. Here, we predict via molecular dynamics simulations the effect of grain interactions on the elastic strain state of a particular class of highly-textured polycrystal under shock-loading conditions. We find that cooperative elastic deformation of grains in directions transverse to the shock allows each crystallite to reach a state of reduced shear stress. We compare the extent of this relaxation for two different columnar geometries, in which the grains have either square or hexagonal cross-sections. Finally, we calculate the shifts in the x-ray diffraction (XRD) peaks that would result from these grain interactions, and hence assess the feasibility of detecting these interactions using ultrafast XRD techniques.

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