

# Shock Compression, Release And Spall Fracture Along The Closest Packed [111] Crystallographic Direction In Single Crystal Iron

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## Abstract

Understanding the microphysical processes that underline the shock compression and release behavior and subsequent spall fracture of solid materials is a scientific challenge relevant for both fundamental and industrial applications [1,2]. Such processes can be characterized at the atomic level by using large-scale Molecular Dynamics simulation, which now gives access to spatial and temporal scales comparable to those available in experiment [3]. Thus, in this work, Non-Equilibrium Molecular Dynamics (NEMD) simulations have been used to study the coupling between phase transitions and spall damage in single crystal iron when a shock wave propagates along the closest packed [111] crystallographic direction. The modified version of the Ackland potential was used [4]. Consistent with the literature [5], no plastic deformation was observed under compression before the phase transition. Then, both direct bcc to hcp and reverse hcp to bcc phase transitions occur at onset pressures that increase with shock pressure. The microstructure behind the incident release wave is mainly composed of defects such as dislocations, with some residual hcp and fcc atoms within the matrix of the released bcc phase. In contrast to

the high symmetry [001]-direction [6], no release shock wave was observed to form upon unloading, leading to large-width Gaussian tensile pulses upon reflection from the free surface. Voids nucleation sites are found to be directly correlated with the bcc to hcp phase transition under compression, since they are located where both phases coexisted before the arrival of the reflected rarefaction wave. On the other hand, the spall strength evaluated from the acoustic approximation is systematically higher than that measured within the maximum tensile plane, which is also higher than that evaluated at the weak sites plane. References [1] M. A. Meyers, Dynamic behavior of Materials (John Wiley and Sons, Inc, New-York, 1994) [2] T. Antoun, et al., Spall Fracture (Springer, New-York, 2002) [3] P. Wen, G. Tao, D. E. Spearot, and S. R. Phillpot, , J. Appl. Phys. 131, 051101 (2022). [4] N. Gunkelmann et al., Phys. Rev. B 86, 144111 (2012) [5] K. Kadau, et al., Phys. Rev. B 72, 064120 (2005). [6] N. Amadou, T. de Ressaiguier, Phys. Rev B 108, 174109 (2023)

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