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The relation between solitons and interactions in bcc materials

JOHANNES ROTH, ITAP, Universitaet Stuttgart — Shock waves in simple crystal structures are frequently accompanied by solitons, at least in molecular dynamics simulations. In this paper results for the case of bcc-materials shocked along a three-fold axis are reported. Pair potentials and generalized EAM potentials are studied. The influence of the Cauchy pressure is investigated by comparing iron and chromium. Solitons are observed for all interactions, but their strength and velocity varies. A modification of the Zhou-Wadley two- and three-body potential [Comp. Mat. Sci., in press] is introduced which permits a controlled variation of the Cauchy pressure in contrast to EAM. For this type of interaction the solitons are strongly depressed for negative Cauchy pressures. For the Dzugutov potential [PRB **72** (2005) 14126] a close relation between a subsonic phase transformation into an ω -phase and supersonic solitons has been observed. A similar relation has not been found for iron and other interactions, although it might be favorable energetically. By ab-initio calculations with VASP it is shown that the ω -phase transition in iron is surpassed by the transition into the hcp-phase.

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