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Abstract

We investigate the bcc-fcc transformation in the new shape memory alloy FeMnAlNi utilizing density functional theory calculations for double shear. We formulate an energy expression to derive the fcc martensite formation stress, incorporating the transformation shear energy and the elastic interactions of the dislocations. The critical bcc-fcc transformation stress was determined as 191 MPa, which is close to the experiments. Concurrently, we also establish the fcc twinning and slip stresses as 201 MPa and 335 MPa respectively. The higher slip resistance ensures recoverability of the transformation. We observe that the Bogers-Burgers double shear mechanism proceeds with a much lower energy barrier and is favored over the 'classical' Bain deformation. Overall, the parameters obtained from DFT calculations are devoid of any empiricism and the prediction of these critical stresses permit the design of new iron based SMAs.