Atomistic simulations of the formation of <c>-type dislocation loops in α-zirconium

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Abstract

The formation of <c>-type dislocation loops in α-Zr is believed to be responsible for the breakaway irradiation growth experimentally observed under high irradiation fluences. Experimental observations have now firmly proven the existence of <c>-type loops, but their formation mechanism is still not well explained experimentally. Atomistic simulations have been extensively employed to investigate the structure of materials at nanometer scale, and their successes provide reasonable explanations to observed experimental phenomenon and provide guidance to understand unknown mechanisms. Due to the length scale of dislocation loops and the time scale of cascades, molecular dynamics (MD) simulations can be an important technique in understanding such phenomenon. In the present work, cascades are introduced onto pre-existing <a>-type dislocation loops in α-Zr with different primary knock-on atom (PKA) energy, using the MD technique. Either a vacancy or an interstitial loop is created, to test if they perform differently during the cascades reaction. The aim of the present study is to show a new potential mechanism for the formation of <c>-type dislocation loops.

Results

Figure. Burgers circuits (BC) were constructed for dislocation loops before and after cascades simulations at initial temperatures 298 K and 573 K, respectively. Before cascades, the Burgers vector for the dislocation loops are 1/3 <1120>; after cascades, the Burgers vectors for two newly formed dislocation loops are 1/3 <1123> and 1/6 <0443>, respectively. Atoms are colored by their bond-angle values, where perfect atoms are not shown. The BC is highlighted with yellow. The starting and the finishing points are colored red and blue, respectively.