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Atomistic simulations of growth mechanisms of hydrogen blisters in copper

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Blistering is a process which usually takes place close to the surface of metals when they are irradiated, as can be seen in radio-frequency quadrupoles accelerating structures. This pronounced change of the surface morphology has been measured when the extended irradiation is done with energetic light ions.

The mechanism of continuous growth of a small bubble to a quantifiable size blister is not completely understood. Frequently, such process is associated to the prismatic dislocation loop punching, which takes place in very short timescale and cannot be covered by experimental techniques. In FCC metals, the pressurized voids yield emitting shear loops, which were suggested to provide explanation on the plastic growth of the bubbles. However, the detachment of these loops has not been demonstrated.

We use molecular dynamics to address the fast bubble growth in Cu, associated with blistering, when exposed to H- irradiation [1]. To do that, we employ a methodology which allows us to closely follow the formation of prismatic loops at different H concentrations. Moreover, we also analyze the interaction of these loops with the different surface orientations of copper. This study sheds light on the mechanism of blister production and, also, to its effect on the surface exposed to irradiation.

We observe the emission of a complete prismatic loop composed by several shear loops, which Burgers vectors are aligned with the gliding direction of the prismatic loop. We show that the prismatic loops are not necessarily smaller than the bubble cross-section. In addition to this, we note that these loops travel toward defects-sinks such as grain boundaries or surfaces, and in the latter case, are creating different shape protrusions. These protrusions'shapes are different depending on the grain orientation, as observed experimentally, and we verify it by our computational method.

[1] Alvaro Lopez-Cazalilla, Flyura Djurabekova, Fredric Granberg, Kenichiro Mizohata, Ana Teresa Perez Fontenla, Sergio Calatroni, Walter Wuensch Acta Materialia, 225 (2022) 12

Topic

Modeling and Simulations

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