

Mechanisms of bubble growth and blistering on metals exposed to hydrogen

Alvaro Lopez-Cazalilla¹, Catarina Serafim^{1,2}, Sergio Calatroni², Walter Wuensch², F. Djurabekova¹

¹ *Department of Physics, P.O. Box 43, FI-00014 University of Helsinki, Finland*

² *CERN, European Organization for Nuclear Research, 1211 Geneva 23, Switzerland*

Increasing demands of energy, along with the yet increasing concern for the development of environmentally friendly technologies, call for exploring new ways of cost-efficient energy production. Hydrogen is one of the primary candidates for this purpose, due to its abundance and diverse ways of how it can be used. Moreover, hydrogen-based technologies are carbon-neutral, and hence their use could have a major effect on slowing down the climate change. One of the most promising green energy production sources, nuclear fusion reactors, is based on reactions between hydrogen isotopes. Hence, the insights on the interaction of H with metals will shed light on processes developing in fusion-related materials as well.

Blistering is a process that 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 extended irradiation is done with energetic light ions.

We use computational methods to address the fast bubble growth in Cu, associated with blistering, when exposed to H⁻ irradiation [1]. We analyze the interaction of the formed dislocation loops with the different surface orientations of copper. Furthermore, we focus on the H depth profile and vacancy distributions along low-index crystallographic directions [2]. In addition, we present a new H-Cu machine-learned (ML) interatomic potential using GAP methodology, which opens the gate to a full understanding of bubble growth.

We find a strong correlation between the blistering and crystallographic orientations. The distance between the mean penetration depth of H and the vacancies (recoils) creation is considerably different along the considered directions, and provides an explanation of the resistance to blistering of some grain orientations. Furthermore, we introduce some successful initial tests performed with the newly developed ML potential.

References

- [1] Alvaro Lopez-Cazalilla, Flyura Djurabekova, Fredric Granberg, Kenichiro Mizohata, Ana Teresa Perez Fontenla, Sergio Calatroni, Walter Wuensch *Acta Materialia*, **225** (2022) 12
- [2] Alvaro Lopez-Cazalilla, Catarina Serafim, Jyri Kimari, Milad Ghaemi, Ana Teresa Perez-Fontenla, Sergio Calatroni, Alexej Grudiev, W. Wuensch, F. Djurabekova submitted (2023)