Growth Mechanisms of Hydrogen Blisters in Copper: Role of grain orientation

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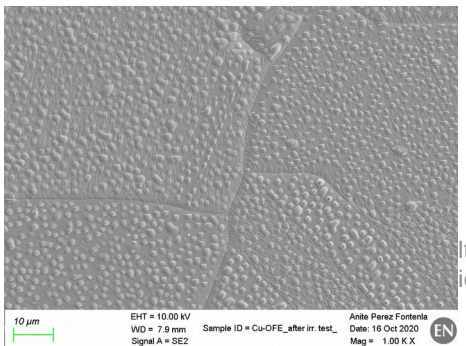
Outline

- Introduction & Motivation:
  - Dislocations, hydrogen and surface behavior.
- Effect on surfaces (MD). Influence of grain orientation at low fluences
- Cu-H machine-learned interatomic potential
- Conclusions

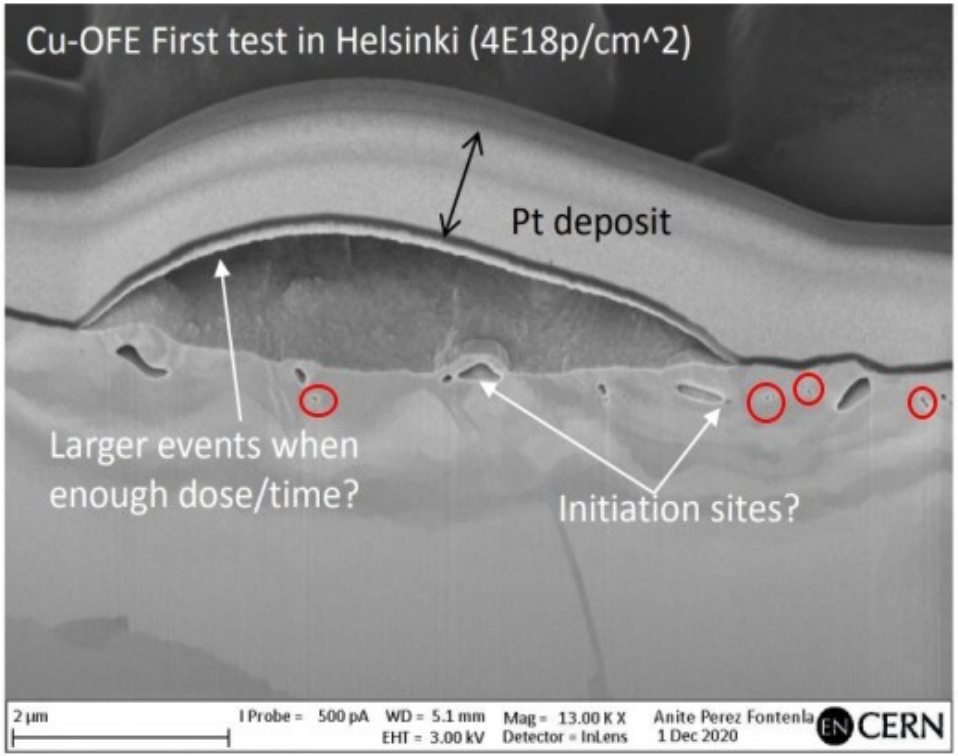
Motivation

- Blistering is common effect in the surface of metal exposed to light species. This detrimental effect has been observed in Al, Fe an steel, and in certain conditions in Nb ([1]). On the other hand, Ti has been experimentally probed to not blister under H fluence ([2]).
- In nuclear fusion (W), this phenomenon is observed under exposure of H and He, being “one” of the bottlenecks of the future nuclear power plants, despite its superior properties such as high melting point, good thermal conductivity, etc.
- Similarly, this is happening in Cu, which is the first candidate for particle accelerators in the field of high energy physics structures
- The role of the solubility is crucial in this phenomenon, as it is the temperature and fluence.



The role of the plastically deformed region between the blister/bubble and surface, affect the mechanical response of the material.

Motivation



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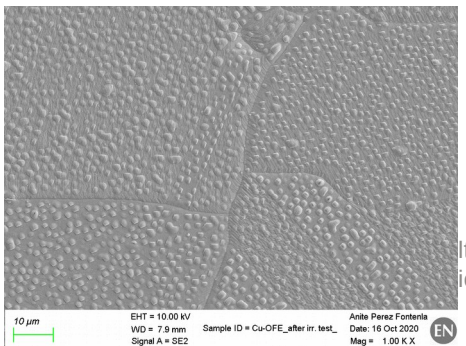
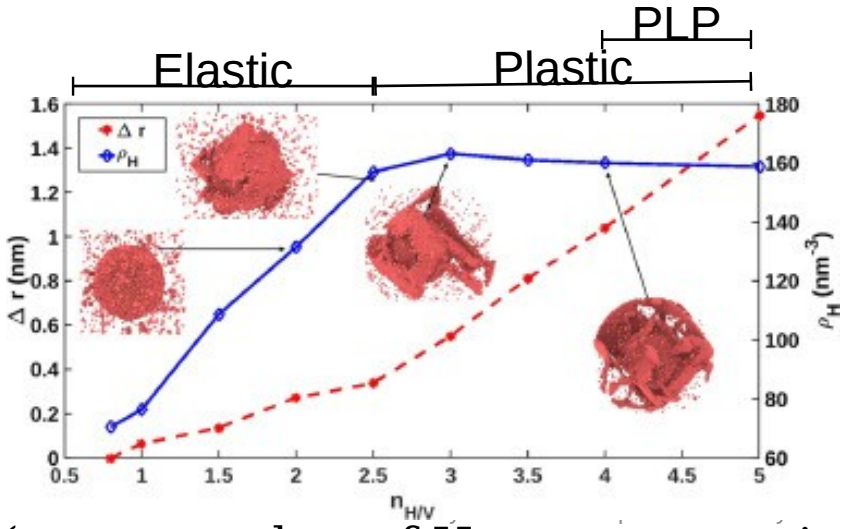


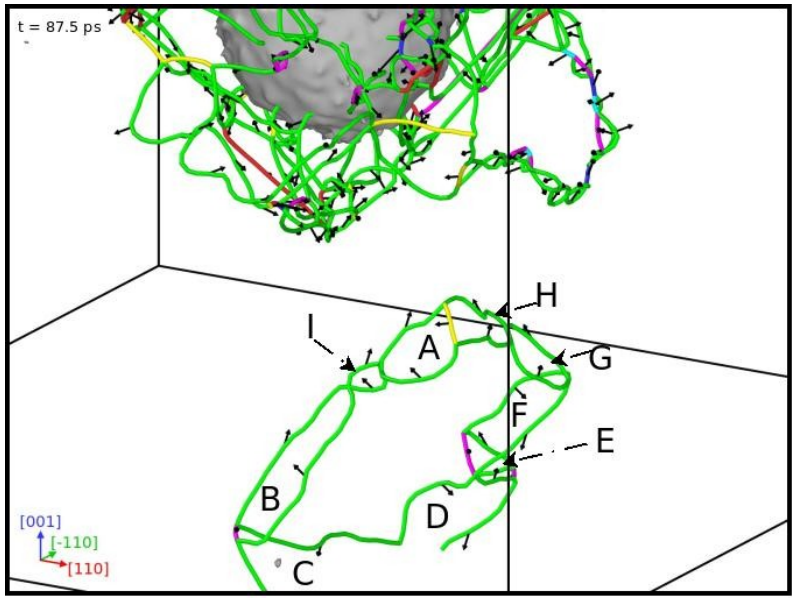
The role of the plastically deformed region between the blister/bubble and surface, affect the mechanical response of the material.

Bubble growth in Cu

- To model this effect, some computational approaches have been implemented before with different outcomes.
- The growth of tiny He bubble was followed in Cu, showing the dissociation of small prismatic loops [Jin et al., Sci. Rep. 11 (2021) 12839]
- We showed that even much larger bubbles grow via prismatic loop punching (PLP). In this case the network of shear loops is forming on adjacent {111} planes with Burgers vector either aligned or opposite to the gliding direction of the prismatic loop [A. Lopez, F. Djurabekova et al. Acta Materialia 225 (2022) 117554]

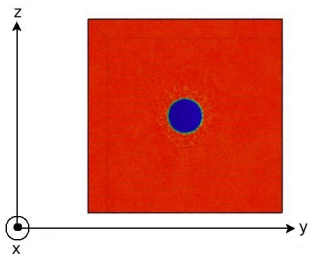


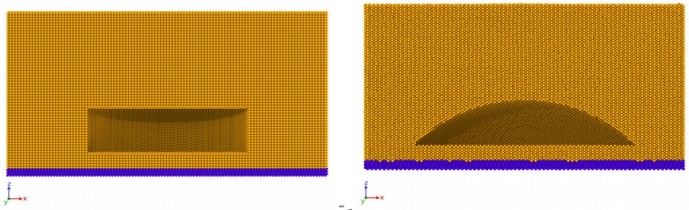
($n_{H/Vac}$: number of H per vacancy in the void)



Simulation details

- The several shapes of blisters formed in surface made us study the bubble growth under differently oriented surfaces.
- We use molecular dynamics (MD) to study this effect. Mishin Embedded Atom Method (EAM) potential for Cu, EAM for H-H and purely repulsive H-Cu.
- MD is limited in the time and size of the cell, however, it provides a good description of the atomic interactions using interatomic potentials
- Problem of H accumulation and complete creation of defects is beyond the MD time span.
  - Solution for H accumulation: introducing directly high concentrations (high pressures) of H ($n_{H/Vac}$: number of H per vacancy in the void), we can speed up the process.
  - Lower paces have been tried with similar results

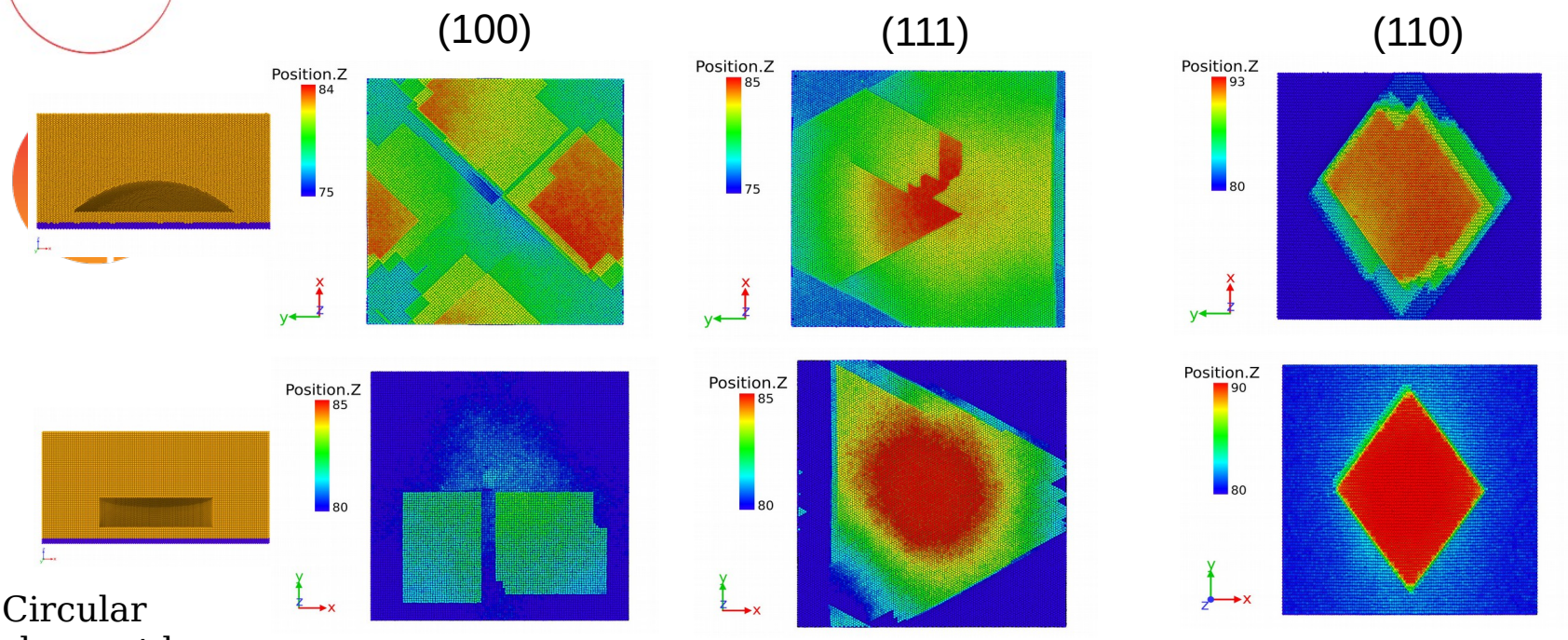




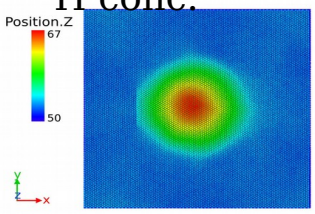
To enable large void simulations, we use different void shapes (sphere, hemisphere, disk) and surface orientations ({100}, {111}, {110}).

Hemispherical and disk bubbles ($n_{H/Vac=}$ 2)

- We consider bubbles with large projection on the surface, as the blisters observed experimentally.



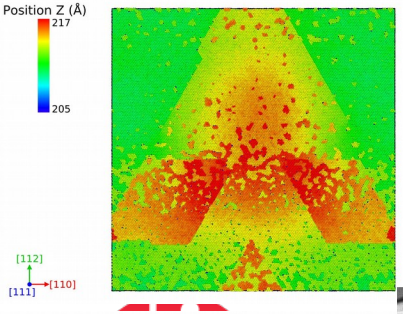
Circular shape at low H conc.



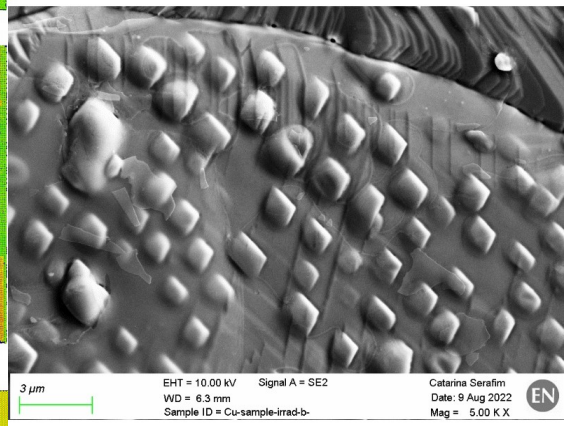
- Similar surface features as in the spherical void, but for lower pressures.
- However the disk-bubble generates clearer protrusions.

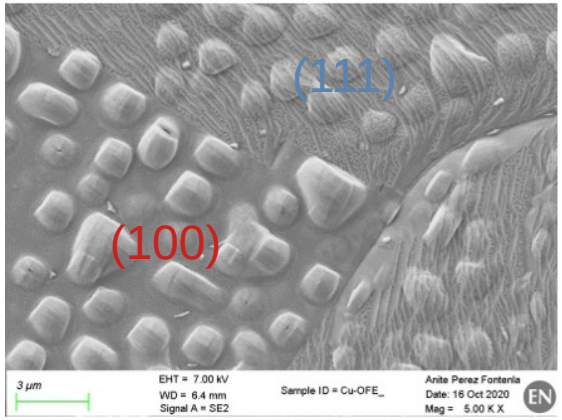
A. Lopez-Cazalilla, C. Serafim, submitted (2023)

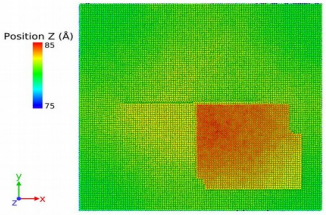
Comparison with experiments

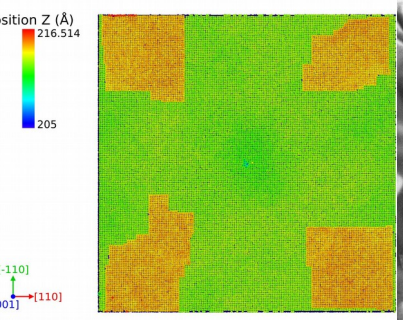


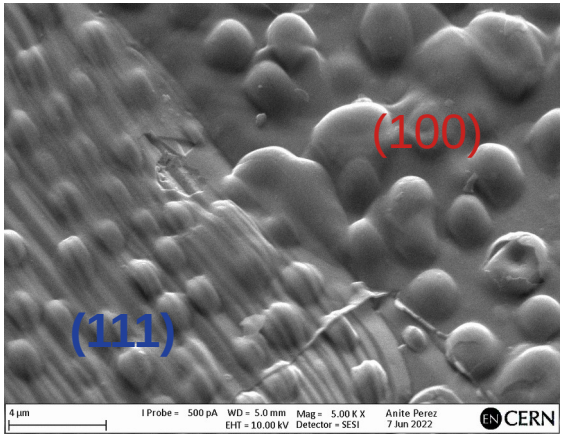
(110)

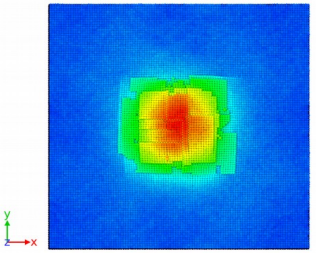


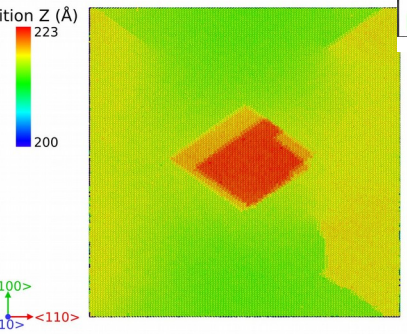


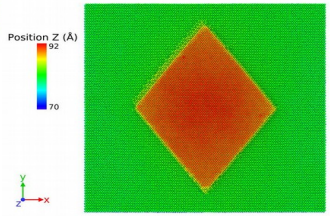


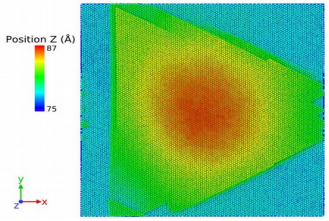


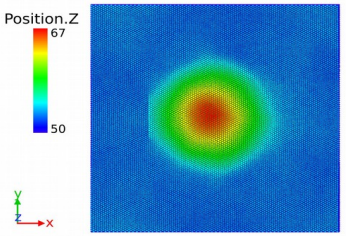






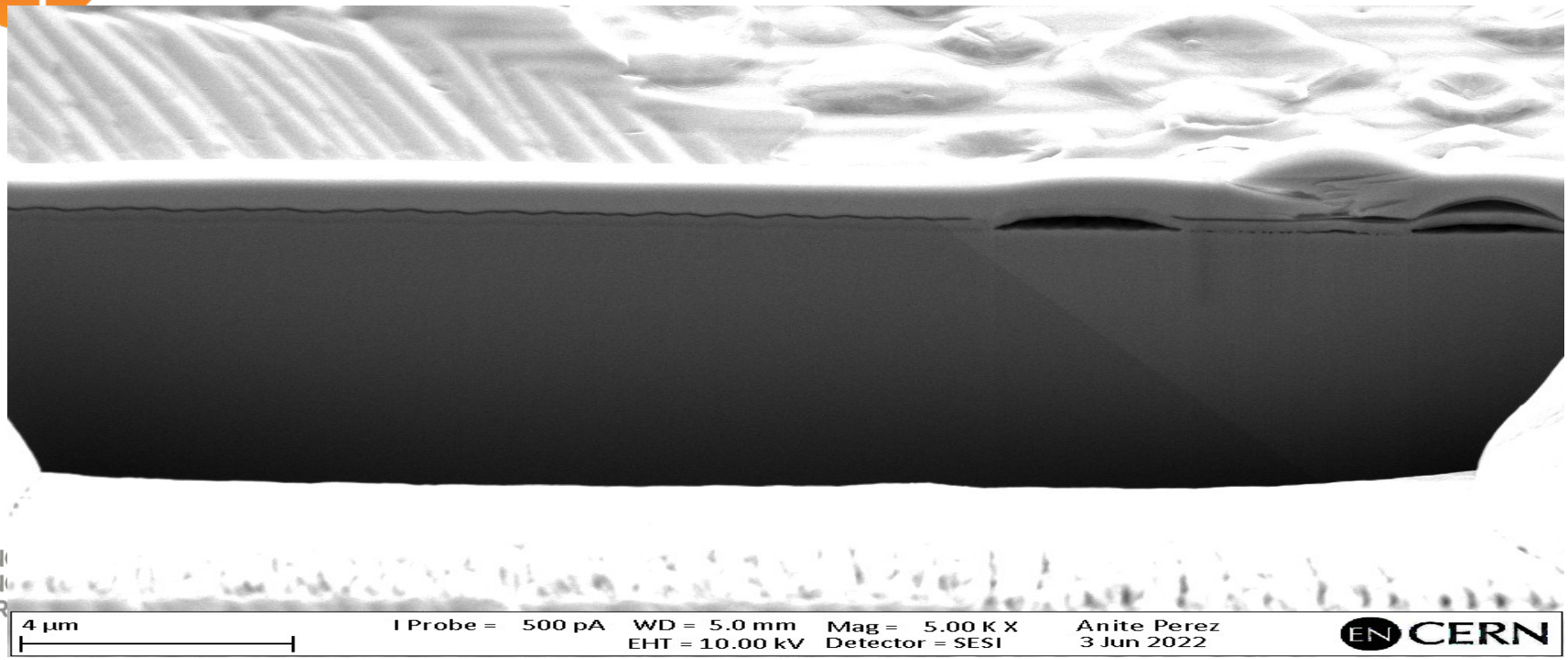






MDRANGE vs BCA

- The MD results do not provide information on why (110)/(111) are not the first surface yielding, being the glide direction/plane. We see (110) is the first yielding, contradicting the experiments.
- Since the initiation sites are formed at different depths depending on the grain orientation, we need to know how the penetration depths are for 45 keV H in Cu. For that we use MDRANGE, when typically Monte Carlo methods are commonly applied to this problem.
- MDRANGE* is an MD approach specifically designed for high-energy interactions and allows for consideration of different crystallographic orientations.



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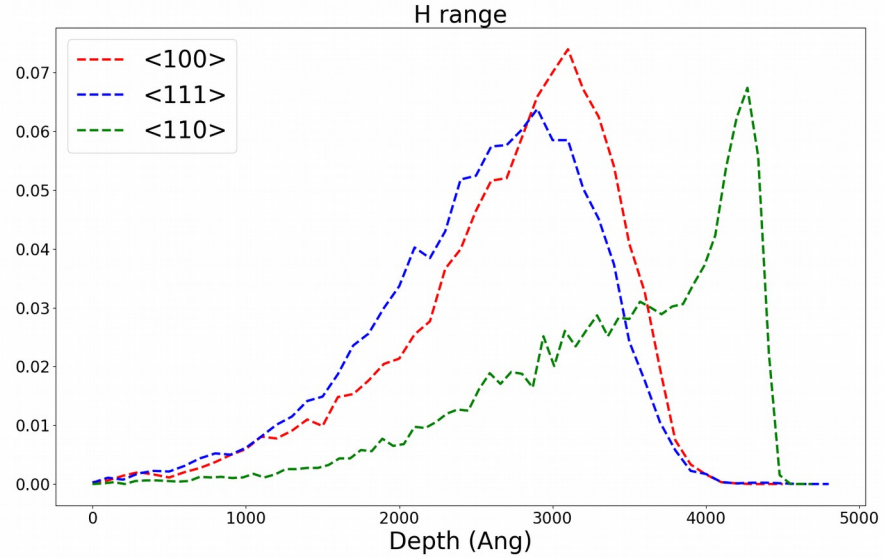
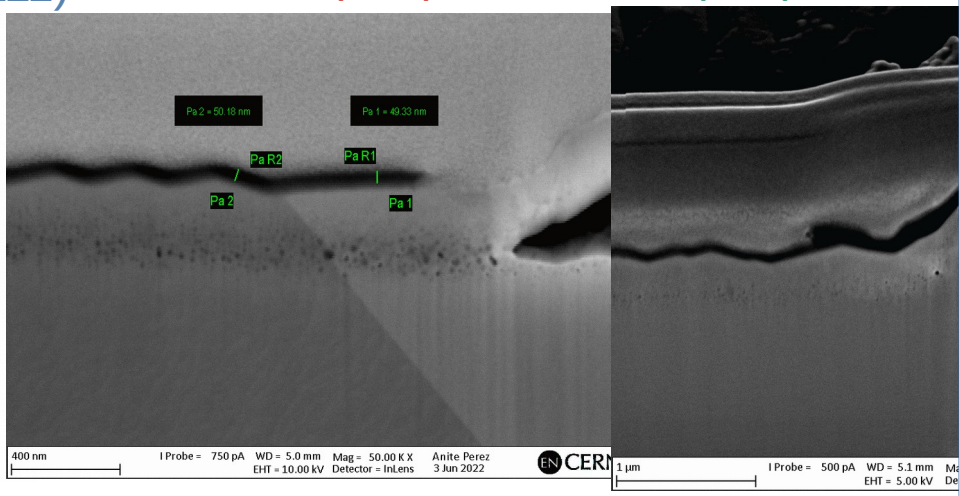
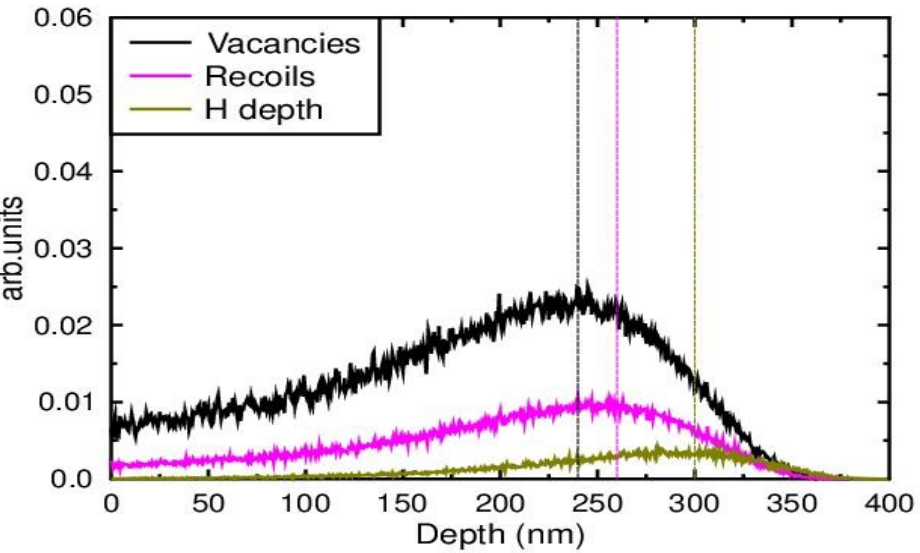


(111) (100) (110)





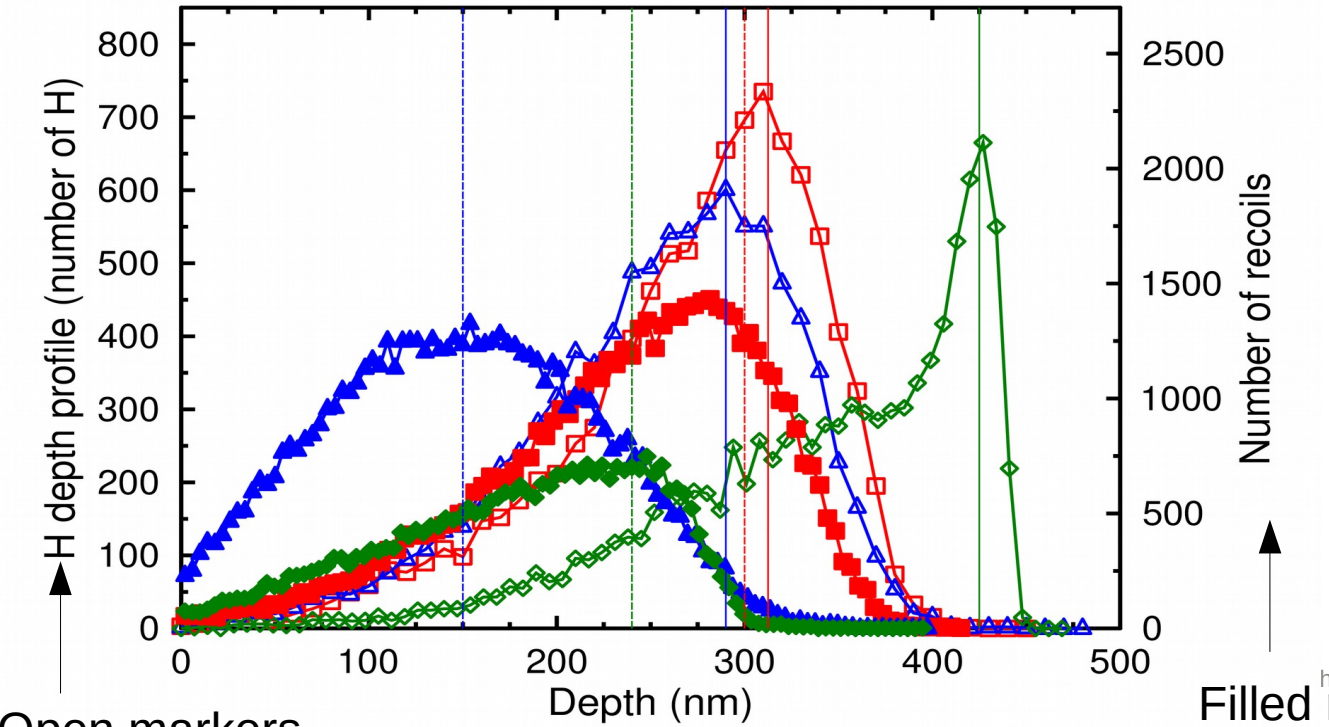
- The studied grains under low fluence show that bubbles are formed at different distances, which is consistent with MDRANGE results, observing a deeper formation in (110) grains.
- After a complete dataset of blisters/protrusions is obtained with MD, we understand the mechanisms of surface modification. However, we observe that under low fluences, only (100) grains experience blistering.

Recoils formation ~ vacancy formation

Comparison with experiments

- We filter those recoils with kinetic energy lower than 40 eV (approximately the energy needed to create a vacancy), and we observe that for <100> the peaks are close, however the distances between them in <111> and <110> (specially the latter)

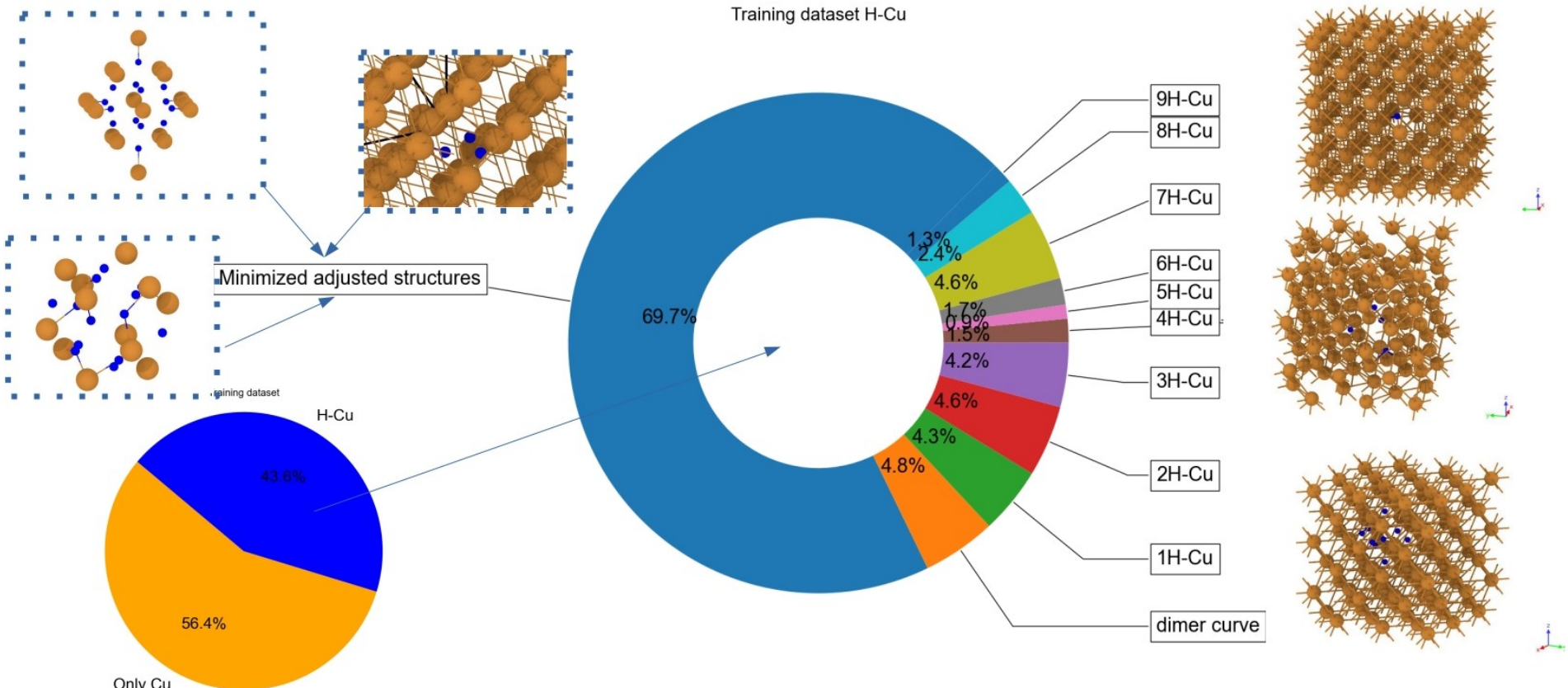
A. Lopez-Cazalilla, C. Serafim, submitted (2023)



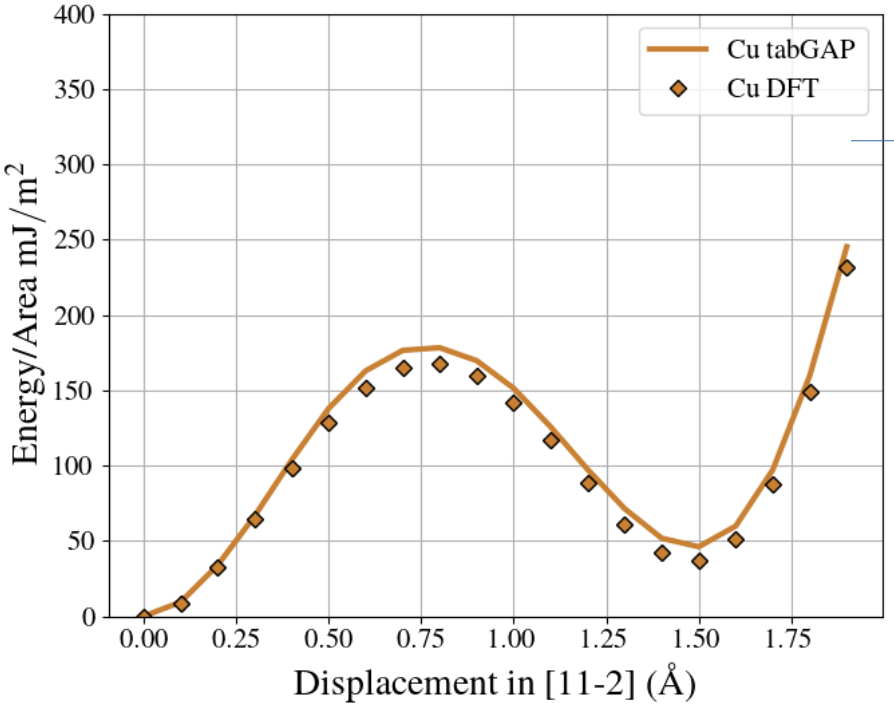
- The formation of vacancies occurs closer to the surface in <111> and <110>grains, but the hydrogen atoms need more time (fluence) to fill these gaps and develop larger blisters visible in the surface, while in <100> is immediate

Cu-H MLIP. Training dataset

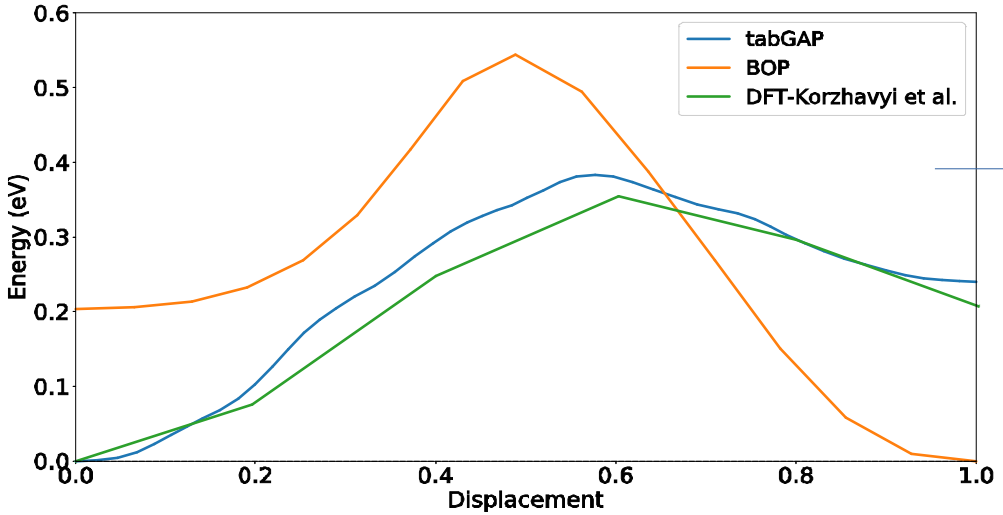
We use VASP DFT code to obtain energy, forces and virials of the considered structures in order to train the (tabulated) Gaussian Approximation Potential (tabGAP). Previously, a pure Cu tabGAP potential was created and its original dataset is employed in the new potential.



Cu-H MLIP. Performance tests

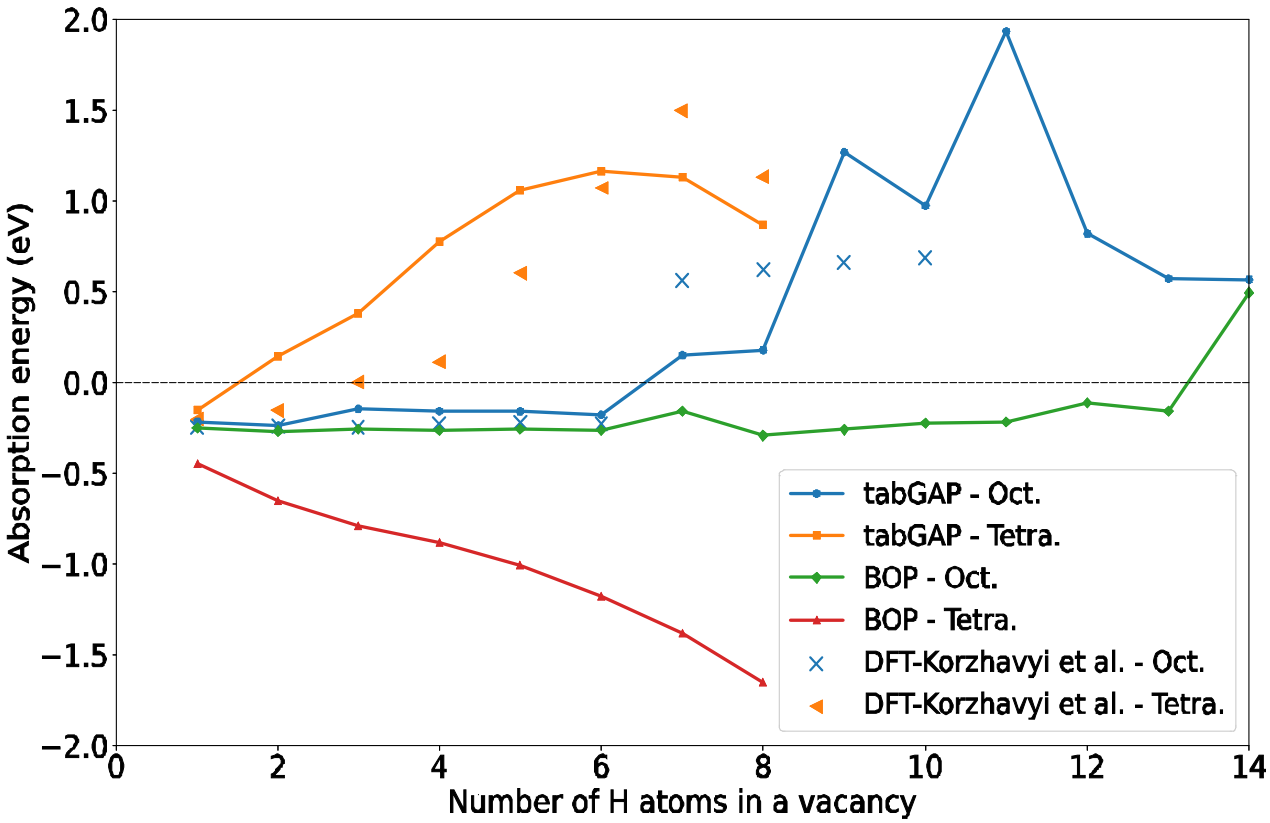


The insertion of the H dataset did not modify the mechanical properties of the copper part



The barrier of a H atom moving from an octahedral to a tetrahedral position is predicted close to DFT precision. And better than the other available potential (BOP)

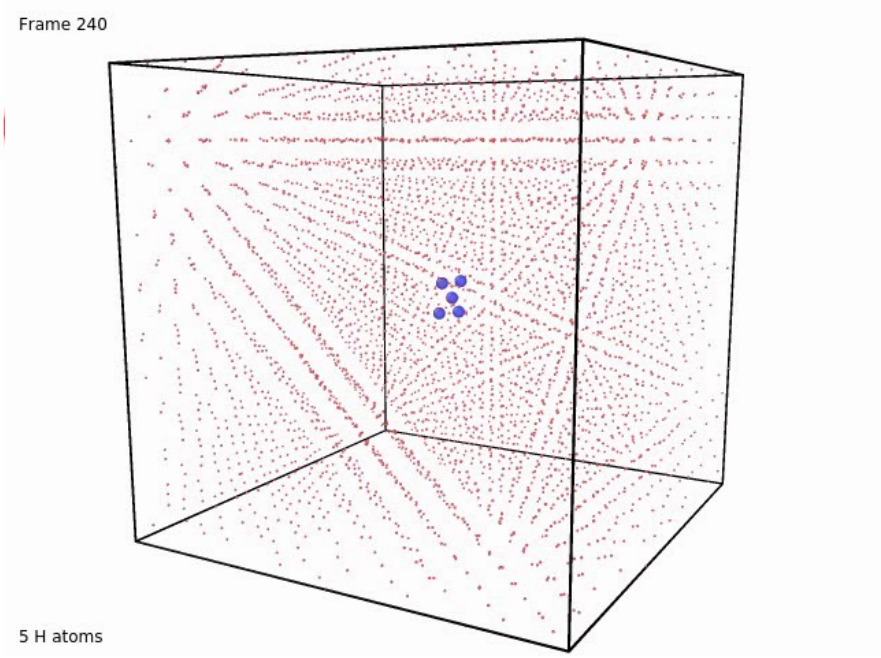
Cu-H MLIP. Performance tests

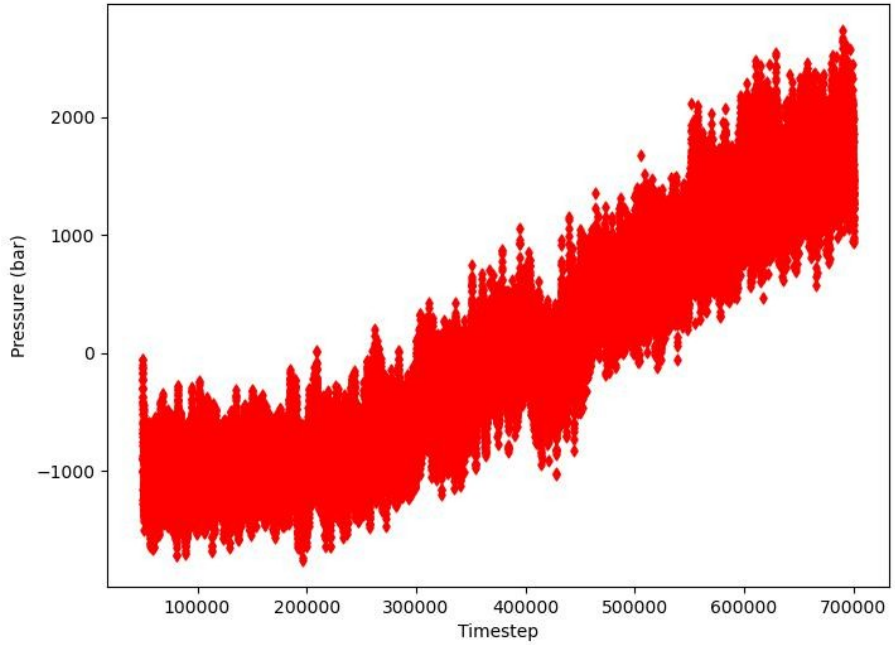


Comparing with the BOP, we see that the trends observed with tabGAP in the absorption energy are accurate when compared with DFT results.

DFT provides that no more than 6 H can be acommodated in 1 vacancy being energetically favourable.

Cu-H MLIP. Sequential insertion of H





This potential allows to follow processes such as the accumulation of H in small defects such as small vacancy clusters, and assist on what experimentally is not possible to follow.

Conclusions

- In our simulations we clearly see the atomistic mechanisms of bubble and blister growth under hydrostatic internal H pressure .We identify the effect of surface orientation on the shape of appearing protrusion.
- The observed differences in the protrusion shapes with MD are consistent with those seen in experiment
- The difference between the formation of vacancies area and the penetration depth of H in (110) and (111) grains explain the later development of blisters, complementing the penetration depth as previous models predicted.
- The ML potential, with DFT precision, enables the exploration of mechanisms behind the blistering effect.

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([1]):

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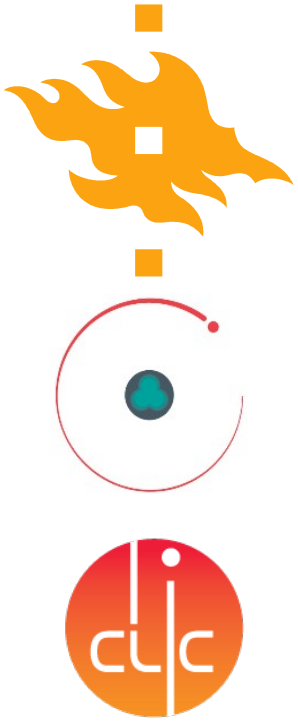
([2])Internal communication with CERN for Titanium not-blistering



Thank you for you attention!