doi:10.1017/S1431927622003452
Microsc. Microanal. 28 (Suppl 1), 2022

Are vacancies in field ion microscopy artefacts? A DFT study

Shyam Katnagallu[1*], Christoph Freysoldt[1] and Joerg Neugebauer[1]

[1.] Computational Materials design, Max-Planck-Institut für Eisensforschung, Düsseldorf, Germany.
* Corresponding author: s.katnagallu@mpie.de

Resolving the atomic structure of engineering materials in 3D continues to be an extensive research field. Field ion microscopy under evaporating conditions (3D-FIM)[1] is one of the few techniques capable of delivering such atomic scale information, allowing to even image vacancies and their interactions with solute atoms in alloys. However, the quantification of the observed vacancies and their origins are still a matter of debate[2–4]. It was suggested that high electric fields (1-10 V/Å) used in FIM could introduce artefact vacancies. To investigate the possibility of this mechanism, we used density functional theory (DFT) simulations. Stepped Ni surfaces with kinks were modelled in the repeated slab approach with a (971) surface orientation. A field of up to 4 V/Å was introduced on one side of the slab using the generalized dipole correction[5]. Contrary to conventional wisdom, we show that the reaction barrier to form vacancies on the electrified metal surface increases compared to the field-free case. We also find that the electric field can introduce kinetic barriers to a potential "vacancy-killing" mechanism as shown in Figure 1. We compare these findings with field evaporation models proposed in literature.

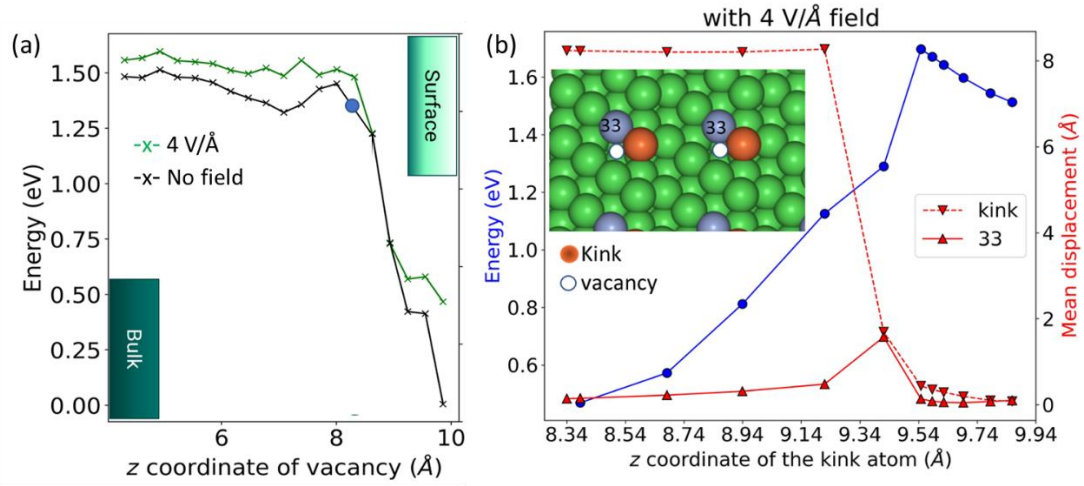

Figure 1. (a) Vacancy formation energies as a function of vacancy position in the slab with 4 V/A and without an electric field. The potential vacancy killing mechanism is highlighted with a circle in the field free case. (b) Introduction of a barrier on the kink atom with electric field stops it from moving to the vacancy's position.

References:

[1] F. Vurpillot, M. Gilbert, B. Deconihout, Towards the three-dimensional field ion microscope, Surf. Interface Anal. 39 (2007) 273–277. https://doi.org/10.1002/sia.2490.

[2]C.A. Speicher, W.T. Pimbley, M.J. Attardo, J.M. Galligan, S.S. Brenner, Observation of vacancies in

the field-ion microscope, Phys. Lett. 23 (1966) 194–196. https://doi.org/10.1016/0031-9163(66)90860-2.

[3] T.F. Page, B. Ralph, The occurrence of field-induced surface vacancies on iridium field-ion microscope specimens, Surf. Sci. 36 (1973) 9–28. https://doi.org/10.1016/0039-6028(73)90243-4.

[4] F.F. Morgado, S. Katnagallu, C. Freysoldt, B. Klaes, F. Vurpillot, J. Neugebauer, D. Raabe, S. Neumeier, B. Gault, L.T. Stephenson, Revealing atomic-scale vacancy-solute interaction in nickel, Scr. Mater. 203 (2021) 114036. https://doi.org/10.1016/j.scriptamat.2021.114036.

[5] C. Freysoldt, A. Mishra, M. Ashton, J. Neugebauer, Generalized dipole correction for charged surfaces in the repeated-slab approach, Phys. Rev. B. 102 (2020) 45403. https://doi.org/10.1103/PhysRevB.102.045403.

https://doi.org/10.1017/S1431927622003452 Published online by Cambridge University Press