Contribution ID: **34** Type: **Oral**

Ab initio investigation of Cu nanoparticle behavior under high electric field

Friday 12 March 2021 16:45 (30 minutes)

Metal cathodes have inevitable surface defects, such as dust, protrusions or small-scale roughness caused by manufacturing. Under high electric field, these defects will generate local electric field enhancement, that can help to initiate vacuum breakdown. When in large, the classical vacuum breakdown mechanism has already been clarified, it demonstrates that small protrusions could be vaporized under external electric field and leave a breakdown crater, the exact mechanism how such tips could form and lead to local electric field enhancement is still unexplained. As such, we consider that extreme electric field could interact with the electronic structure of the metal atoms, thus distorting the classical interatomic potentials (used in molecular dynamics) and opening a way to field enhanced surface diffusion.
In the current study, we investigate several Cu nanoparticle systems using the Gaussian DFT package. Gaussian allows us to focus on nonperiodic structures, thus opening the possibility to extend the understanding of electric field influenced surface behavior beyond structures of the size of a few atoms. The investigated systems consist of a Cu dimer and different nanoparticles such as 1FCC, 2FCC and 4FCC structures. Already simple energy scan of Cu dimer under field, shows a noticeable change in the interatomic potential. In order to get generalized results, the scale of simulation models is increased. Larger systems, such as nanoparticles consisting of 1FCC, 2FCC and 4FCC unit cells, demonstrate a significant field dependent straining that can cause even bending. While the current study focuses on the electric field effects on nanoparticles, our results strongly indicate that electric field may have strong influence to large scale surface defects as well.

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Session Classification: Modelling and simulations