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Experiments and simulations of nanoscale surface-field interaction

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The measured field enhancement factors of 50-100 in CLIC accelerating structures are associated with high aspect ratio surface irregularities. The formation of these surface structures is thought to occur due to subsurface dislocation activity and field-assisted surface atom diffusion. In the current work, we investigate these aspects using computer simulations and experimental approaches. Surface diffusion in the absence of field was studied for FCC metals using nanowires as model systems. Experimental observations and kinetic Monte Carlo simulations showed that nanowire junction disintegrate due to surface atom diffusion at temperatures much lower than the melting temperature. This was due to increased surface roughness at the junction spots. The stability of surfaces was further investigated with molecular dynamics and DFT calculations to estimate the change in work function due to surface roughness. It was found that surface tips and ridges can significantly reduce the work function. Further generalization of conducted studies resulted in in-situ SEM experiments with applied field between metal tips. Images were taken before and after voltage application. FEM simulations were used to reconstruct possible electric field distributions and surface behavior in observed situations.

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