Contribution ID: **6** Type: **Oral**

Thermal runaway and the Pre-breakdown characteristics of FCC, BCC and HCP metal nanotips under the high electric field using PIC-ED-MD simulations

Wednesday 21 September 2022 10:00 (30 minutes)

The most important physical parameter that determines the microstructure evolution in the thermal runaway and the subsequent electric pre-breakdown behaviors of nano-size metal field emitters and micro-protrusions on the metal surfaces is yet to be elucidated. In this work, we conduct a systematic multiscale-multiphysics simulations for FCC (Cu, Au and Al), BCC (Mo, W and Zr) and HCP (Ti, V and Zn) metal nano-tips (R0=1 nm and H0=100 nm) based on the latest developed PIC-ED-MD computational methodology. The structural evolution and thermal runaway mechanism are found to be decisively determined by the thermal conductivity and boiling point of metal. The nano-tip made of metal with low thermal conductivity and high boiling point (Mo, W, Zr, V and Ti), the field emission induced heating processes (Joule and Nottingham heats) lead to formation of nano-protrusion because of the continuous thinning and sharpening of the molten region at the apex of the tip, and the thermal runaway usually occurs at the tip of atomically sharp nano-protrusion. Meanwhile, the metal nanotips made of Cu, Al, Au and Zn are prone to the melting and recrystallization. The high electric-field stress excreted on the surface of nanotip strongly deforms the whole molten region, and the detachment of the large liquid droplet from the nano-tip base is prevalent during the thermal runaway process. We further apply the multi-variable linear regression method to analysis the influences of some intrinsic physical properties of metals (boiling/melting point, work function, crystal structure, surface crystallographic orientation and thermal/electric conductivity) on the pre-breakdown characteristics including on-set pre-breakdown time and the critical E-field strength. The results strongly support the use of boiling point of metals as the most decisive descriptor to indicate the pre-breakdown resilient of various metal nano-tips. A quantitative expression is also obtained between the pre-breakdown E-field and boiling point, based on the current PIC-ED-MD simulations for nine metal materials.

Topic

Modeling and Simulations

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Session Classification: Modelling & Simulation

Track Classification: Simulations