Poster Session | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[PO-F2]Poster Session 2
Symposium F
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[P2-50]Atomic surface treatment of copper nanowires by electron beam irradiation simulated by first principle calculation

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Atomic surface treatment of copper nanowires by electron beam irradiation simulated by first principle calculation

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Recently, the techniques of atomic surface treatment by electron beam etching has developed vigorously. However, the improvement and more details should be understood specially in atomic scale. In the experiment when we applied the electron beam on copper nanowires with copper oxide (111) surface without heating, it was found the reduction reaction and the following Cu clusters slip on Cu (111) surface. For further complete the mechanism, we provide the Vienna ab initio simulation package (vasp) to perform the GGA calculation with PAW pseuodopotentials. For reduction reaction, we compare the energy between the theoretical structure of Cu with oxide surface and Cu (111) surface to predict the binding energy of oxygen. For the slip of Cu clusters, we calculate the energy mapping of slip path on Cu (111) surface to find the most probable routine of slip. The calculation data should help us control the intensity of electron beam radiation when we do the surface treatment of material and be the complement of slip observation.