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First principles study of the impact of grain boundaries on Nb_3Sn

Tuesday, 10 November 2020 09:30 (20 minutes)

We present the first comprehensive study of grain boundaries in Nb_3Sn from first principles. While most conventional superconductors, such as Nb, are not significantly impacted by the presence of grain boundaries, Nb_3Sn is much more sensitive to defects and disorder owing to its relatively short coherence length of ~3 nm. Indeed, experiments suggest a link between grain-boundary stoichiometry and the performance of Nb_3Sn superconducting radio frequency (SRF) cavities, and mesoscopic simulations point to grain boundaries as a candidate mechanism that lowers the vortex-entry field in SRF cavities. Our density-functional theory (DFT) calculations on tilt and twist grain boundaries provide insight into general trends on quantities such as the local Fermi-level density of states, antisite defect formation free energies, local electronic properties from grain boundaries with added point defects, and how grain boundary composition affects the local Tc around grain boundaries in Nb_3Sn. In this talk we will use our findings to explain recent experimental findings and provide insight on promising modifications to the growth procedure of the material to optimize the performance of SRF cavities.

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