New Recipes to Optimize the Niobium Oxide Surface From First-Principles Calculations

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We investigate Nb$_3$Sn nucleation and the SRF properties of Nb$_2$O$_5$ and NbO using density functional theory.

Growth conditions such as pH determine the properties of the pentoxide surface. These properties in turn can affect Nb$_3$Sn nucleation and SRF performance.

OH binding energies vs OH ion: -0.4, -0.6 eV
Corresponding debinding: pH 9, 5.5

OH groups eliminate unpaired electrons on the surface, while O->N substitutions eliminate them in the bulk.

Diffusion barriers in NbO are enormous due to ordered Nb vacancies. N destabilizes these vacancies, reducing barriers to a level similar to diffusion barriers in Nb.

We perform calculations on a realistic Nb$_2$O$_5$ nanoparticle to further understand Nb$_3$Sn nucleation.

Based on our findings, we recommend a lower-pH surface preparation and lower-temperature nucleation.

During Nb3Sn nucleation, OH groups compete with Cl atoms for binding sites (i.e. exposed Nb atoms) on the Nb2O5 surface.

- Low-pH pre-treatment may produce more binding sites and better nucleation.
- Low-temperature nucleation may help maximize surface area and presence of edge/corner sites, which also appear to be favorable binding sites.

- This may also delay a phase crystalline transition to high-T crystalline Nb$_2$O$_5$ phases which are generally more inert than the low-T “amorphous” phase.

- Unpaired electrons in Nb$_2$O$_5$ exert a significant magnetic field on the superconductor, possibly enhancing pair breaking.

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- Dry, low-pressure atmosphere may result in slower native oxide growth with fewer defects associated with unpaired electrons. N may also be beneficial.

- We investigate the effect of N on vacancy mobility in the passivating NbO layer, which may impact sub-surface doping levels.

- We also investigate the electron and phonon properties of the surface to determine how impurities may affect the superheating field.

Rocksalt NbO/N compounds can achieve very high Tc.

- Low-frequency phonon density of states and Fermi-level electronic density of states can distinguish poor superconductors from good ones.

- Rocksalt NbO/N compounds can achieve very high Tc.

- Preliminary calculations find that Nb, NbO surfaces have soft phonon modes.

- This property is correlated with enhanced electron-phonon coupling in the bulk rocksalt system.

- Hydrogen and nitrogen also affect the electronic properties of the surface.

- Here we find additional evidence for a beneficial effect of nitrogen.

OH binding energies vs SnCl$_2$ molecule (vacuum) -0.2 eV +0.6 eV