FIRST PRINCIPLES INVESTIGATION OF HYDROGEN IN NIOBIUM

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Abstract

Niobium hydride is a contributor to degraded niobium SRF cavity performance by Q-slope and Q-disease. Hydrogen is easily absorbed into niobium when the protective oxide layer is disturbed, such as during electropolishing and chemical treatments, and the structure and distribution of hydrogen in niobium is altered during other processing steps such as baking. To optimize cavity performance and production efficiency, it is important to understand the structures of hydrogen in niobium, including the interactions of hydrogen with structural defects and other impurities such as oxygen. In this study density functional theory was used to evaluate these interactions. Hydrogen was examined as a dissolved interstitial impurity and in ordered niobium-hydride phases; and the interactions between hydrogen, niobium, vacancies on niobium sites, and oxygen dissolved in niobium were evaluated. The results yield information about the thermodynamic, electronic, magnetic, and geometric properties of these systems, which lead to important implications concerning the mobilities of impurities and vacancies in niobium and the precipitation of phases that are detrimental to cavity performance.

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