ACCELERATOR SEMINAR

"Density Functional Theory Calculations to Understand the Role of Impurity and Defect Structures in Nb SRF Cavities"

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Niobium is susceptible to the absorption and redistribution of the chemical impurities H, O, N, and C while it is being formed into and processed for use as superconducting radio-frequency cavities. These impurities may reside in niobium lattice interstitial sites, interact with each other and structural defects, and form precipitates. The various impurity and defect states in niobium affect the properties of SRF cavities, resulting in changes in the cavity quality factor, and potentially the cause or cure of Q-slope and Q-disease. A first-principles approach using density functional theory is taken to gain insight into the interactions between these impurities, niobium, and niobium structural defects. I will describe the relationship between impurities, structural defects, and the SRF cavity forming and processing procedure; the application of density functional theory to materials design and processing problems; and the insights gained by studying impurity and defect structures in niobium with density functional theory. Particular emphasis will be given to thermodynamics, charge transfer and bonding in the structures, lattice strain, and interfaces between the niobium and precipitates.

Thursday, April 30, 2015
11:00 a.m.
CEBAF Center, Room F113

Coffee before seminar beginning at 10:45 a.m.

Jefferson Lab

For further info, please contact Joe Grames at x7097