First-Principles Analysis of Nb_3Sn Surface Configurations in SRF Cavities through DFT-Guided Genetic Algorithms

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The development of Nb_3Sn-coated superconducting radiofrequency (SRF) cavities represents a significant leap forward in particle accelerator technology, primarily due to their enhanced critical fields and operability at elevated temperatures. However, the practical implementation of Nb_3Sn coatings on Nb cavities faces substantial challenges, particularly in achieving effective and consistent coating. A crucial factor in addressing these challenges is the detailed understanding of the surface characteristics of Nb_3Sn, as these largely dictate the superconducting properties of the coated cavities. In this study, we focus on elucidating the surface structure of Nb_3Sn using an innovative approach that integrates genetic algorithms with density functional theory (DFT) computations. This methodology is adapted to simulate vapor deposition processes commonly employed for Nb_3Sn coatings. Our research successfully generates comprehensive data, enabling the construction of a detailed surface phase diagram for the $Nb_3Sn(100)$ surface. This diagram provides critical insights into the stable surface configurations under varying temperature and tin (Sn) vapor pressure conditions. Remarkably, our theoretical phase diagram exhibits a strong correlation with the conditions typically utilized in experimental settings for Nb_3Sn deposition, validating the practical relevance of our model. Further, our results reveal that tin anti-site defects, which are known to adversely affect superconductivity, predominantly stabilize near the material's surface.