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The mechanism of non-uniform distribution of tin sites on the surface of niobium during the nucleation process

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A uniform distribution of nucleation tin sites is essential to the growth of high quality Nb3Sn thin film by vapor diffusion method. The less-nuclear zones were commonly observed in previous nucleation experiments. However, a fully understanding of the occurrence of less-nuclear zones has not yet been achieved. Here, the adsorption energy of nuclear agent SnCl2 on different crystal planes of niobium (Nb) including Nb (110), Nb (100), Nb (211) are studied through density functional theory (DFT) calculations and several types of adsorption configurations are optimized. The large differences of calculated adsorption energy of SnCl2 on three different crystal planes reveal strong crystal direction selectivity during nucleation stage. In addition, the phenomenon of nucleation experiment on large grain samples further consolidates the accuracy of the calculation results. The calculation results explain the presence of less-nuclear zones during nucleation process and provide guidance for the subsequent suppression of these regions.

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