Thermodynamic Stability of Nb_3Ge, Nb_3Al, and Nb_3Ga A15 Phases

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In this work, we investigate the thermodynamic stability of Nb-based A15 phases- Nb_3Ge, Nb_3Ga, and Nb_3Al. These Nb-based A15 phases can be used as potential alternatives to Nb_3Sn coatings in superconducting radio-frequency particle accelerator cavities. These A15 phases, like Nb_3Sn coatings, might lead to shorter cavity lengths, higher operating temperatures, and lower power consumption. We use a density functional theory (DFT) and cluster expansion based approach to calculate the thermodynamic stability ranges of these A15 phases. We use PBE functional for the construction of the DFT based cluster expansion model. We find that Nb_X (X = Ge, Ga, Al) antisite defects helps in stabilizing these phases at off-stoichiometric composition. Also, our calculated composition stability ranges for Nb_3Ge differ from the stability ranges found in the phase diagrams.