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Structural phase transformations in Ti_3Al_2Nb system, a first-principles approach[1] MAHDI SANATI, Texas Tech University, DAMIEN WEST, Texas Tech Univesrity — First-principles method is employed to determine the vibrational entropy and Gibbs free energy as a function of temperature of the homogenous Ti_3Al_2Nb system. Calculated energies at T=0 K show instabilities in ternary B2 Ti_3Al_2Nb alloy against the ω and $B8_2$ structures. We show that at high temperatures the B2 phase is stabilized by the vibrational entropy. The transition temperatures for B2 $\rightarrow$ ω and B2 $\rightarrow$ $B8_2$ have been calculated and are in excellent agreement with experiment.

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Mahdi Sanati
Texas Tech University

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